



BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

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FACULTAD DE CIENCIAS QUÍMICAS  
LABORATORIO DE FISICOQUÍMICA TEÓRICA

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Reporte de resultados para el programa  
alignandcomparemolecules

Título del proyecto:

**Desarrollo de software para comparar y resolver estructuras  
isoméricas mediante el tensor de inercia**

PRESENTA  
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DIRECTOR DE TESIS

Dr. Juan Manuel Solano Altamirano  
FQ-BUAP

29 de abril de 2019

# **1. Resultados**

## **1.1. Pruebas realizadas**

Las Pruebas que ya se realizaron son las siguientes y los resultados son óptimos y satisfactorios en todas las pruebas.

Realicé todas las pruebas que muestro a continuación, para hacer todas las comparaciones programé unos scripts que me ayudaran a automatizar todo el trabajo.

# Rendimeinto del programa

Tiempo más corto de cálculo = 0.001 s

Tiempo más largo de cálculo = 0.064 s

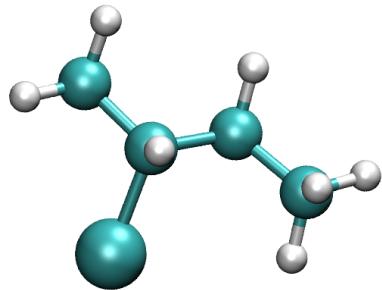
Tiempo total de todos los cálculos = 2.067 s

Número de comparaciones = 663

Promedio de tiempo = 0.00311765 s

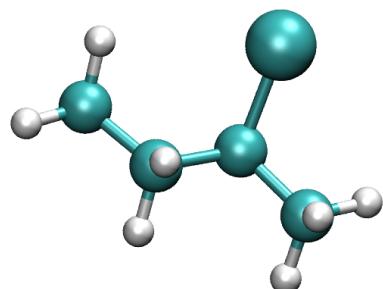
# AsymmetricEnantiomers Número 1

Molecule A r-2-chlorobutane\_out\_G09



Molecule B

r-2-chlorobutane\_out\_G09\_inversion



Inertia Tensor - Molecule A

113.621	-8.52391	-0.0867925
-8.52391	164.234	-0.885702
-0.0867925	-0.885702	257.008

Inertia Tensor - Molecule B

113.621	-8.52381	-0.0867846
-8.52381	164.234	-0.885691
-0.0867846	-0.885691	257.008

EingenVectors - Molecule A

-0.986829	-0.161759	-0.00158111
0.161767	-0.986784	-0.00941026
-3.80259e-05	-0.00954208	0.999954

EingenVectors - Molecule B

-0.986829	-0.161756	-0.00158103
0.161764	-0.986785	-0.00941017
-3.79835e-05	-0.00954198	0.999954

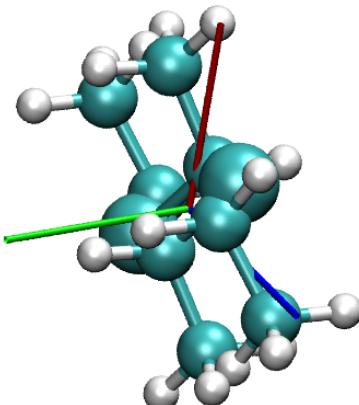
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

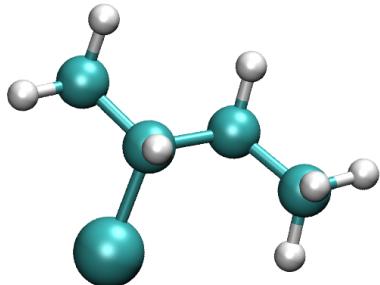
112.224	165.623	257.016
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Enantiomers



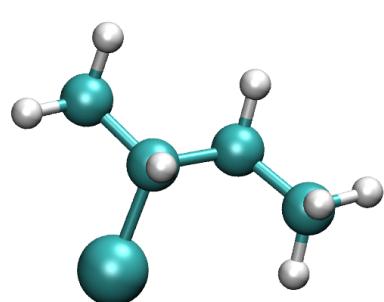
# AsymmetricEnantiomers Número 2

Molecule A r-2-chlorobutane\_out\_G09



Molecule B

r-2-chlorobutane\_rotated\_out\_G09



Inertia Tensor - Molecule A

113.621	-8.52391	-0.0867925
-8.52391	164.234	-0.885702
-0.0867925	-0.885702	257.008

Inertia Tensor - Molecule B

113.621	-8.52391	-0.0867928
-8.52391	164.234	-0.885702
-0.0867928	-0.885702	257.008

EingenVectors - Molecule A

-0.986829	-0.161759	-0.00158111
0.161767	-0.986784	-0.00941026
-3.80259e-05	-0.00954208	0.999954

EingenVectors - Molecule B

-0.986829	-0.161759	-0.00158112
0.161767	-0.986784	-0.00941025
-3.80279e-05	-0.00954208	0.999954

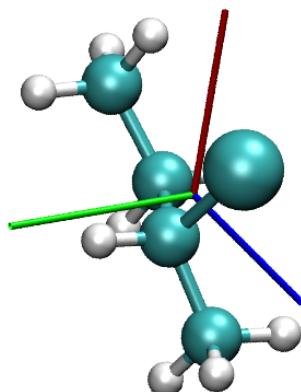
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

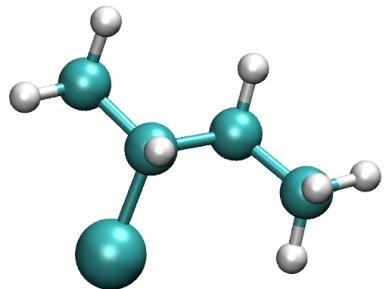
112.224	165.623	257.016
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Equal

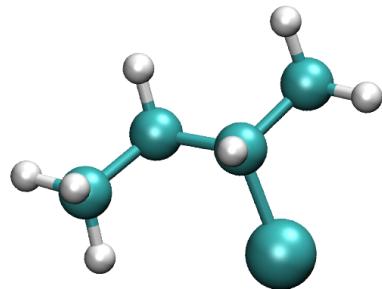


# AsymmetricEnantiomers Número 3

Molecule A r-2-chlorobutane\_out\_G09



Molecule B s-2-chlorobutane\_out\_G09



Inertia Tensor - Molecule A

113.621	-8.52391	-0.0867925
-8.52391	164.234	-0.885702
-0.0867925	-0.885702	257.008

Inertia Tensor - Molecule B

113.621	8.52396	0.0868155
8.52396	164.235	-0.885715
0.0868155	-0.885715	257.008

EingenVectors - Molecule A

-0.986829	-0.161759	-0.00158111
0.161767	-0.986784	-0.00941026
-3.80259e-05	-0.00954208	0.999954

EingenVectors - Molecule B

-0.98683	0.161755	0.00158125
-0.161763	-0.986785	-0.00941041
3.81715e-05	-0.00954226	0.999954

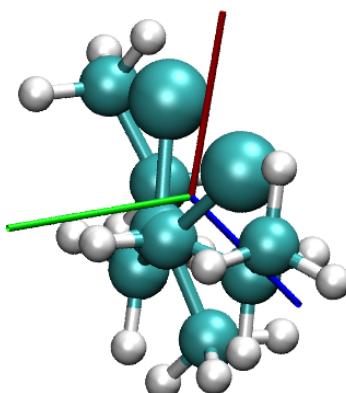
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

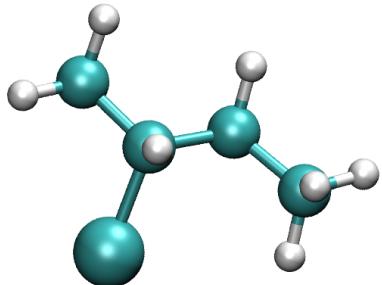
112.224	165.624	257.017
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Enantiomers



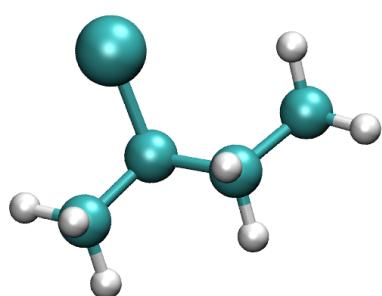
# AsymmetricEnantiomers Número 4

Molecule A r-2-chlorobutane.out\_G09



Molecule B

s-2-chlorobutane.out\_G09\_inversion



Inertia Tensor - Molecule A

113.621	-8.52391	-0.0867925
-8.52391	164.234	-0.885702
-0.0867925	-0.885702	257.008

Inertia Tensor - Molecule B

113.622	8.52398	0.0868204
8.52398	164.235	-0.88572
0.0868204	-0.88572	257.009

EingenVectors - Molecule A

-0.986829	-0.161759	-0.00158111
0.161767	-0.986784	-0.00941026
-3.80259e-05	-0.00954208	0.999954

EingenVectors - Molecule B

-0.986829	0.161757	0.0015813
-0.161765	-0.986785	-0.00941039
3.82053e-05	-0.00954225	0.999954

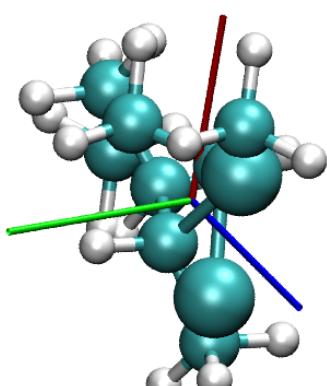
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

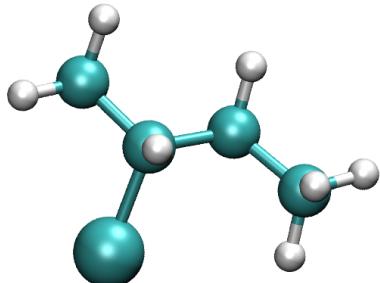
112.224	165.624	257.018
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Equal



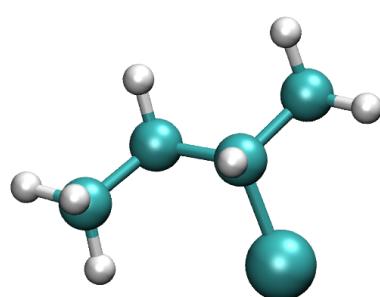
# AsymmetricEnantiomers Número 5

Molecule A r-2-chlorobutane\_out\_G09



Molecule B

s-2-chlorobutane\_rotated\_out\_G09



Inertia Tensor - Molecule A

113.621	-8.52391	-0.0867925
-8.52391	164.234	-0.885702
-0.0867925	-0.885702	257.008

Inertia Tensor - Molecule B

113.621	8.52397	0.0867992
8.52397	164.235	-0.885706
0.0867992	-0.885706	257.008

EingenVectors - Molecule A

-0.986829	-0.161759	-0.00158111
0.161767	-0.986784	-0.00941026
-3.80259e-05	-0.00954208	0.999954

EingenVectors - Molecule B

-0.98683	0.161756	0.00158113
-0.161763	-0.986785	-0.00941034
3.80628e-05	-0.00954217	0.999954

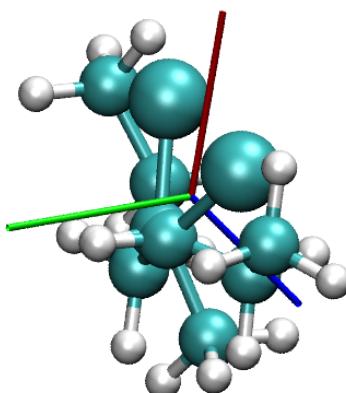
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

112.224	165.624	257.017
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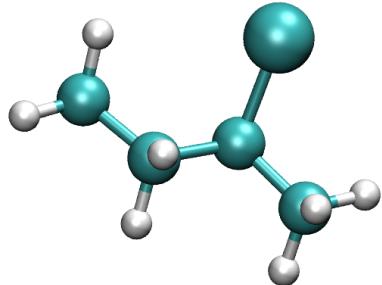
Enantiomers



# Asymmetric Enantiomers Número 6

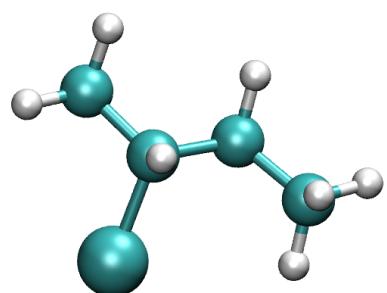
Molecule A

r-2-chlorobutane\_out\_G09\_inversion



Molecule B

r-2-chlorobutane\_rotated\_out\_G09



Inertia Tensor - Molecule A

113.621	-8.52381	-0.0867846
-8.52381	164.234	-0.885691
-0.0867846	-0.885691	257.008

Inertia Tensor - Molecule B

113.621	-8.52391	-0.0867928
-8.52391	164.234	-0.885702
-0.0867928	-0.885702	257.008

EigenVectors - Molecule A

-0.986829	-0.161756	-0.00158103
0.161764	-0.986785	-0.00941017
-3.79835e-05	-0.00954198	0.999954

EigenVectors - Molecule B

-0.986829	-0.161759	-0.00158112
0.161767	-0.986784	-0.00941025
-3.80279e-05	-0.00954208	0.999954

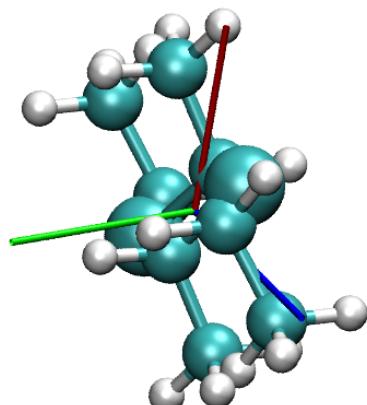
EigenValues - Molecule A

112.224	165.623	257.016
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EigenValues - Molecule B

112.224	165.623	257.016
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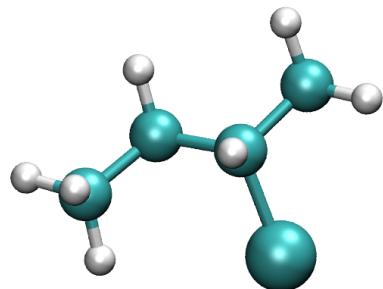
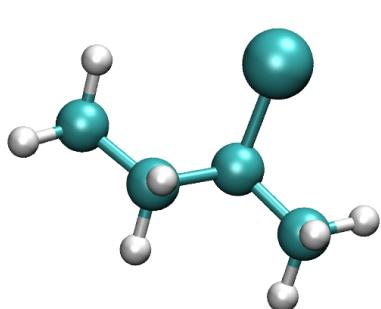
Enantiomers



# AsymmetricEnantiomers Número 7

Molecule A  
r-2-chlorobutane\_out\_G09\_inversion

Molecule B s-2-chlorobutane\_out\_G09



Inertia Tensor - Molecule A		
113.621	-8.52381	-0.0867846
-8.52381	164.234	-0.885691
-0.0867846	-0.885691	257.008

Inertia Tensor - Molecule B		
113.621	8.52396	0.0868155
8.52396	164.235	-0.885715
0.0868155	-0.885715	257.008

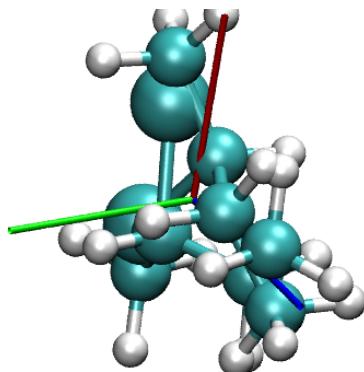
EingenVectors - Molecule A		
-0.986829	-0.161756	-0.00158103
0.161764	-0.986785	-0.00941017
-3.79835e-05	-0.00954198	0.999954

EingenVectors - Molecule B		
-0.98683	0.161755	0.00158125
-0.161763	-0.986785	-0.00941041
3.81715e-05	-0.00954226	0.999954

EingenValues - Molecule A		
112.224	165.623	257.016

EingenValues - Molecule B		
112.224	165.624	257.017

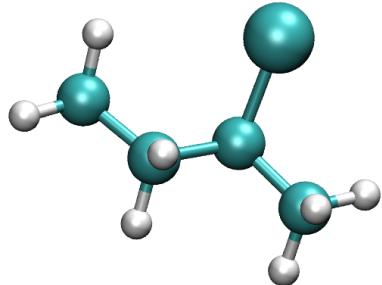
Equal



# AsymmetricEnantiomers Número 8

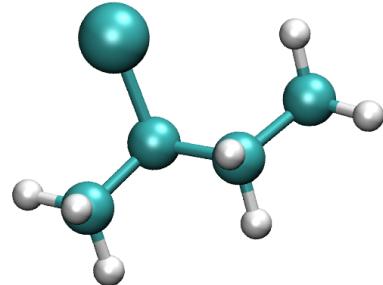
Molecule A

r-2-chlorobutane.out\_G09\_inversion



Molecule B

s-2-chlorobutane.out\_G09\_inversion



Inertia Tensor - Molecule A

113.621	-8.52381	-0.0867846
-8.52381	164.234	-0.885691
-0.0867846	-0.885691	257.008

Inertia Tensor - Molecule B

113.622	8.52398	0.0868204
8.52398	164.235	-0.88572
0.0868204	-0.88572	257.009

EingenVectors - Molecule A

-0.986829	-0.161756	-0.00158103
0.161764	-0.986785	-0.00941017
-3.79835e-05	-0.00954198	0.999954

EingenVectors - Molecule B

-0.986829	0.161757	0.0015813
-0.161765	-0.986785	-0.00941039
3.82053e-05	-0.00954225	0.999954

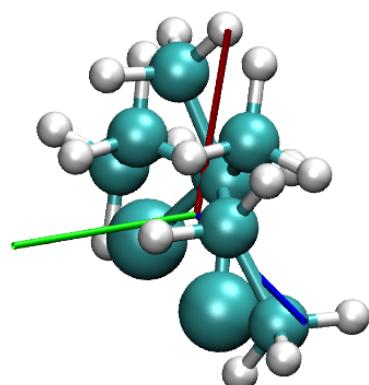
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

112.224	165.624	257.018
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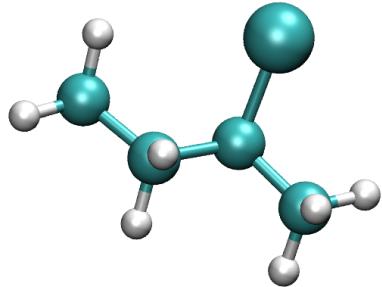
Enantiomers



# AsymmetricEnantiomers Número 9

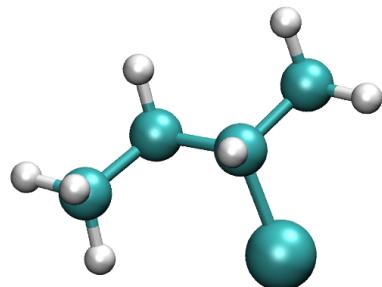
Molecule A

r-2-chlorobutane\_out\_G09\_inversion



Molecule B

s-2-chlorobutane\_rotated\_out\_G09



Inertia Tensor - Molecule A

113.621	-8.52381	-0.0867846
-8.52381	164.234	-0.885691
-0.0867846	-0.885691	257.008

Inertia Tensor - Molecule B

113.621	8.52397	0.0867992
8.52397	164.235	-0.885706
0.0867992	-0.885706	257.008

EingenVectors - Molecule A

-0.986829	-0.161756	-0.00158103
0.161764	-0.986785	-0.00941017
-3.79835e-05	-0.00954198	0.999954

EingenVectors - Molecule B

-0.98683	0.161756	0.00158113
-0.161763	-0.986785	-0.00941034
3.80628e-05	-0.00954217	0.999954

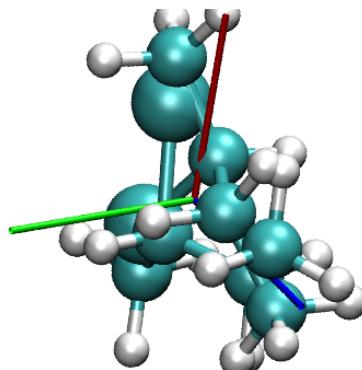
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

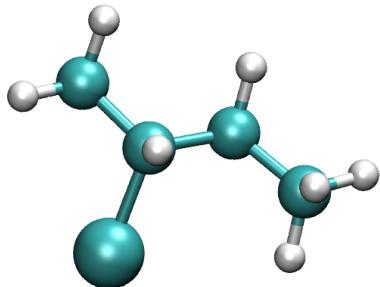
112.224	165.624	257.017
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Equal

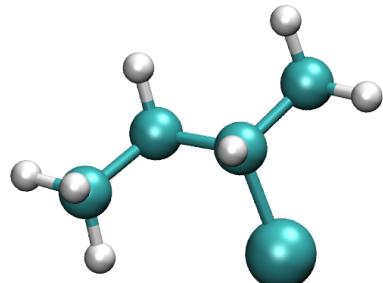


# AsymmetricEnantiomers Número 10

Molecule A  
r-2-chlorobutane\_rotated\_out\_G09



Molecule B s-2-chlorobutane\_out\_G09



Inertia Tensor - Molecule A		
113.621	-8.52391	-0.0867928
-8.52391	164.234	-0.885702
-0.0867928	-0.885702	257.008

Inertia Tensor - Molecule B		
113.621	8.52396	0.0868155
8.52396	164.235	-0.885715
0.0868155	-0.885715	257.008

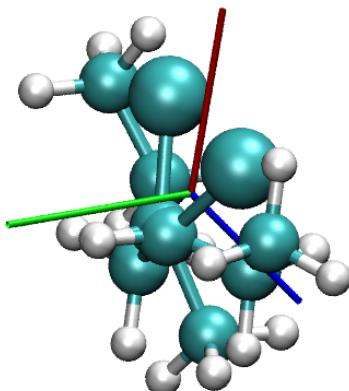
EingenVectors - Molecule A		
-0.986829	-0.161759	-0.00158112
0.161767	-0.986784	-0.00941025
-3.80279e-05	-0.00954208	0.999954

EingenVectors - Molecule B		
-0.98683	0.161755	0.00158125
-0.161763	-0.986785	-0.00941041
3.81715e-05	-0.00954226	0.999954

EingenValues - Molecule A		
112.224	165.623	257.016

EingenValues - Molecule B		
112.224	165.624	257.017

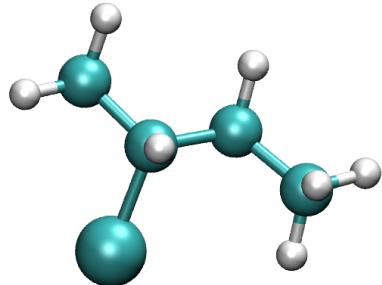
Enantiomers



# AsymmetricEnantiomers Número 11

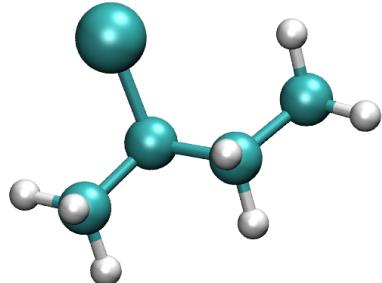
Molecule A

r-2-chlorobutane\_rotated\_out\_G09



Molecule B

s-2-chlorobutane\_out\_G09\_inversion



Inertia Tensor - Molecule A

113.621	-8.52391	-0.0867928
-8.52391	164.234	-0.885702
-0.0867928	-0.885702	257.008

Inertia Tensor - Molecule B

113.622	8.52398	0.0868204
8.52398	164.235	-0.88572
0.0868204	-0.88572	257.009

EingenVectors - Molecule A

-0.986829	-0.161759	-0.00158112
0.161767	-0.986784	-0.00941025
-3.80279e-05	-0.00954208	0.999954

EingenVectors - Molecule B

-0.986829	0.161757	0.0015813
-0.161765	-0.986785	-0.00941039
3.82053e-05	-0.00954225	0.999954

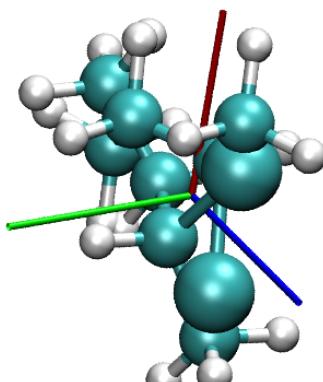
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

112.224	165.624	257.018
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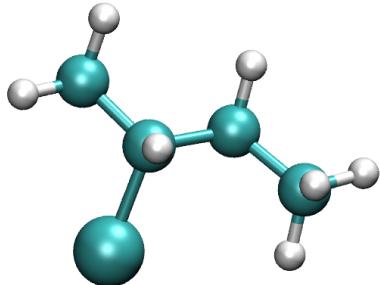
Equal



# AsymmetricEnantiomers Número 12

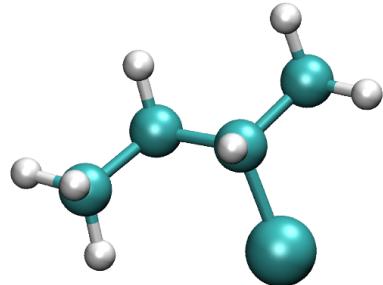
Molecule A

r-2-chlorobutane\_rotated\_out\_G09



Molecule B

s-2-chlorobutane\_rotated\_out\_G09



Inertia Tensor - Molecule A

113.621	-8.52391	-0.0867928
-8.52391	164.234	-0.885702
-0.0867928	-0.885702	257.008

Inertia Tensor - Molecule B

113.621	8.52397	0.0867992
8.52397	164.235	-0.885706
0.0867992	-0.885706	257.008

EingenVectors - Molecule A

-0.986829	-0.161759	-0.00158112
0.161767	-0.986784	-0.00941025
-3.80279e-05	-0.00954208	0.999954

EingenVectors - Molecule B

-0.98683	0.161756	0.00158113
-0.161763	-0.986785	-0.00941034
3.80628e-05	-0.00954217	0.999954

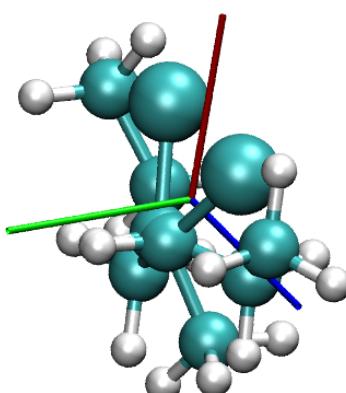
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

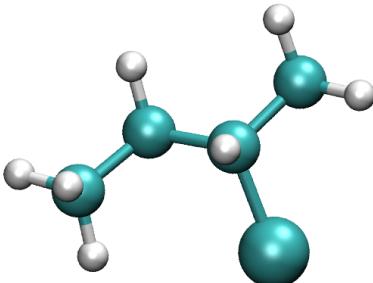
112.224	165.624	257.017
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Enantiomers



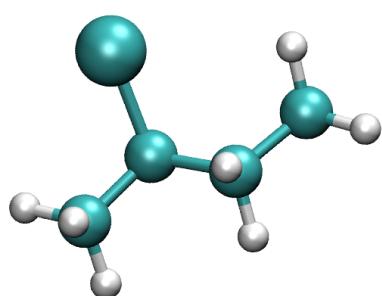
# AsymmetricEnantiomers Número 13

Molecule A s-2-chlorobutane\_out\_G09



Molecule B

s-2-chlorobutane.out\_G09.inversion



Inertia Tensor - Molecule A

113.621	8.52396	0.0868155
8.52396	164.235	-0.885715
0.0868155	-0.885715	257.008

Inertia Tensor - Molecule B

113.622	8.52398	0.0868204
8.52398	164.235	-0.88572
0.0868204	-0.88572	257.009

EingenVectors - Molecule A

-0.98683	0.161755	0.00158125
-0.161763	-0.986785	-0.00941041
3.81715e-05	-0.00954226	0.999954

EingenVectors - Molecule B

-0.986829	0.161757	0.0015813
-0.161765	-0.986785	-0.00941039
3.82053e-05	-0.00954225	0.999954

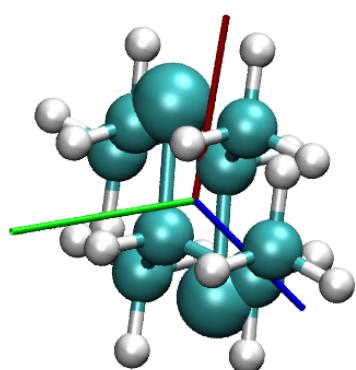
EingenValues - Molecule A

112.224	165.624	257.017
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EingenValues - Molecule B

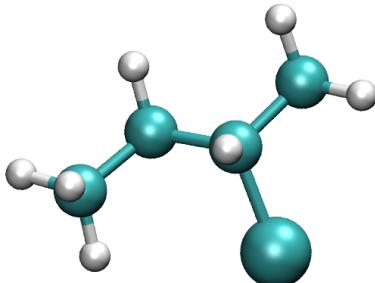
112.224	165.624	257.018
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Enantiomers



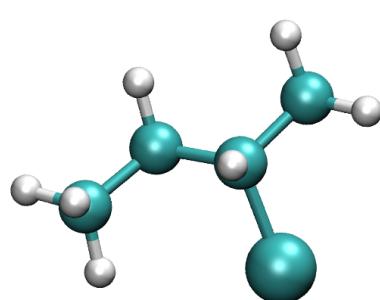
# AsymmetricEnantiomers Número 14

Molecule A s-2-chlorobutane\_out\_G09



Molecule B

s-2-chlorobutane\_rotated\_out\_G09



Inertia Tensor - Molecule A

113.621	8.52396	0.0868155
8.52396	164.235	-0.885715
0.0868155	-0.885715	257.008

Inertia Tensor - Molecule B

113.621	8.52397	0.0867992
8.52397	164.235	-0.885706
0.0867992	-0.885706	257.008

EingenVectors - Molecule A

-0.98683	0.161755	0.00158125
-0.161763	-0.986785	-0.00941041
3.81715e-05	-0.00954226	0.999954

EingenVectors - Molecule B

-0.98683	0.161756	0.00158113
-0.161763	-0.986785	-0.00941034
3.80628e-05	-0.00954217	0.999954

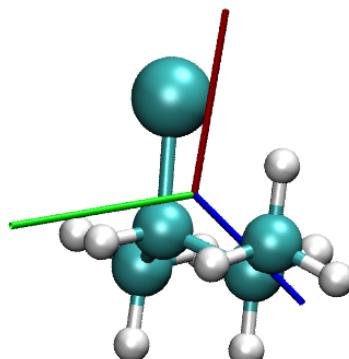
EingenValues - Molecule A

112.224	165.624	257.017
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EingenValues - Molecule B

112.224	165.624	257.017
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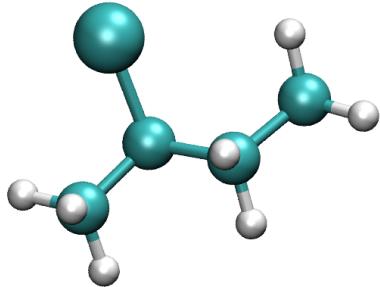
Equal



# AsymmetricEnantiomers Número 15

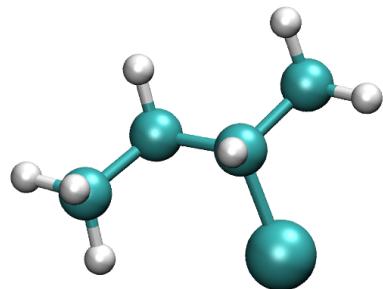
Molecule A

s-2-chlorobutane\_out\_G09\_inversion



Molecule B

s-2-chlorobutane\_rotated\_out\_G09



Inertia Tensor - Molecule A

113.622	8.52398	0.0868204
8.52398	164.235	-0.88572
0.0868204	-0.88572	257.009

Inertia Tensor - Molecule B

113.621	8.52397	0.0867992
8.52397	164.235	-0.885706
0.0867992	-0.885706	257.008

EingenVectors - Molecule A

-0.986829	0.161757	0.0015813
-0.161765	-0.986785	-0.00941039
3.82053e-05	-0.00954225	0.999954

EingenVectors - Molecule B

-0.98683	0.161756	0.00158113
-0.161763	-0.986785	-0.00941034
3.80628e-05	-0.00954217	0.999954

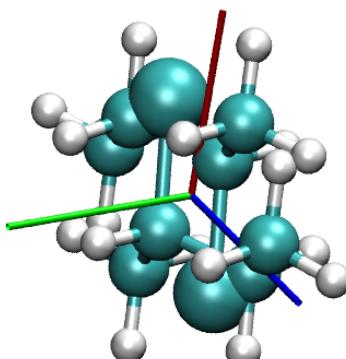
EingenValues - Molecule A

112.224	165.624	257.018
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EingenValues - Molecule B

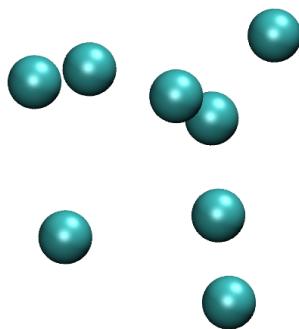
112.224	165.624	257.017
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Enantiomers

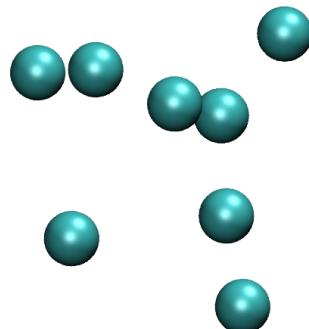


# ClustersCu Número 16

Molecule A G\_08\_Cu



Molecule B G\_08\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1654.82	51.548	-216.332
51.548	1555.14	-242.791
-216.332	-242.791	1259.16

Inertia Tensor - Molecule B

1597.81	73.7499	-186.12
73.7499	1509.17	-199.941
-186.12	-199.941	1250.28

EingenVectors - Molecule A

0.286837	0.406743	0.867343
0.655465	-0.743609	0.13195
0.698634	0.530665	-0.479901

EingenVectors - Molecule B

0.274867	0.38536	0.880878
0.652168	-0.747915	0.123691
0.706488	0.540482	-0.456897

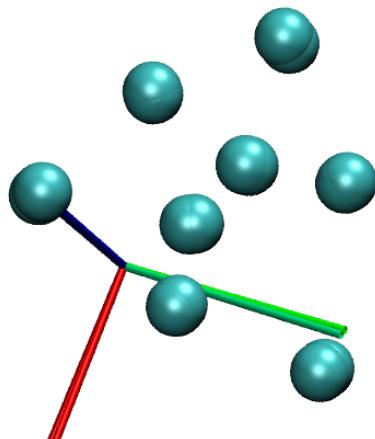
EingenValues - Molecule A

1073.76	1552.79	1842.57
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EingenValues - Molecule B

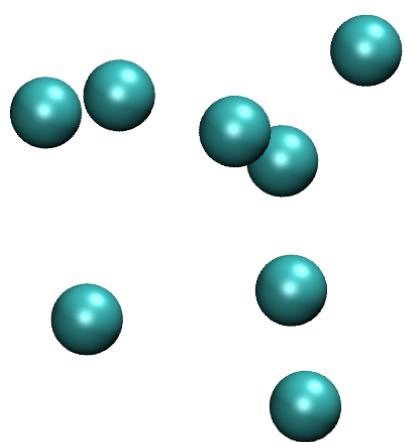
1104.74	1477.93	1774.59
---------	---------	---------

Different



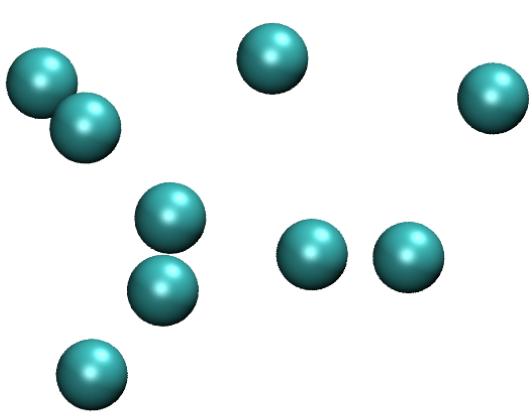
ClustersCu Número 17

Molecule A



G\_08\_Cu

Molecule B

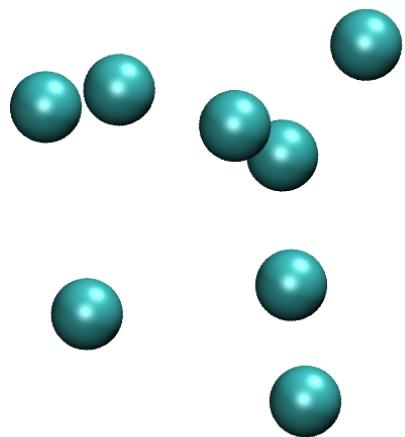


G\_09\_Cu

Different

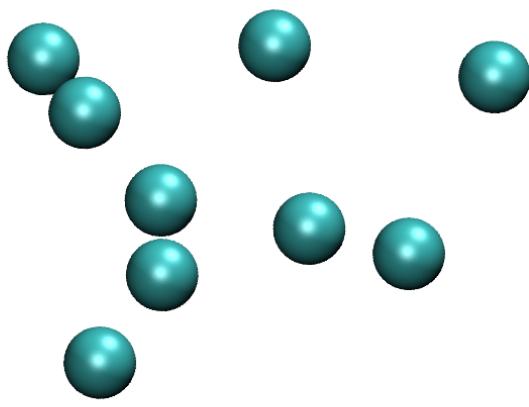
ClustersCu Número 18

Molecule A



G\_08\_Cu

Molecule B

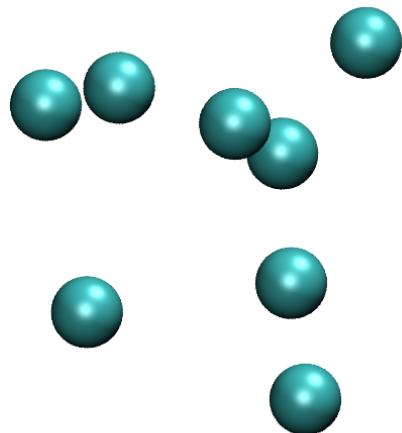


G\_09\_Cu\_AFTER\_DFT

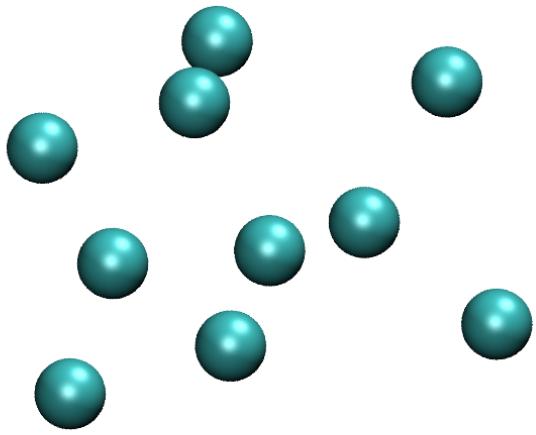
Different

ClustersCu Número 19

Molecule A



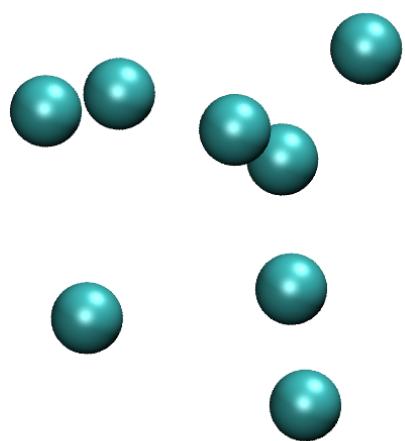
Molecule B



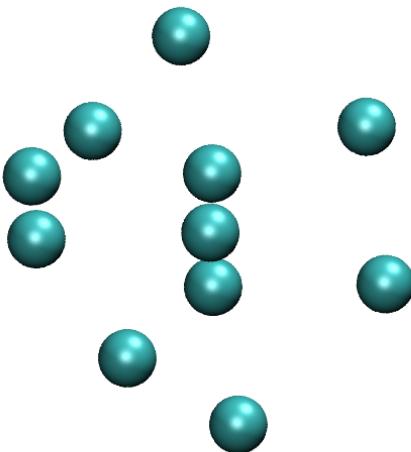
Different

ClustersCu Número 20

Molecule A



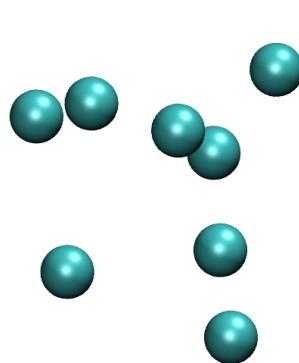
Molecule B



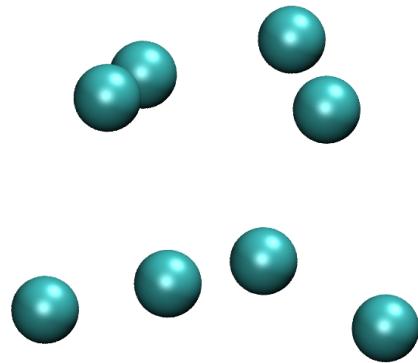
Different

# ClustersCu Número 21

Molecule A G\_08\_Cu



Molecule B SC\_08\_Cu



Inertia Tensor - Molecule A

1654.82	51.548	-216.332
51.548	1555.14	-242.791
-216.332	-242.791	1259.16

Inertia Tensor - Molecule B

1331.27	0.00958178	0.0062677
0.00958178	1331.26	0.00713637
0.0062677	0.00713637	1331.28

EingenVectors - Molecule A

0.286837	0.406743	0.867343
0.655465	-0.743609	0.13195
0.698634	0.530665	-0.479901

EingenVectors - Molecule B

-0.515886	0.847718	-0.123437
-0.684575	-0.321331	0.654296
0.514994	0.422044	0.746096

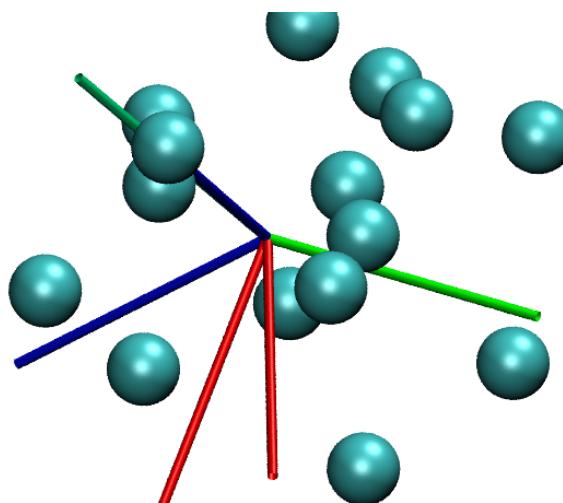
EingenValues - Molecule A

1073.76	1552.79	1842.57
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EingenValues - Molecule B

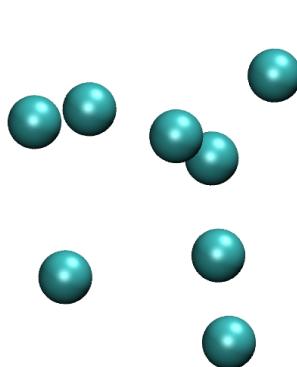
1331.25	1331.27	1331.28
---------	---------	---------

Different

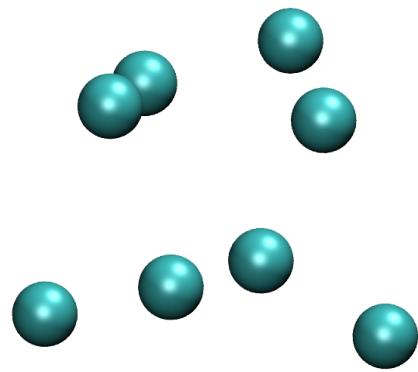


# ClustersCu Número 22

Molecule A G\_08\_Cu



Molecule B SC\_08\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1654.82	51.548	-216.332
51.548	1555.14	-242.791
-216.332	-242.791	1259.16

Inertia Tensor - Molecule B

1394.63	1.12138	-5.89124
1.12138	1385.89	0.251188
-5.89124	0.251188	1398.86

EingenVectors - Molecule A

0.286837	0.406743	0.867343
0.655465	-0.743609	0.13195
0.698634	0.530665	-0.479901

EingenVectors - Molecule B

0.189307	-0.97651	0.102909
0.794609	0.213922	0.568184
-0.576853	-0.0257885	0.816441

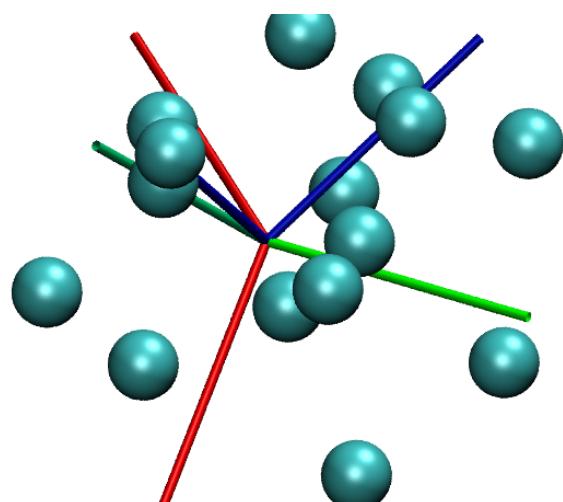
EingenValues - Molecule A

1073.76	1552.79	1842.57
---------	---------	---------

EingenValues - Molecule B

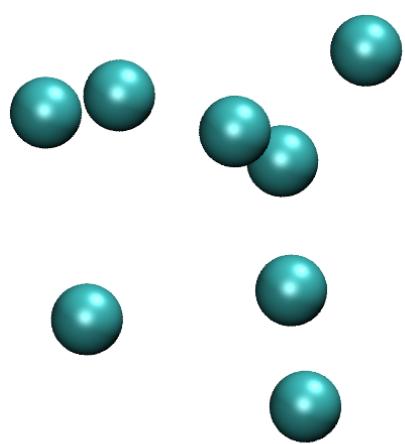
1385.64	1390.72	1403.02
---------	---------	---------

Different



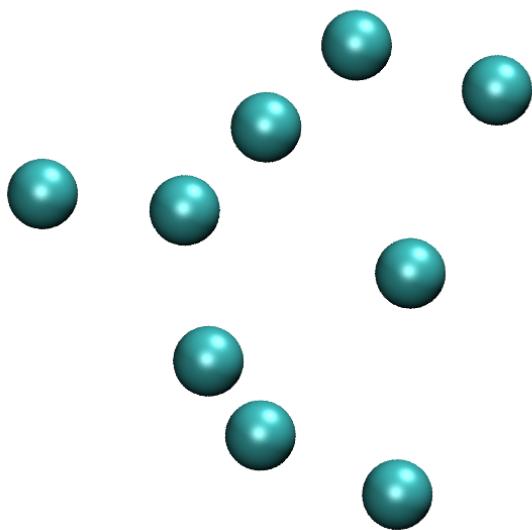
ClustersCu Número 23

Molecule A



G\_08\_Cu

Molecule B

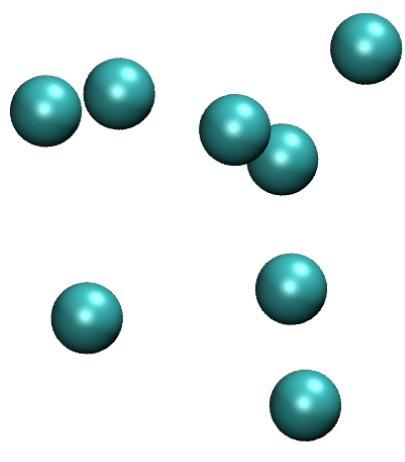


SC\_09\_Cu

Different

ClustersCu Número 24

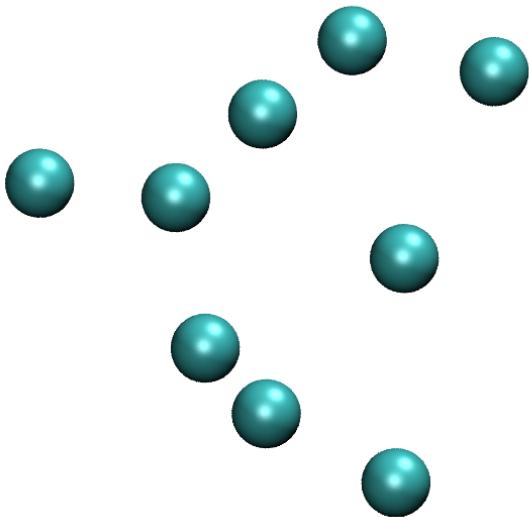
Molecule A



G\_08\_Cu

Molecule B

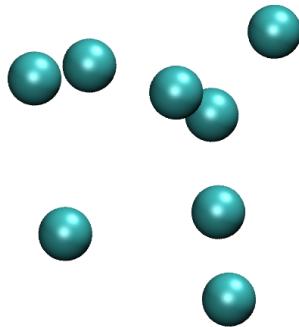
SC\_09\_Cu\_AFTER\_DFT



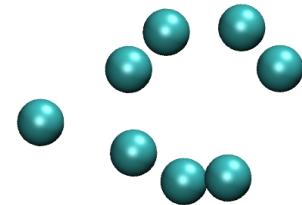
Different

# ClustersCu Número 25

Molecule A G\_08\_Cu



Molecule B lj\_08\_Cu



Inertia Tensor - Molecule A

1654.82	51.548	-216.332
51.548	1555.14	-242.791
-216.332	-242.791	1259.16

Inertia Tensor - Molecule B

1617.21	-91.1093	-437.808
-91.1093	1798.78	-179.618
-437.808	-179.618	957.828

EigenVectors - Molecule A

0.286837	0.406743	0.867343
0.655465	-0.743609	0.13195
0.698634	0.530665	-0.479901

EigenVectors - Molecule B

0.43919	0.180681	0.880038
-0.601213	-0.668782	0.437348
-0.667574	0.721169	0.185095

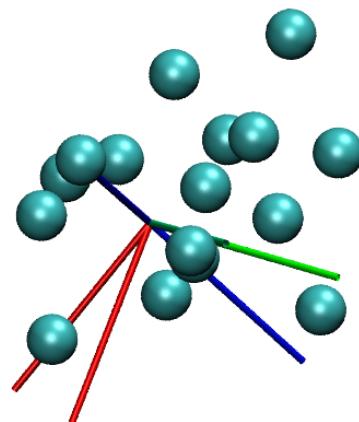
EigenValues - Molecule A

1073.76	1552.79	1842.57
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EigenValues - Molecule B

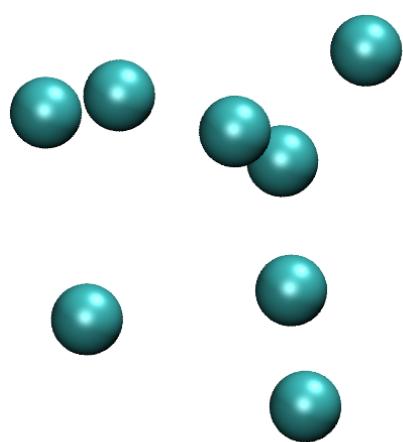
702.459	1834.34	1837.02
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Different



ClustersCu Número 26

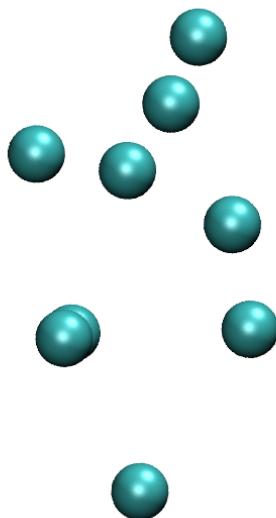
Molecule A



G\_08\_Cu

Molecule B

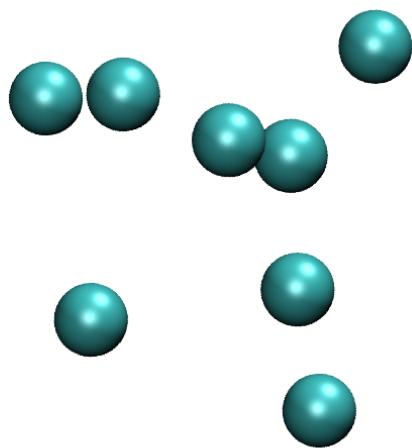
lj\_09\_Cu\_AFTER\_DFT



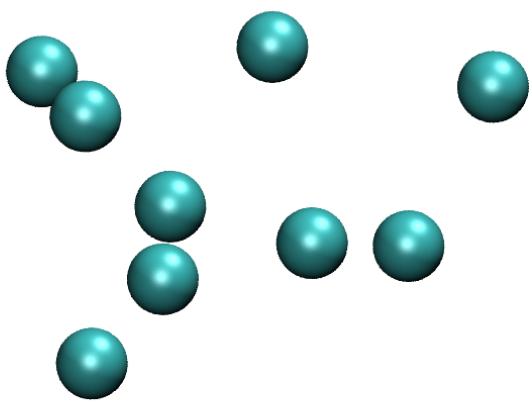
Different

ClustersCu Número 27

Molecule A



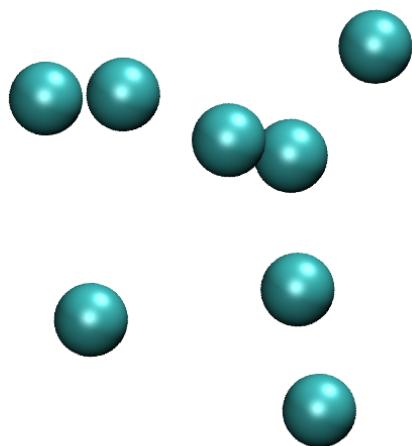
Molecule B



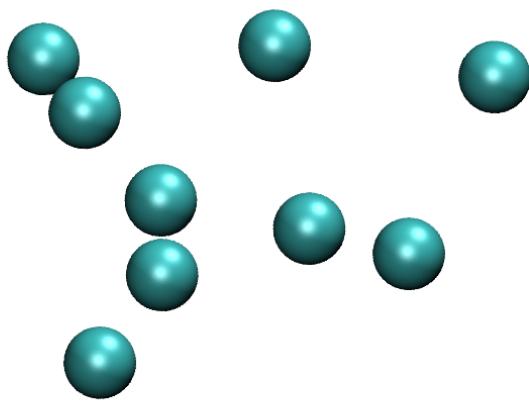
Different

ClustersCu Número 28

Molecule A



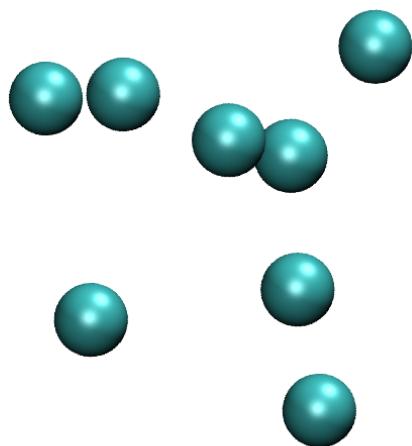
Molecule B



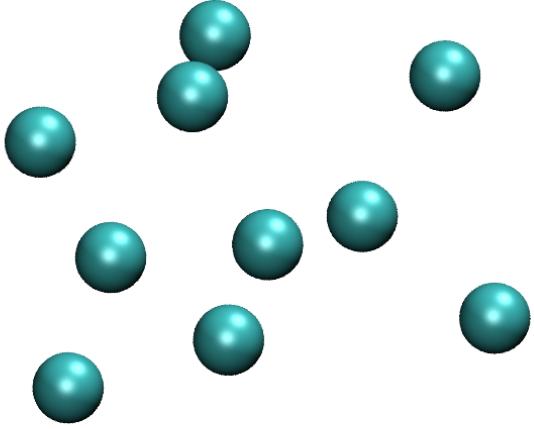
Different

ClustersCu Número 29

Molecule A



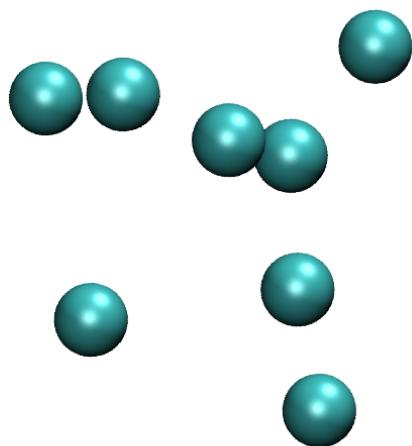
Molecule B



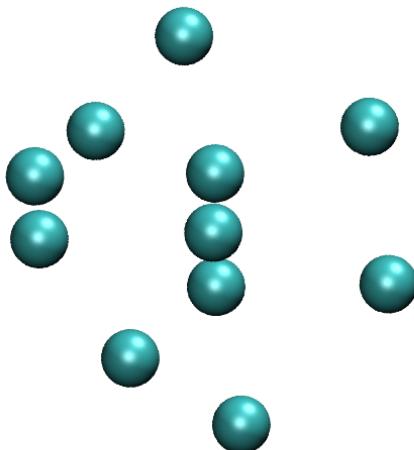
Different

ClustersCu Número 30

Molecule A



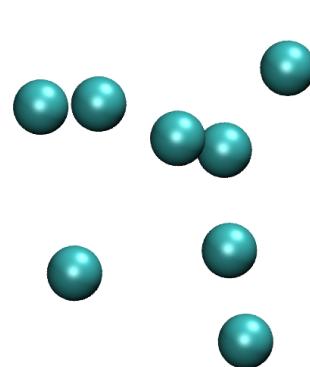
Molecule B



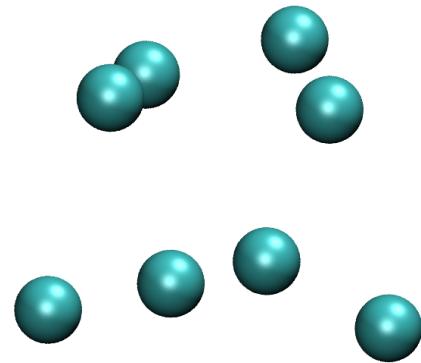
Different

# ClustersCu Número 31

Molecule A G\_08\_Cu\_AFTER\_DFT



Molecule B SC\_08\_Cu



Inertia Tensor - Molecule A

1597.81	73.7499	-186.12
73.7499	1509.17	-199.941
-186.12	-199.941	1250.28

Inertia Tensor - Molecule B

1331.27	0.00958178	0.0062677
0.00958178	1331.26	0.00713637
0.0062677	0.00713637	1331.28

EingenVectors - Molecule A

0.274867	0.38536	0.880878
0.652168	-0.747915	0.123691
0.706488	0.540482	-0.456897

EingenVectors - Molecule B

-0.515886	0.847718	-0.123437
-0.684575	-0.321331	0.654296
0.514994	0.422044	0.746096

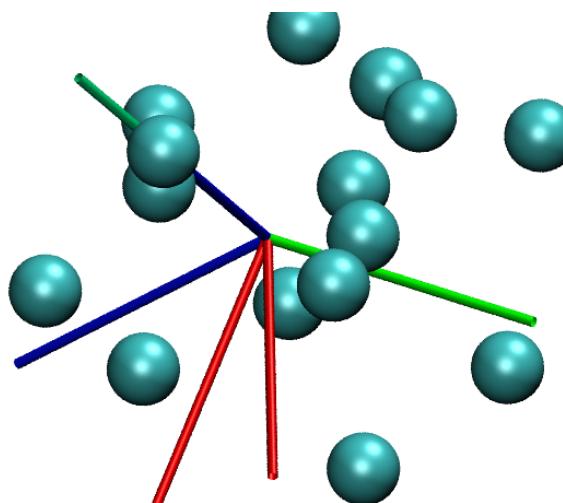
EingenValues - Molecule A

1104.74	1477.93	1774.59
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EingenValues - Molecule B

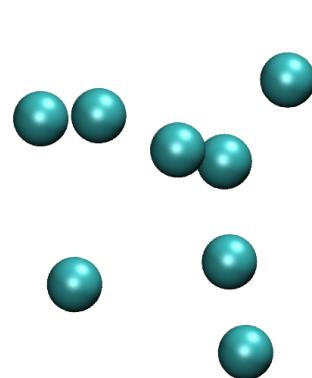
1331.25	1331.27	1331.28
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Different

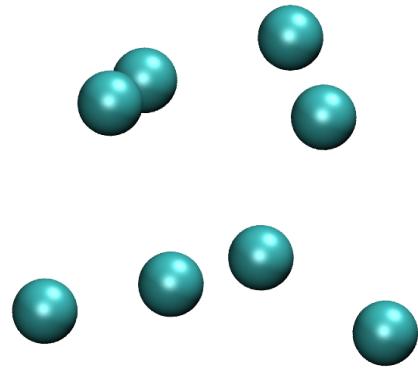


# ClustersCu Número 32

Molecule A G\_08\_Cu\_AFTER\_DFT



Molecule B SC\_08\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1597.81	73.7499	-186.12
73.7499	1509.17	-199.941
-186.12	-199.941	1250.28

Inertia Tensor - Molecule B

1394.63	1.12138	-5.89124
1.12138	1385.89	0.251188
-5.89124	0.251188	1398.86

EingenVectors - Molecule A

0.274867	0.38536	0.880878
0.652168	-0.747915	0.123691
0.706488	0.540482	-0.456897

EingenVectors - Molecule B

0.189307	-0.97651	0.102909
0.794609	0.213922	0.568184
-0.576853	-0.0257885	0.816441

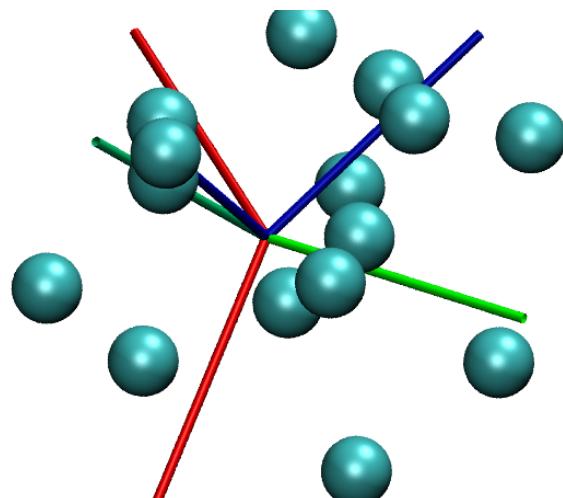
EingenValues - Molecule A

1104.74	1477.93	1774.59
---------	---------	---------

EingenValues - Molecule B

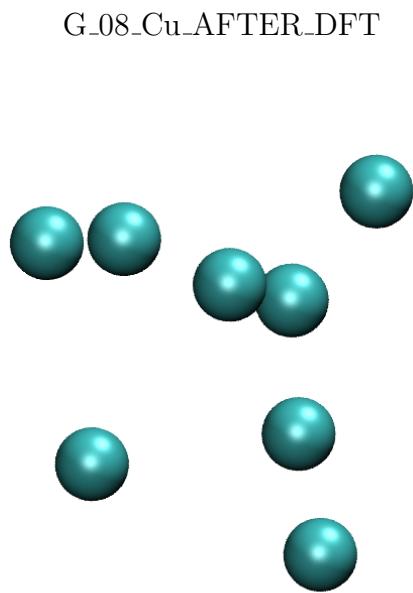
1385.64	1390.72	1403.02
---------	---------	---------

Different

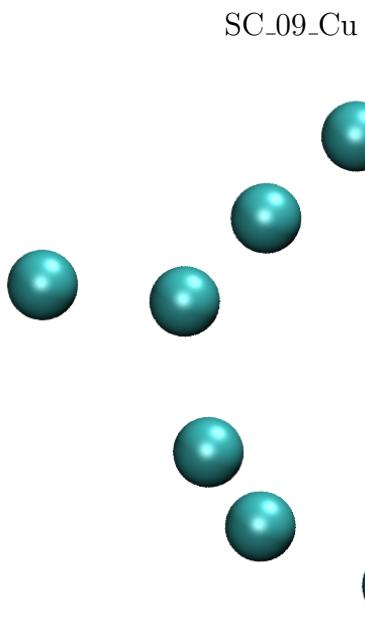


ClustersCu Número 33

Molecule A



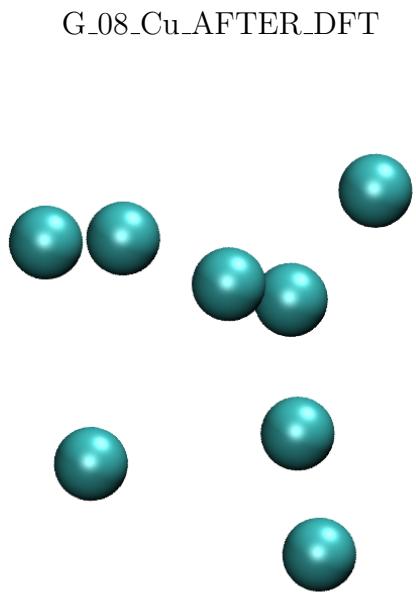
Molecule B



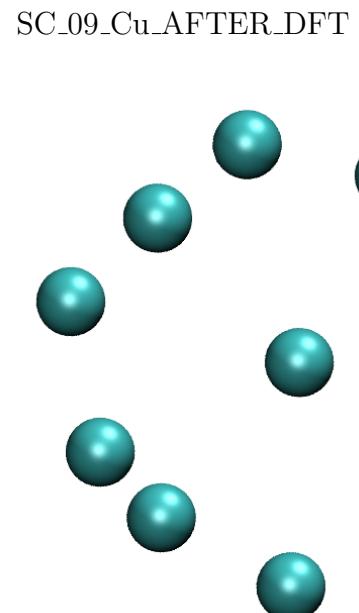
Different

ClustersCu Número 34

Molecule A



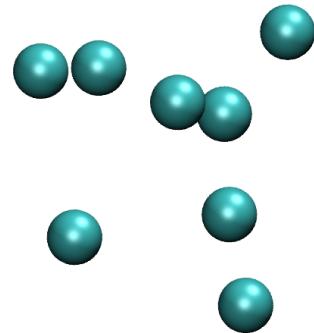
Molecule B



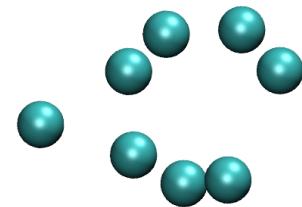
Different

# ClustersCu Número 35

Molecule A G\_08\_Cu\_AFTER\_DFT



Molecule B lj\_08\_Cu



Inertia Tensor - Molecule A

1597.81	73.7499	-186.12
73.7499	1509.17	-199.941
-186.12	-199.941	1250.28

Inertia Tensor - Molecule B

1617.21	-91.1093	-437.808
-91.1093	1798.78	-179.618
-437.808	-179.618	957.828

EingenVectors - Molecule A

0.274867	0.38536	0.880878
0.652168	-0.747915	0.123691
0.706488	0.540482	-0.456897

EingenVectors - Molecule B

0.43919	0.180681	0.880038
-0.601213	-0.668782	0.437348
-0.667574	0.721169	0.185095

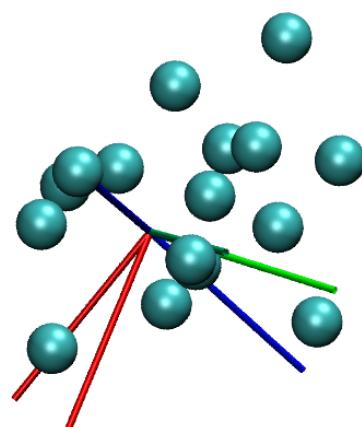
EingenValues - Molecule A

1104.74	1477.93	1774.59
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EingenValues - Molecule B

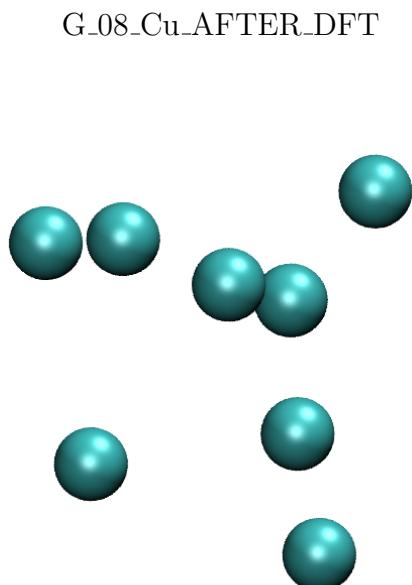
702.459	1834.34	1837.02
---------	---------	---------

Different

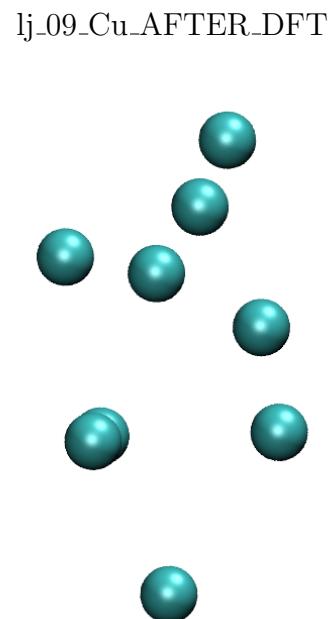


ClustersCu Número 36

Molecule A



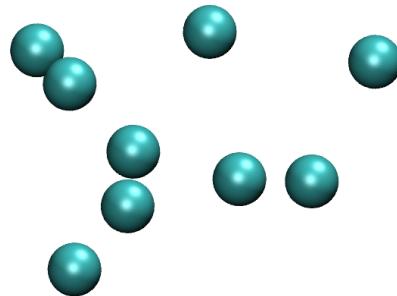
Molecule B



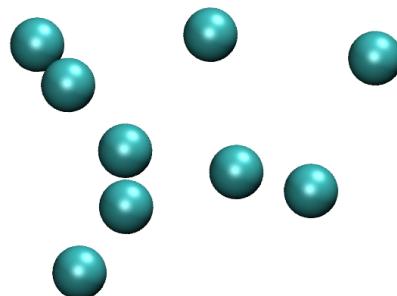
Different

# ClustersCu Número 37

Molecule A G\_09\_Cu



Molecule B G\_09\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1643.08	-103.447	113.093
-103.447	2240.72	205.863
113.093	205.863	1748.04

Inertia Tensor - Molecule B

1625.38	-92.1303	110.251
-92.1303	2185.43	185.921
110.251	185.921	1731.97

EingenVectors - Molecule A

-0.747587	-0.277171	0.603564
0.657992	-0.185481	0.729825
-0.0903363	0.942748	0.321039

EingenVectors - Molecule B

-0.760255	-0.26577	0.592773
0.644373	-0.192718	0.740029
-0.0824395	0.944577	0.317769

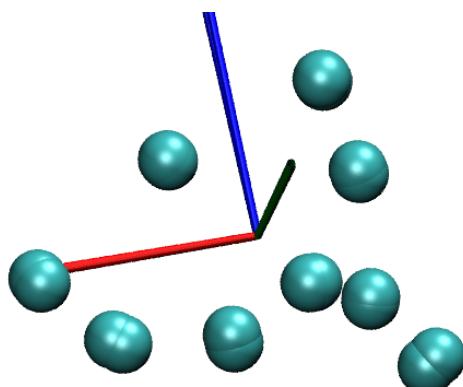
EingenValues - Molecule A

1513.42	1797.68	2320.74
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EingenValues - Molecule B

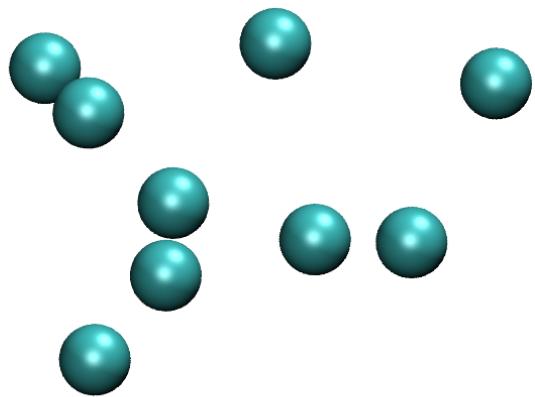
1507.21	1779.55	2256.02
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Different



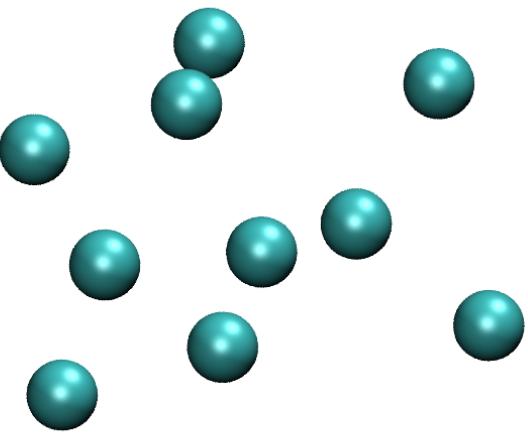
ClustersCu Número 38

Molecule A



G\_09\_Cu

Molecule B

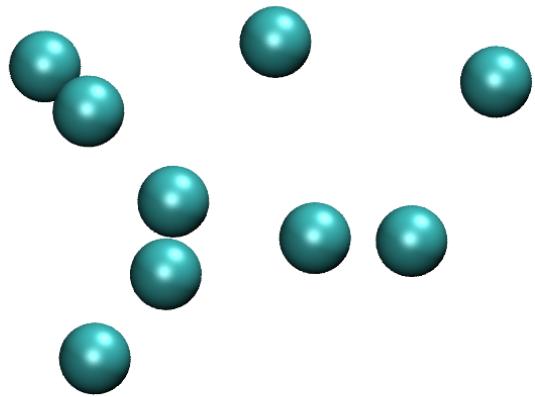


G\_10\_Cu

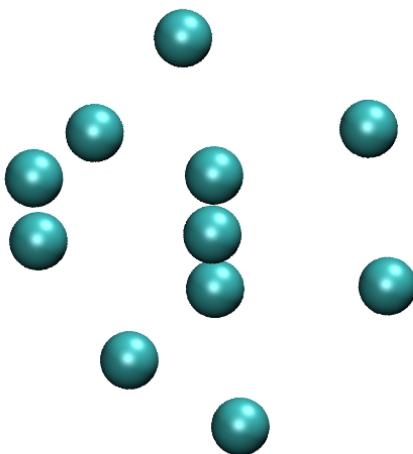
Different

ClustersCu Número 39

Molecule A



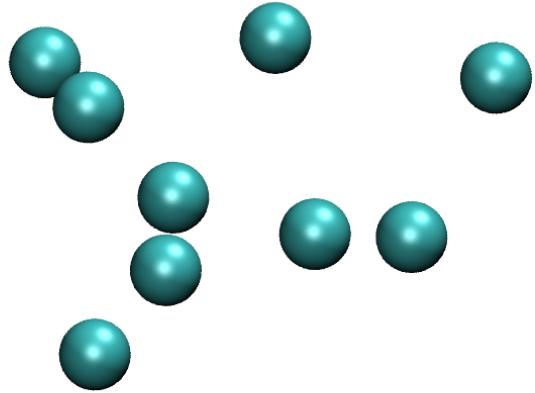
Molecule B



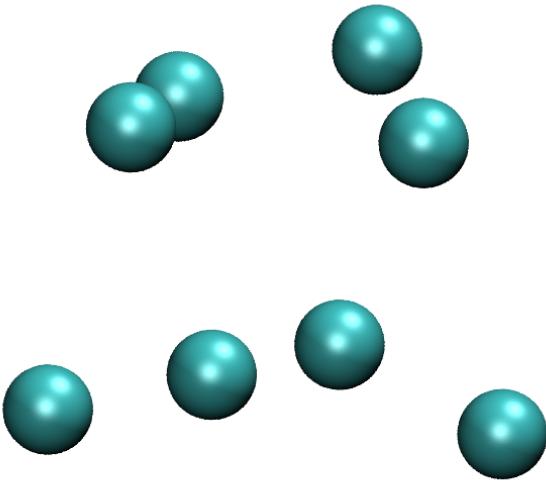
Different

ClustersCu Número 40

Molecule A



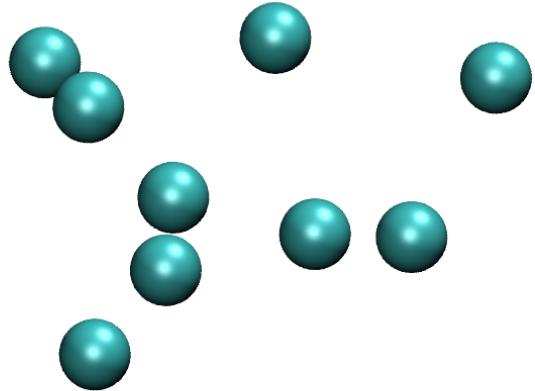
Molecule B



Different

ClustersCu Número 41

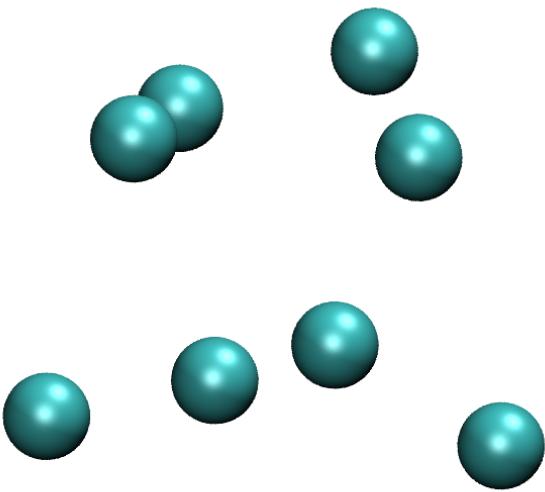
Molecule A



G\_09\_Cu

Molecule B

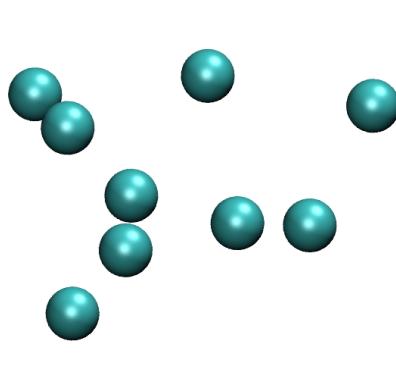
SC\_08\_Cu\_AFTER\_DFT



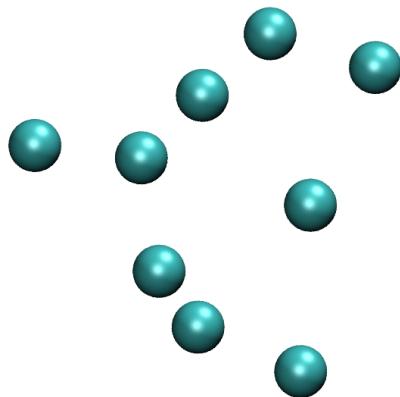
Different

# ClustersCu Número 42

Molecule A G\_09\_Cu



Molecule B SC\_09\_Cu



Inertia Tensor - Molecule A

1643.08	-103.447	113.093
-103.447	2240.72	205.863
113.093	205.863	1748.04

Inertia Tensor - Molecule B

1697.74	-70.4883	5.56477
-70.4883	1438.99	-78.8974
5.56477	-78.8974	2188.92

EingenVectors - Molecule A

-0.747587	-0.277171	0.603564
0.657992	-0.185481	0.729825
-0.0903363	0.942748	0.321039

EingenVectors - Molecule B

0.23798	0.966449	0.0966559
0.970922	-0.234051	-0.0503052
0.025995	-0.105817	0.994046

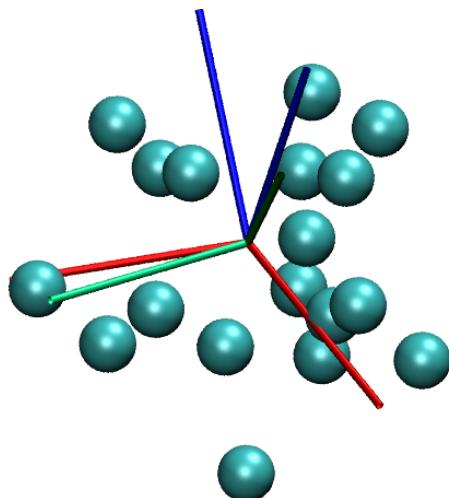
EingenValues - Molecule A

1513.42	1797.68	2320.74
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EingenValues - Molecule B

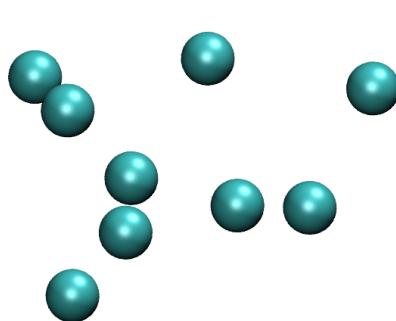
1413.74	1714.44	2197.47
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Different

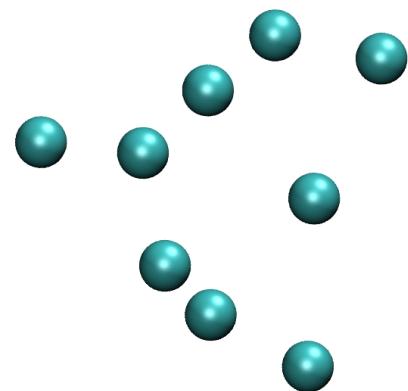


# ClustersCu Número 43

Molecule A G\_09\_Cu



Molecule B SC\_09\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1643.08	-103.447	113.093
-103.447	2240.72	205.863
113.093	205.863	1748.04

Inertia Tensor - Molecule B

1766.59	-64.0178	3.81884
-64.0178	1532.55	-76.7432
3.81884	-76.7432	2248.22

EingenVectors - Molecule A

-0.747587	-0.277171	0.603564
0.657992	-0.185481	0.729825
-0.0903363	0.942748	0.321039

EingenVectors - Molecule B

0.238514	0.966075	0.0990463
0.970895	-0.234926	-0.046613
0.0217631	-0.107281	0.99399

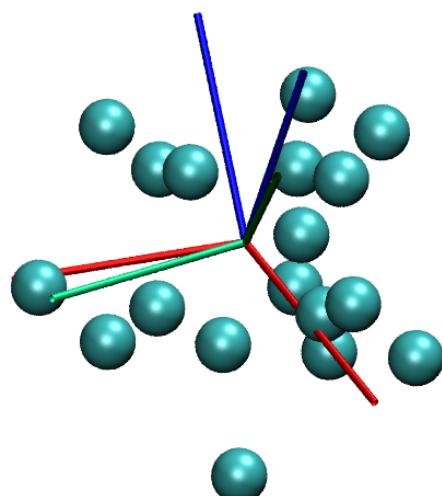
EingenValues - Molecule A

1513.42	1797.68	2320.74
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EingenValues - Molecule B

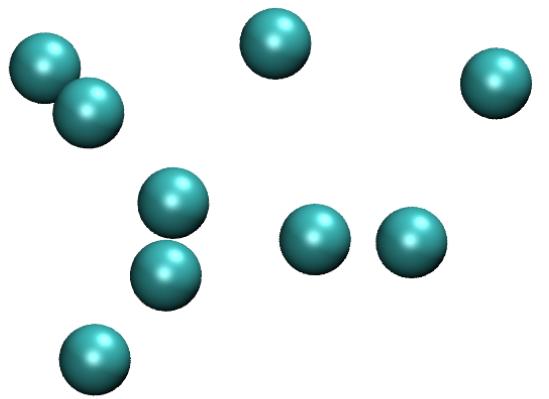
1508.88	1781.9	2256.58
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Different

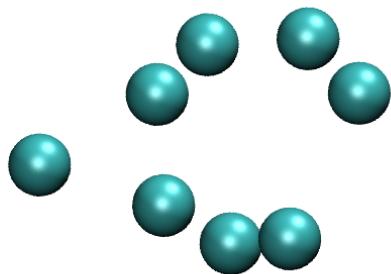


ClustersCu Número 44

Molecule A



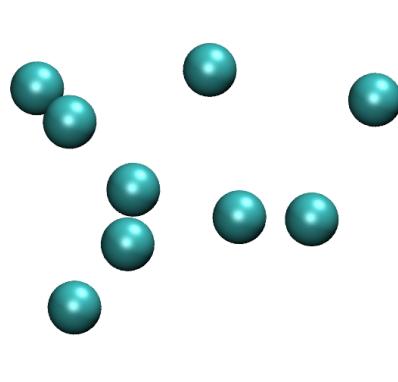
Molecule B



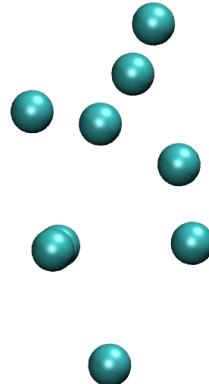
Different

# ClustersCu Número 45

Molecule A G\_09\_Cu



Molecule B lj\_09\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1643.08	-103.447	113.093
-103.447	2240.72	205.863
113.093	205.863	1748.04

Inertia Tensor - Molecule B

2617.21	-111.803	97.8221
-111.803	1523.61	773.326
97.8221	773.326	1971.07

EingenVectors - Molecule A

-0.747587	-0.277171	0.603564
0.657992	-0.185481	0.729825
-0.0903363	0.942748	0.321039

EingenVectors - Molecule B

-0.0874373	-0.795928	0.599044
0.136388	-0.60525	-0.784265
-0.986789	-0.0131283	-0.161476

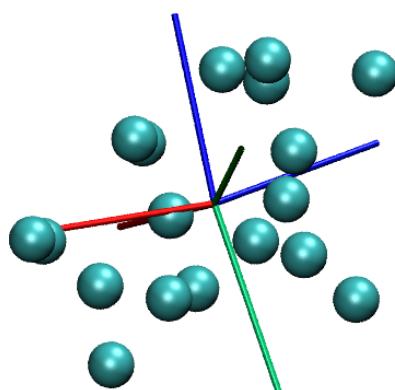
EingenValues - Molecule A

1513.42	1797.68	2320.74
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EingenValues - Molecule B

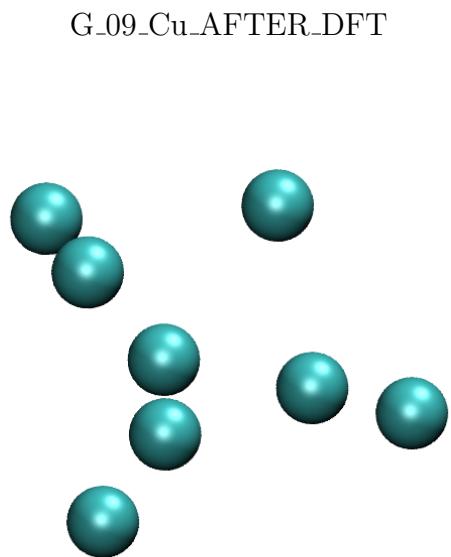
929.299	2550.86	2631.73
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Different

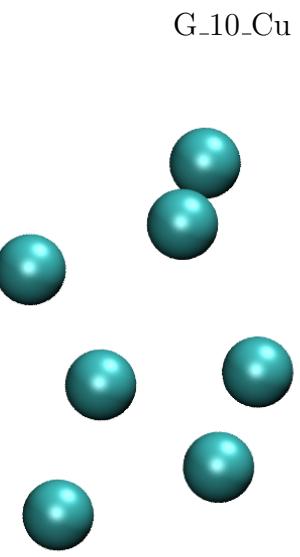


ClustersCu Número 46

Molecule A



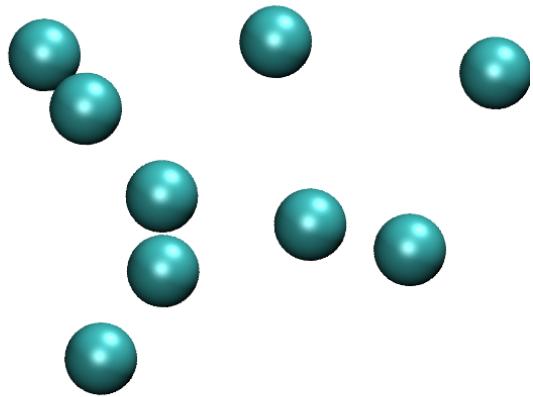
Molecule B



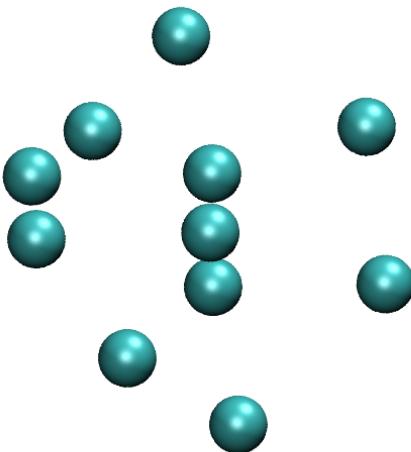
Different

ClustersCu Número 47

Molecule A



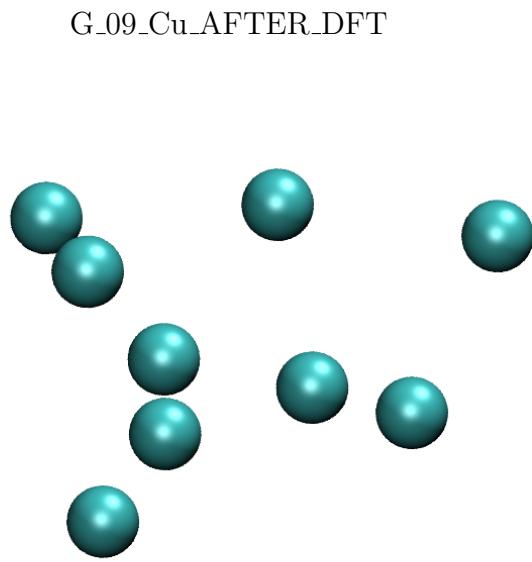
Molecule B



Different

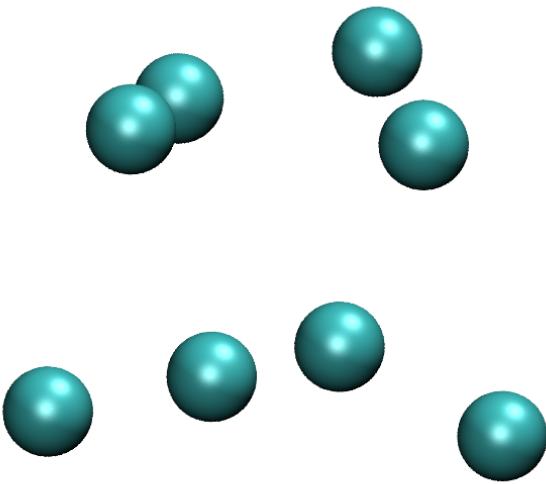
ClustersCu Número 48

Molecule A



Molecule B

SC\_08\_Cu

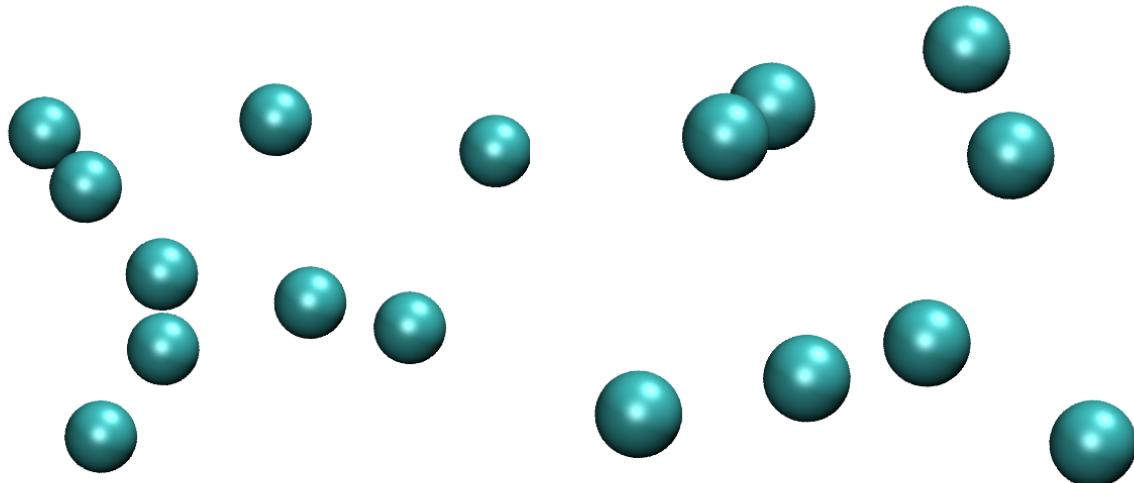


Different

ClustersCu Número 49

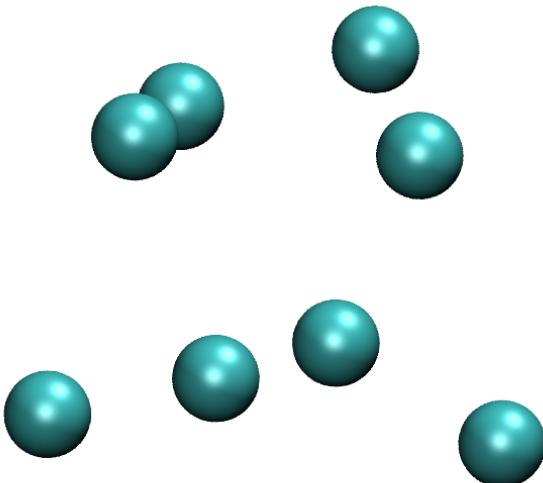
Molecule A

G\_09\_Cu\_AFTER\_DFT



Molecule B

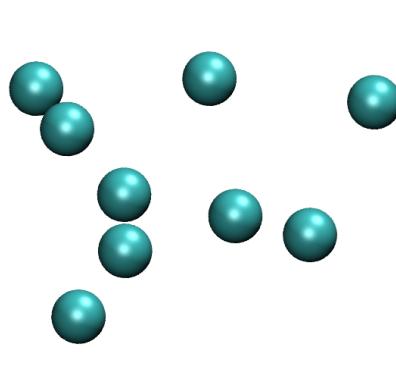
SC\_08\_Cu\_AFTER\_DFT



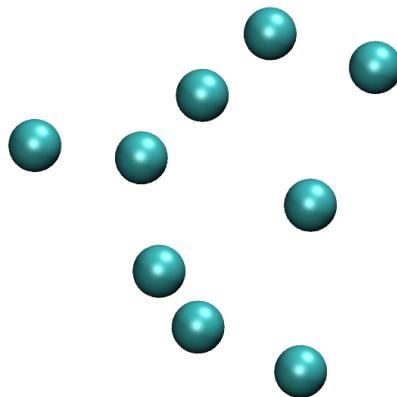
Different

# ClustersCu Número 50

Molecule A G\_09\_Cu\_AFTER\_DFT



Molecule B SC\_09\_Cu



Inertia Tensor - Molecule A

1625.38	-92.1303	110.251
-92.1303	2185.43	185.921
110.251	185.921	1731.97

Inertia Tensor - Molecule B

1697.74	-70.4883	5.56477
-70.4883	1438.99	-78.8974
5.56477	-78.8974	2188.92

EingenVectors - Molecule A

-0.760255	-0.26577	0.592773
0.644373	-0.192718	0.740029
-0.0824395	0.944577	0.317769

EingenVectors - Molecule B

0.23798	0.966449	0.0966559
0.970922	-0.234051	-0.0503052
0.025995	-0.105817	0.994046

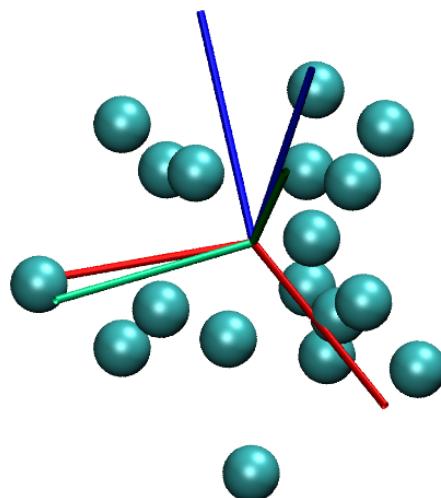
EingenValues - Molecule A

1507.21	1779.55	2256.02
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EingenValues - Molecule B

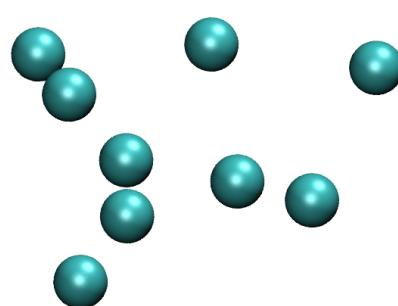
1413.74	1714.44	2197.47
---------	---------	---------

Different

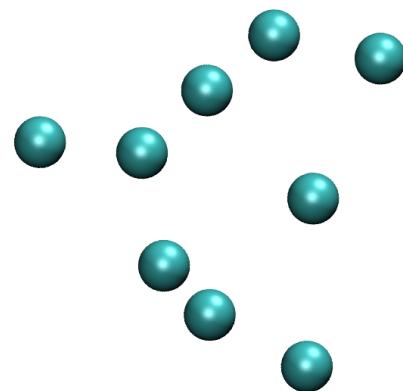


# ClustersCu Número 51

Molecule A G\_09\_Cu\_AFTER\_DFT



Molecule B SC\_09\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1625.38	-92.1303	110.251
-92.1303	2185.43	185.921
110.251	185.921	1731.97

Inertia Tensor - Molecule B

1766.59	-64.0178	3.81884
-64.0178	1532.55	-76.7432
3.81884	-76.7432	2248.22

EingenVectors - Molecule A

-0.760255	-0.26577	0.592773
0.644373	-0.192718	0.740029
-0.0824395	0.944577	0.317769

EingenVectors - Molecule B

0.238514	0.966075	0.0990463
0.970895	-0.234926	-0.046613
0.0217631	-0.107281	0.99399

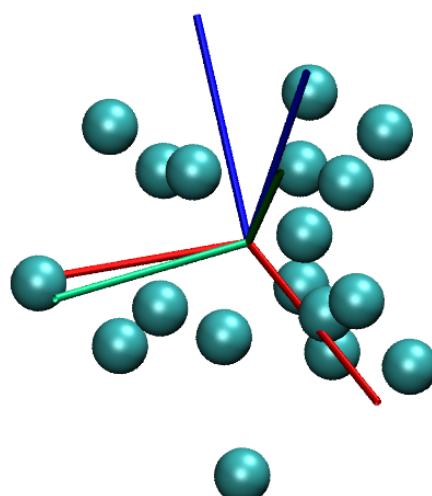
EingenValues - Molecule A

1507.21	1779.55	2256.02
---------	---------	---------

EingenValues - Molecule B

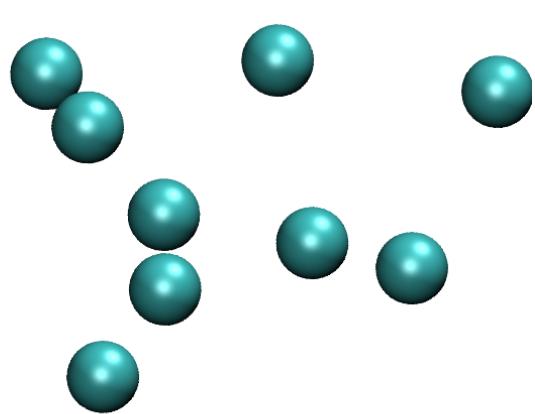
1508.88	1781.9	2256.58
---------	--------	---------

Different



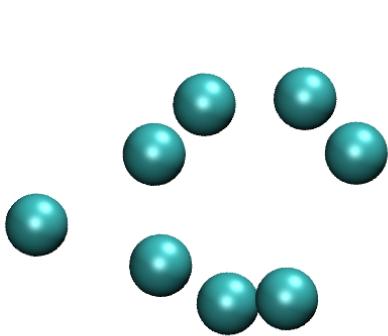
ClustersCu Número 52

Molecule A



Molecule B

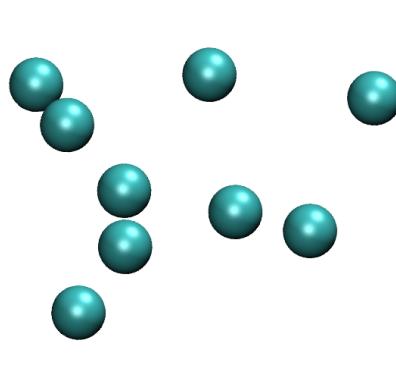
lj\_08\_Cu



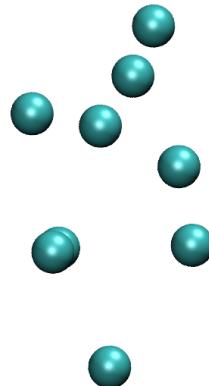
Different

# ClustersCu Número 53

Molecule A G\_09\_Cu\_AFTER\_DFT



Molecule B lj\_09\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1625.38	-92.1303	110.251
-92.1303	2185.43	185.921
110.251	185.921	1731.97

Inertia Tensor - Molecule B

2617.21	-111.803	97.8221
-111.803	1523.61	773.326
97.8221	773.326	1971.07

EingenVectors - Molecule A

-0.760255	-0.26577	0.592773
0.644373	-0.192718	0.740029
-0.0824395	0.944577	0.317769

EingenVectors - Molecule B

-0.0874373	-0.795928	0.599044
0.136388	-0.60525	-0.784265
-0.986789	-0.0131283	-0.161476

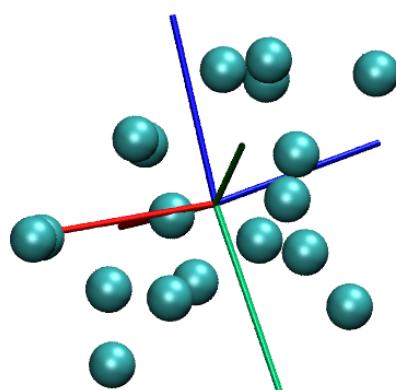
EingenValues - Molecule A

1507.21	1779.55	2256.02
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EingenValues - Molecule B

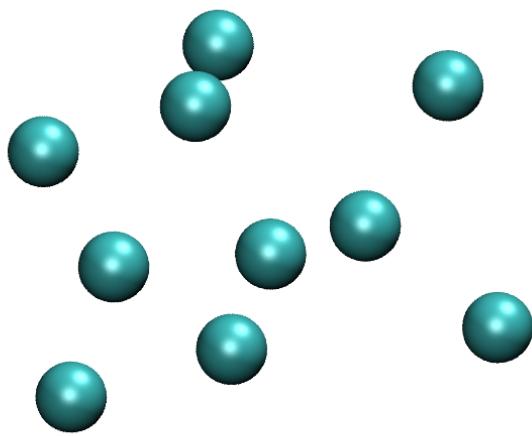
929.299	2550.86	2631.73
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Different



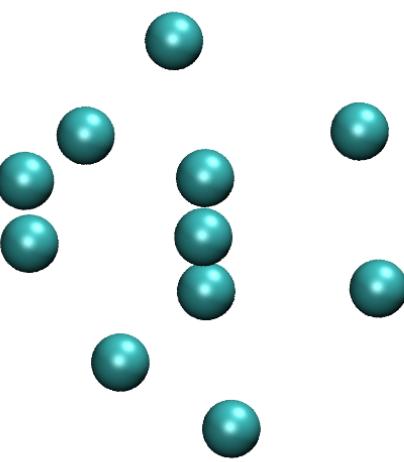
ClustersCu Número 54

Molecule A



G\_10\_Cu

Molecule B

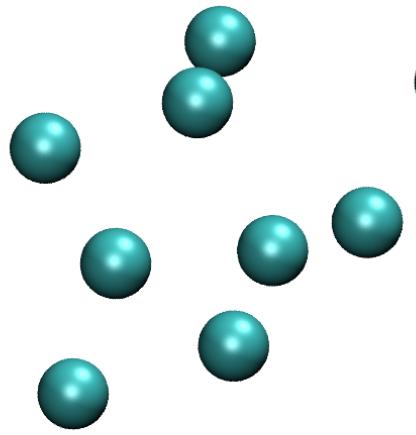


G\_11\_Cu

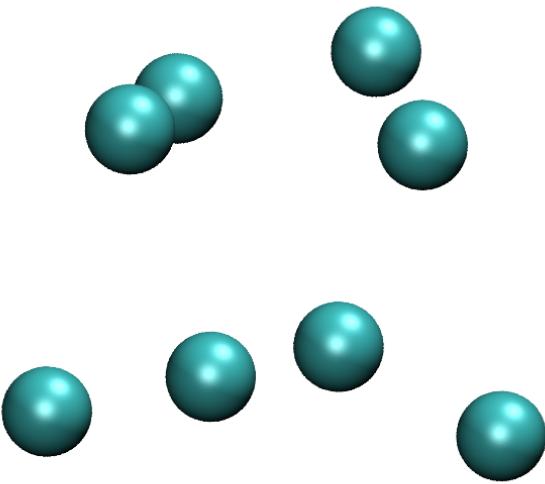
Different

ClustersCu Número 55

Molecule A



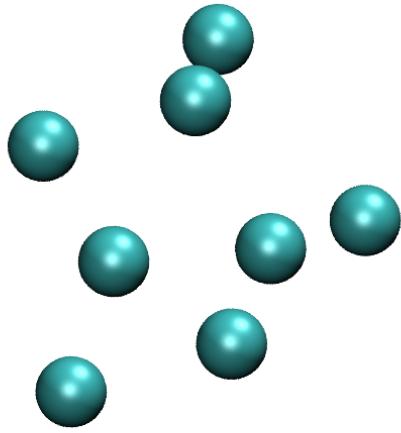
Molecule B



Different

ClustersCu Número 56

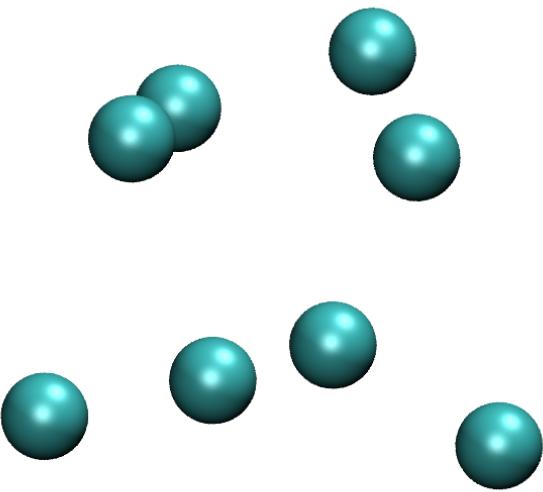
Molecule A



G\_10\_Cu

Molecule B

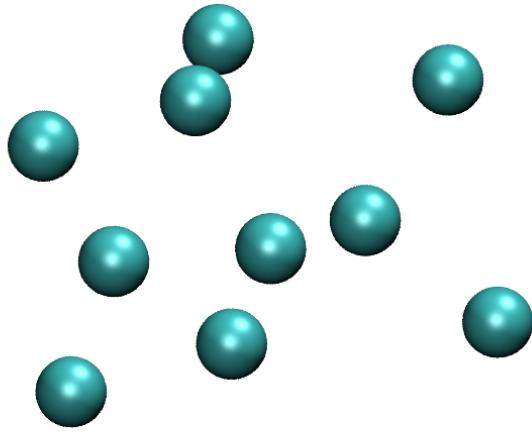
SC\_08\_Cu\_AFTER\_DFT



Different

ClustersCu Número 57

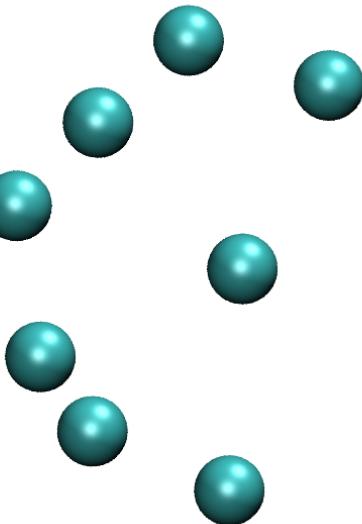
Molecule A



G\_10\_Cu

Molecule B

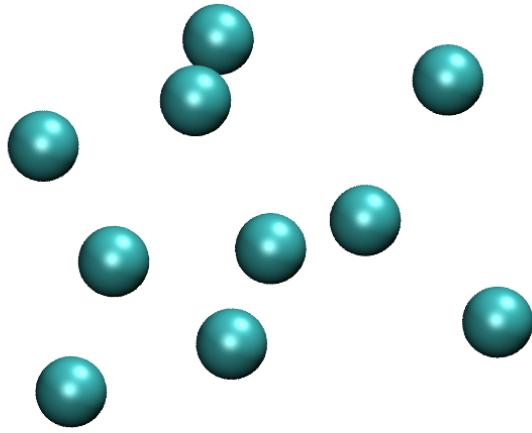
SC\_09\_Cu



Different

ClustersCu Número 58

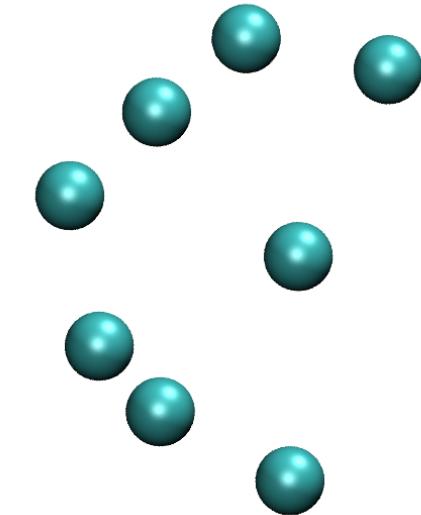
Molecule A



G\_10\_Cu

Molecule B

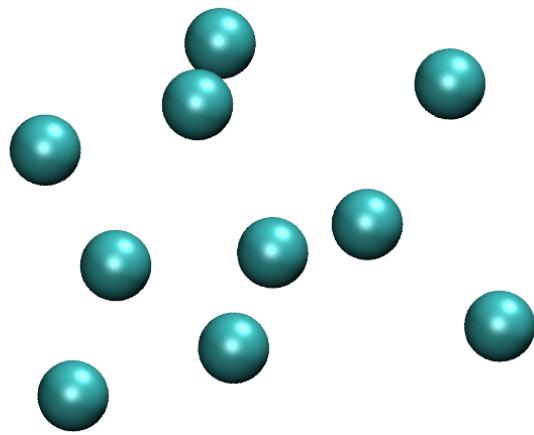
SC\_09\_Cu\_AFTER\_DFT



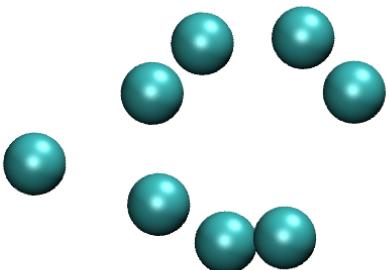
Different

ClustersCu Número 59

Molecule A



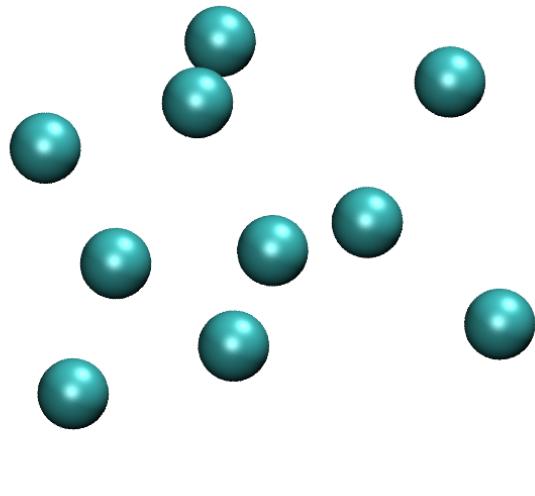
Molecule B



Different

ClustersCu Número 60

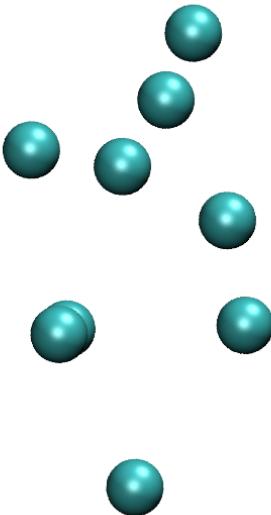
Molecule A



G\_10\_Cu

Molecule B

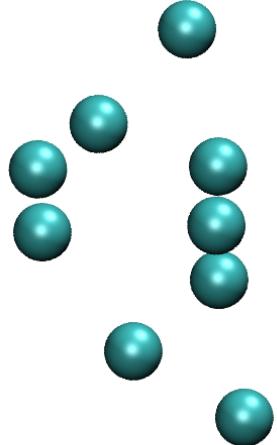
lj\_09\_Cu\_AFTER\_DFT



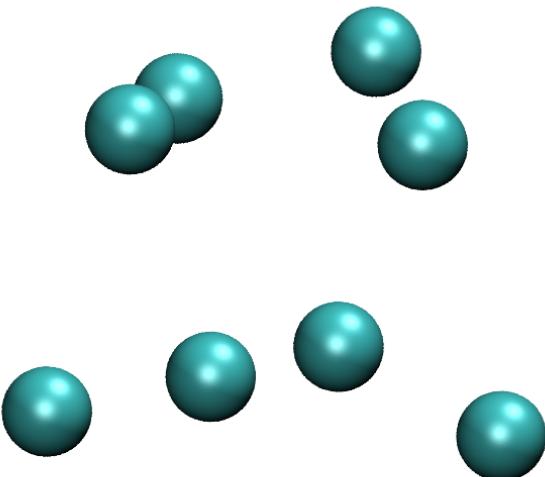
Different

ClustersCu Número 61

Molecule A



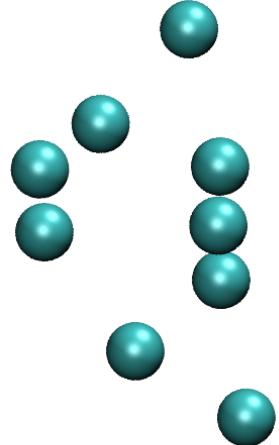
Molecule B



Different

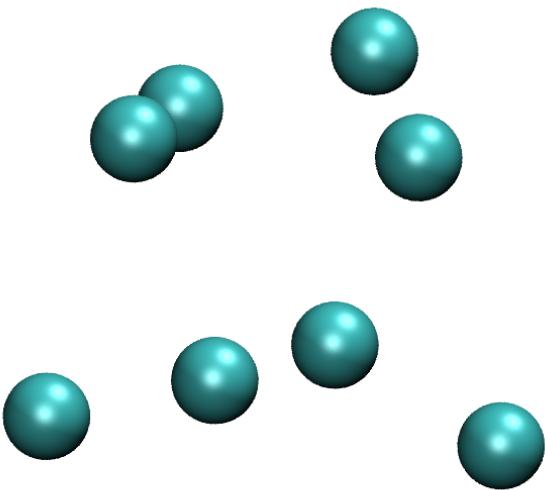
ClustersCu Número 62

Molecule A



Molecule B

SC\_08\_Cu\_AFTER\_DFT

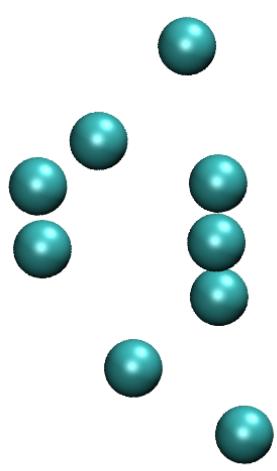


Different

ClustersCu Número 63

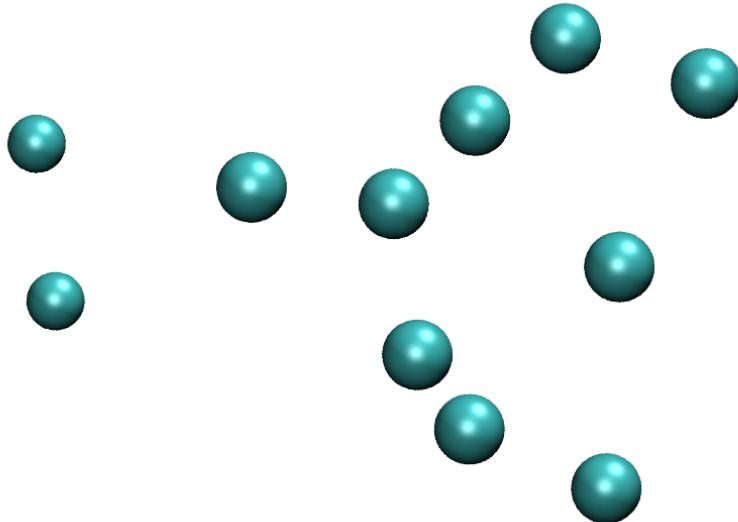
Molecule A

G\_11\_Cu



Molecule B

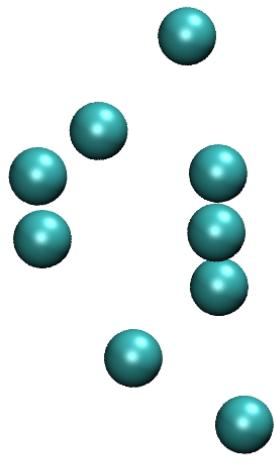
SC\_09\_Cu



Different

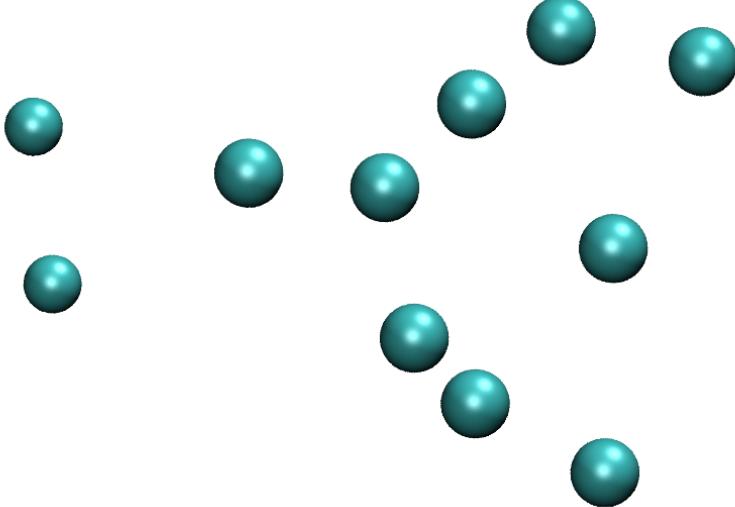
ClustersCu Número 64

Molecule A



Molecule B

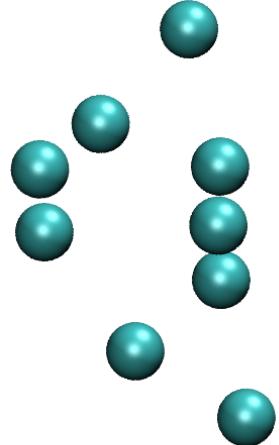
SC\_09\_Cu\_AFTER\_DFT



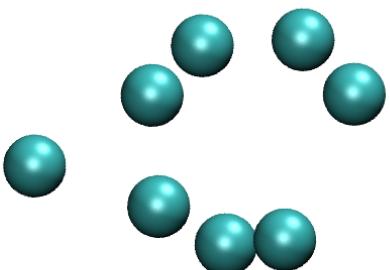
Different

ClustersCu Número 65

Molecule A



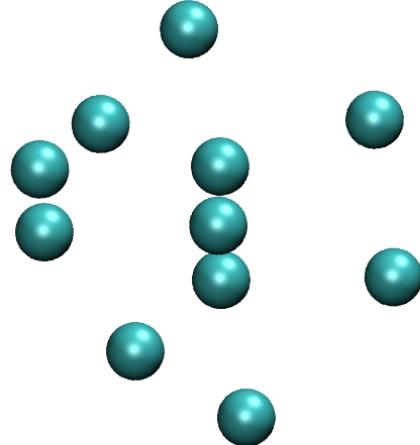
Molecule B



Different

ClustersCu Número 66

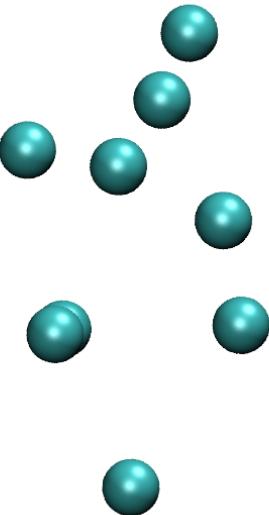
Molecule A



G\_11\_Cu

Molecule B

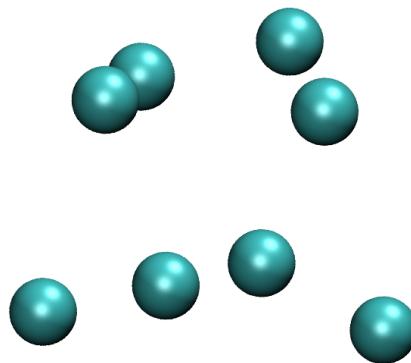
lj\_09\_Cu\_AFTER\_DFT



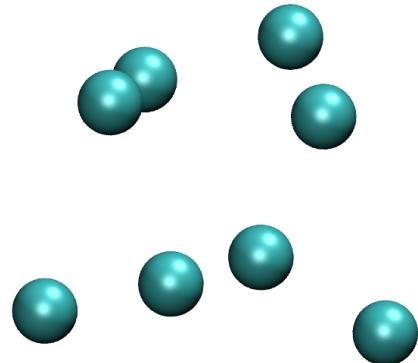
Different

# ClustersCu Número 67

Molecule A SC\_08\_Cu



Molecule B SC\_08\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1331.27	0.00958178	0.0062677
0.00958178	1331.26	0.00713637
0.0062677	0.00713637	1331.28

Inertia Tensor - Molecule B

1394.63	1.12138	-5.89124
1.12138	1385.89	0.251188
-5.89124	0.251188	1398.86

EingenVectors - Molecule A

-0.515886	0.847718	-0.123437
-0.684575	-0.321331	0.654296
0.514994	0.422044	0.746096

EingenVectors - Molecule B

0.189307	-0.97651	0.102909
0.794609	0.213922	0.568184
-0.576853	-0.0257885	0.816441

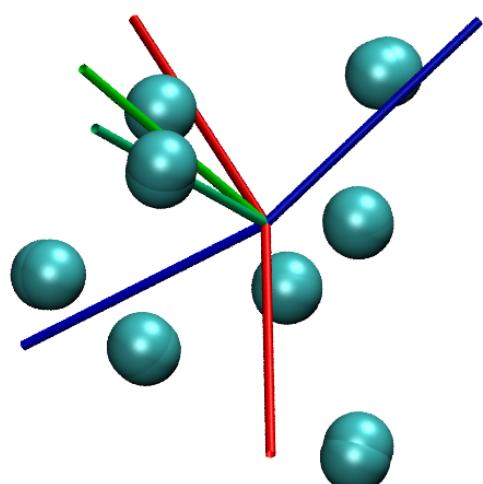
EingenValues - Molecule A

1331.25	1331.27	1331.28
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EingenValues - Molecule B

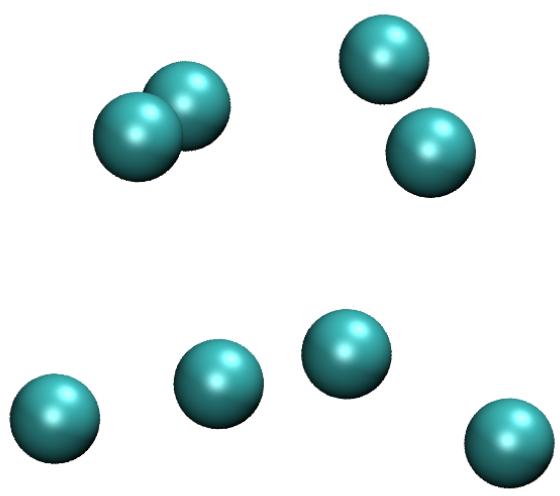
1385.64	1390.72	1403.02
---------	---------	---------

Different



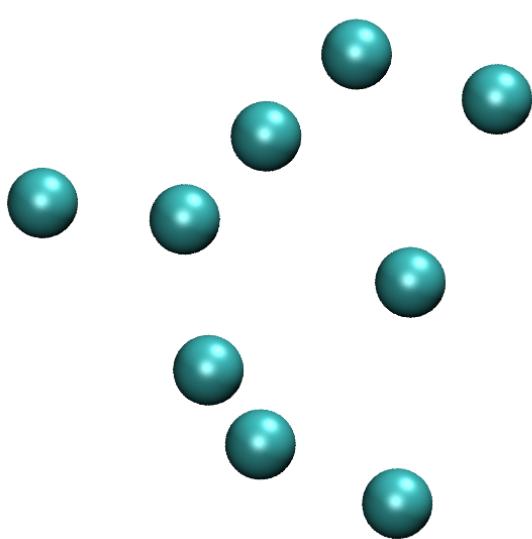
ClustersCu Número 68

Molecule A



SC\_08\_Cu

Molecule B



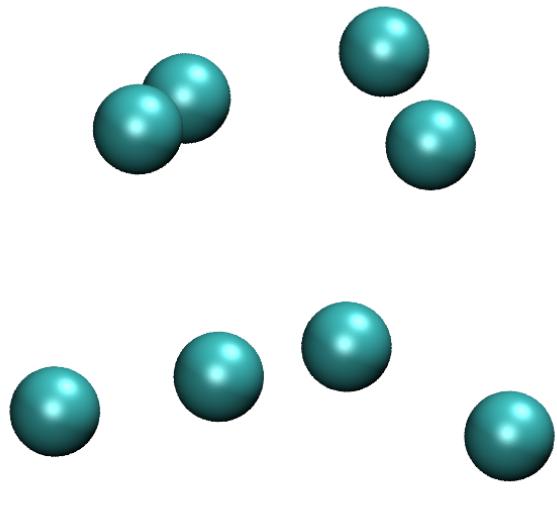
SC\_09\_Cu

Different

ClustersCu Número 69

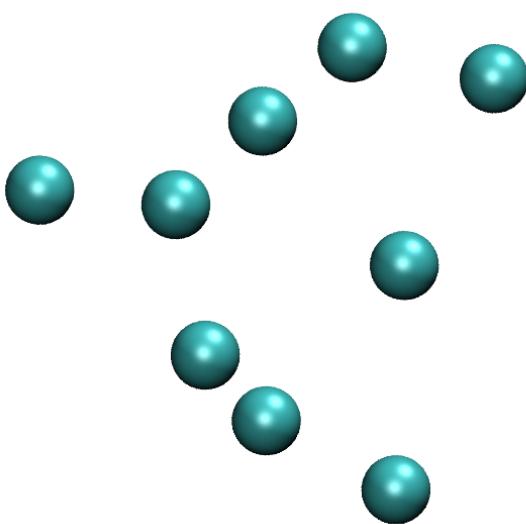
Molecule A

SC\_08\_Cu



Molecule B

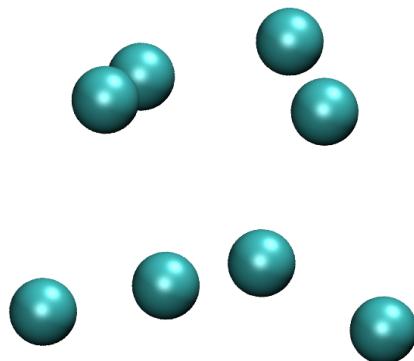
SC\_09\_Cu\_AFTER\_DFT



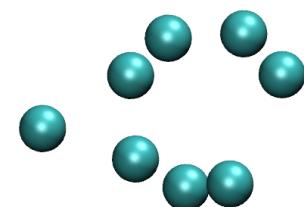
Different

# ClustersCu Número 70

Molecule A SC\_08\_Cu



Molecule B lj\_08\_Cu



Inertia Tensor - Molecule A

1331.27	0.00958178	0.0062677
0.00958178	1331.26	0.00713637
0.0062677	0.00713637	1331.28

Inertia Tensor - Molecule B

1617.21	-91.1093	-437.808
-91.1093	1798.78	-179.618
-437.808	-179.618	957.828

EingenVectors - Molecule A

-0.515886	0.847718	-0.123437
-0.684575	-0.321331	0.654296
0.514994	0.422044	0.746096

EingenVectors - Molecule B

0.43919	0.180681	0.880038
-0.601213	-0.668782	0.437348
-0.667574	0.721169	0.185095

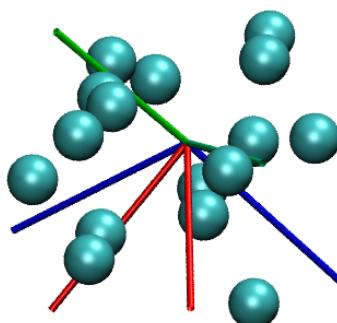
EingenValues - Molecule A

1331.25	1331.27	1331.28
---------	---------	---------

EingenValues - Molecule B

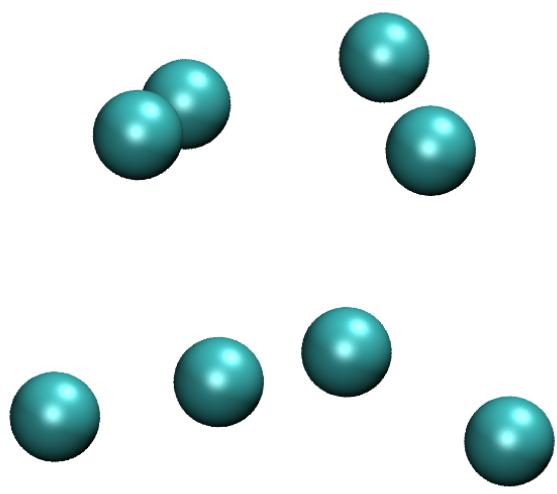
702.459	1834.34	1837.02
---------	---------	---------

Different



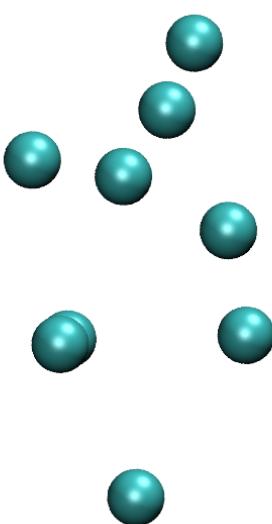
ClustersCu Número 71

Molecule A



Molecule B

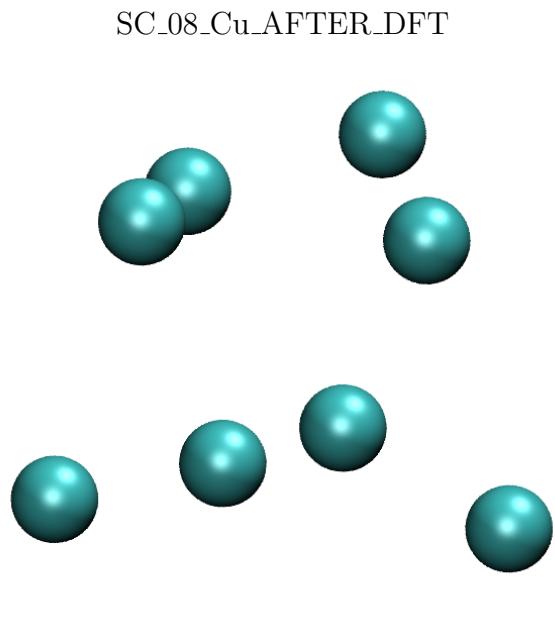
lj\_09\_Cu\_AFTER\_DFT



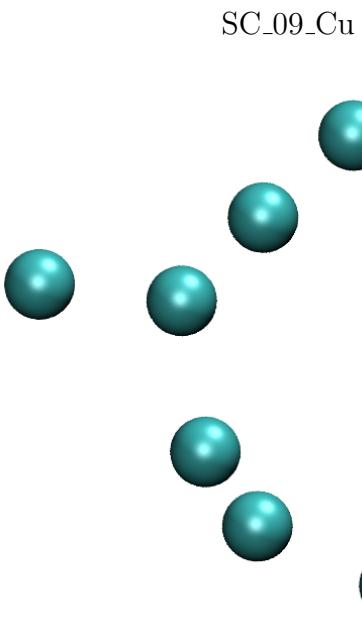
Different

ClustersCu Número 72

Molecule A



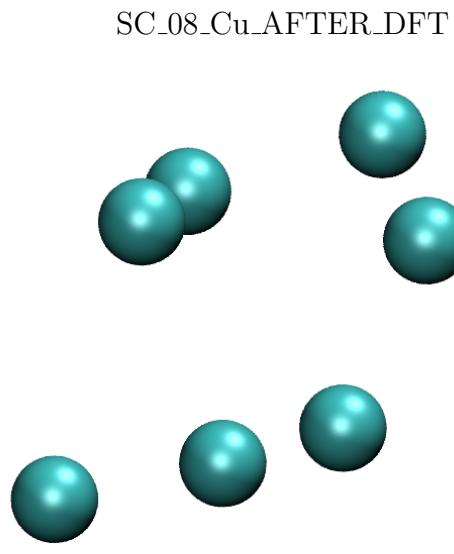
Molecule B



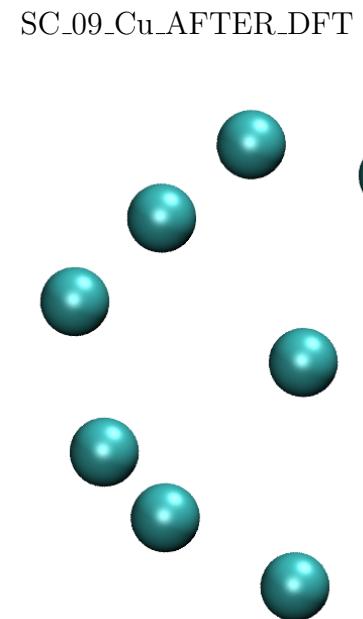
Different

ClustersCu Número 73

Molecule A



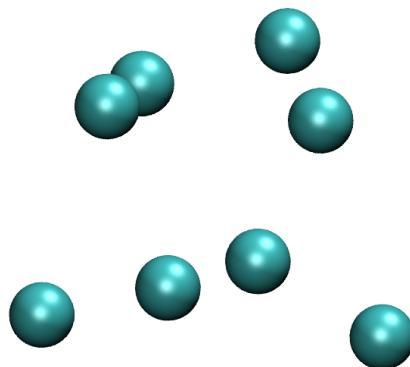
Molecule B



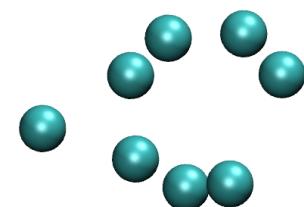
Different

# ClustersCu Número 74

Molecule A SC\_08\_Cu\_AFTER\_DFT



Molecule B lj\_08\_Cu



Inertia Tensor - Molecule A

1394.63	1.12138	-5.89124
1.12138	1385.89	0.251188
-5.89124	0.251188	1398.86

Inertia Tensor - Molecule B

1617.21	-91.1093	-437.808
-91.1093	1798.78	-179.618
-437.808	-179.618	957.828

EingenVectors - Molecule A

0.189307	-0.97651	0.102909
0.794609	0.213922	0.568184
-0.576853	-0.0257885	0.816441

EingenVectors - Molecule B

0.43919	0.180681	0.880038
-0.601213	-0.668782	0.437348
-0.667574	0.721169	0.185095

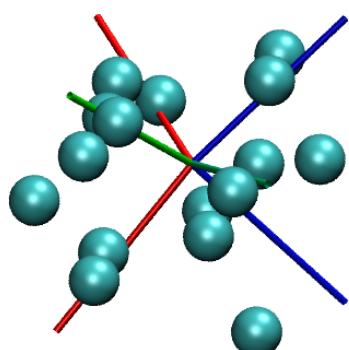
EingenValues - Molecule A

1385.64	1390.72	1403.02
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EingenValues - Molecule B

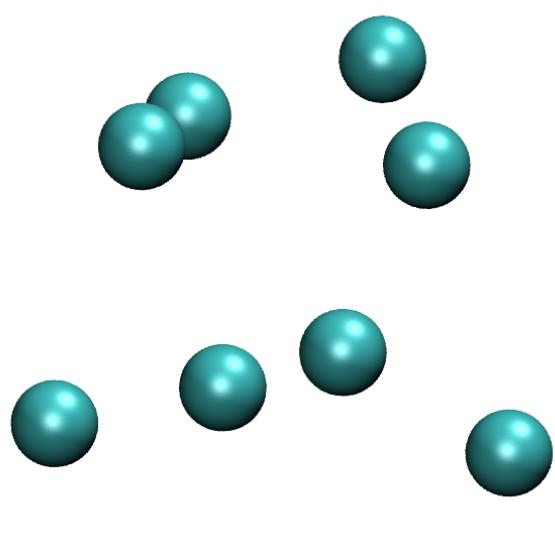
702.459	1834.34	1837.02
---------	---------	---------

Different



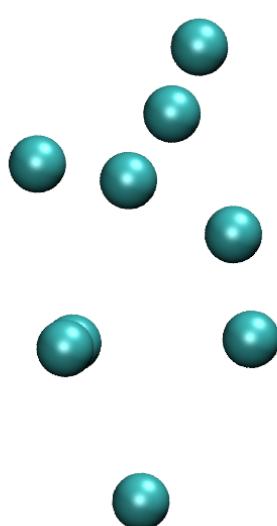
ClustersCu Número 75

Molecule A



Molecule B

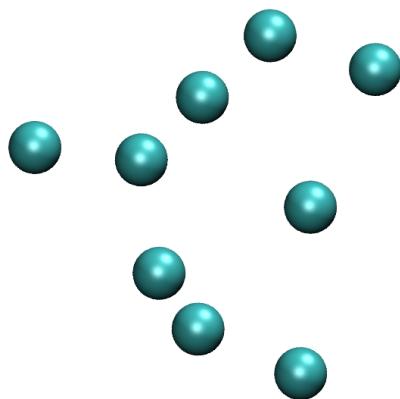
lj\_09\_Cu\_AFTER\_DFT



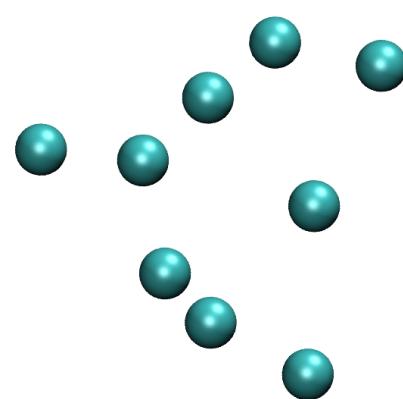
Different

# ClustersCu Número 76

Molecule A SC\_09\_Cu



Molecule B SC\_09\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1697.74	-70.4883	5.56477
-70.4883	1438.99	-78.8974
5.56477	-78.8974	2188.92

Inertia Tensor - Molecule B

1766.59	-64.0178	3.81884
-64.0178	1532.55	-76.7432
3.81884	-76.7432	2248.22

EingenVectors - Molecule A

0.23798	0.966449	0.0966559
0.970922	-0.234051	-0.0503052
0.025995	-0.105817	0.994046

EingenVectors - Molecule B

0.238514	0.966075	0.0990463
0.970895	-0.234926	-0.046613
0.0217631	-0.107281	0.99399

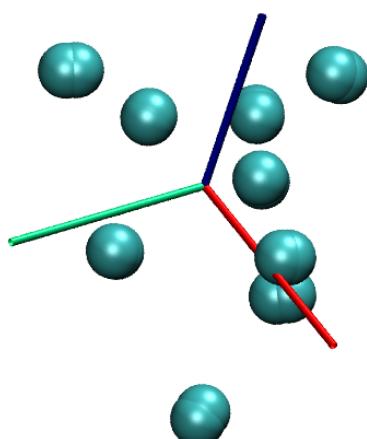
EingenValues - Molecule A

1413.74	1714.44	2197.47
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EingenValues - Molecule B

1508.88	1781.9	2256.58
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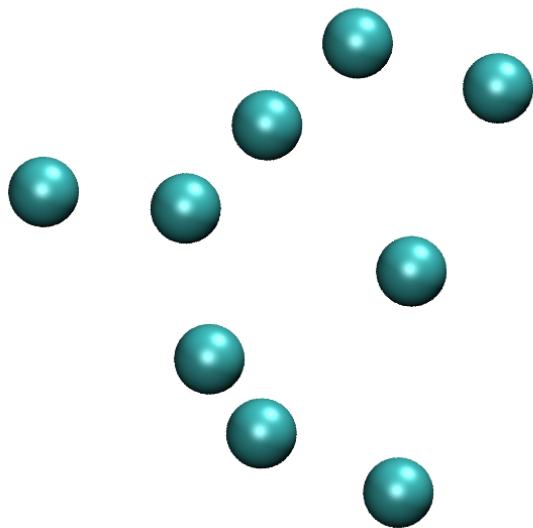
Different



ClustersCu Número 77

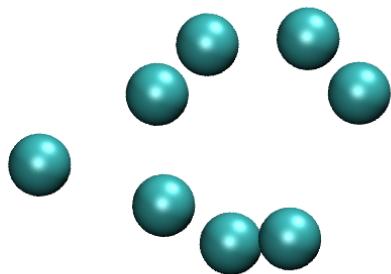
Molecule A

SC\_09\_Cu



Molecule B

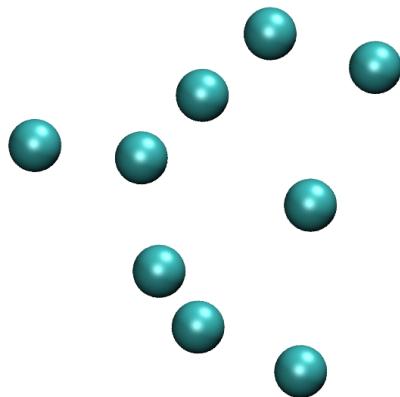
lj\_08\_Cu



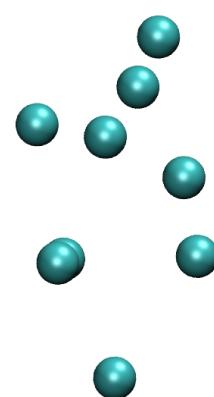
Different

# ClustersCu Número 78

Molecule A SC\_09\_Cu



Molecule B lj\_09\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1697.74	-70.4883	5.56477
-70.4883	1438.99	-78.8974
5.56477	-78.8974	2188.92

Inertia Tensor - Molecule B

2617.21	-111.803	97.8221
-111.803	1523.61	773.326
97.8221	773.326	1971.07

EingenVectors - Molecule A

0.23798	0.966449	0.0966559
0.970922	-0.234051	-0.0503052
0.025995	-0.105817	0.994046

EingenVectors - Molecule B

-0.0874373	-0.795928	0.599044
0.136388	-0.60525	-0.784265
-0.986789	-0.0131283	-0.161476

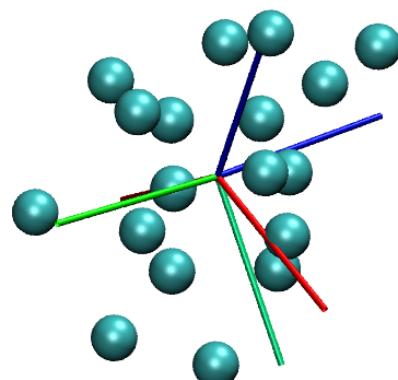
EingenValues - Molecule A

1413.74	1714.44	2197.47
---------	---------	---------

EingenValues - Molecule B

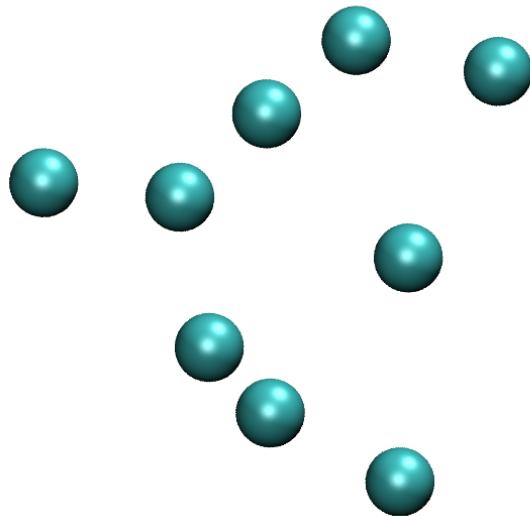
929.299	2550.86	2631.73
---------	---------	---------

Different



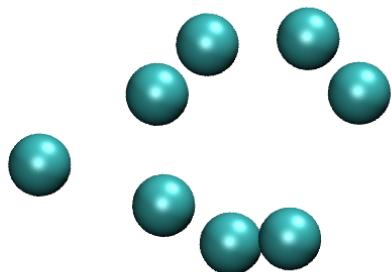
ClustersCu Número 79

Molecule A



Molecule B

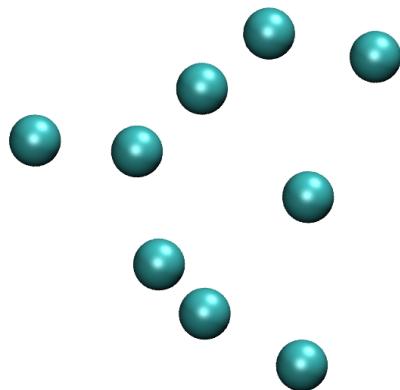
lj\_08\_Cu



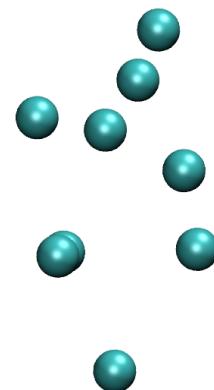
Different

# ClustersCu Número 80

Molecule A SC\_09\_Cu\_AFTER\_DFT



Molecule B lj\_09\_Cu\_AFTER\_DFT



Inertia Tensor - Molecule A

1766.59	-64.0178	3.81884
-64.0178	1532.55	-76.7432
3.81884	-76.7432	2248.22

Inertia Tensor - Molecule B

2617.21	-111.803	97.8221
-111.803	1523.61	773.326
97.8221	773.326	1971.07

EingenVectors - Molecule A

0.238514	0.966075	0.0990463
0.970895	-0.234926	-0.046613
0.0217631	-0.107281	0.99399

EingenVectors - Molecule B

-0.0874373	-0.795928	0.599044
0.136388	-0.60525	-0.784265
-0.986789	-0.0131283	-0.161476

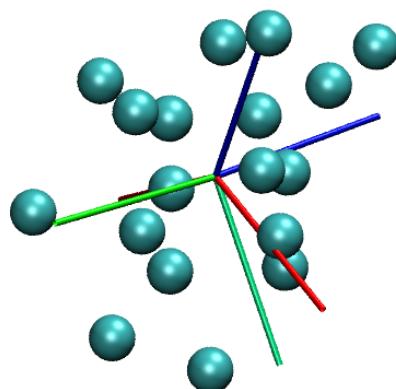
EingenValues - Molecule A

1508.88	1781.9	2256.58
---------	--------	---------

EingenValues - Molecule B

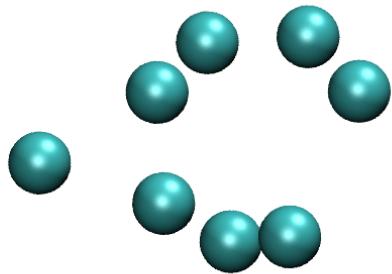
929.299	2550.86	2631.73
---------	---------	---------

Different



ClustersCu Número 81

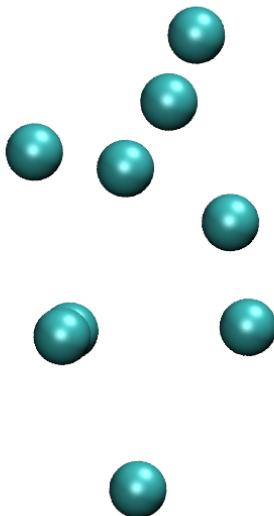
Molecule A



lj\_08\_Cu

Molecule B

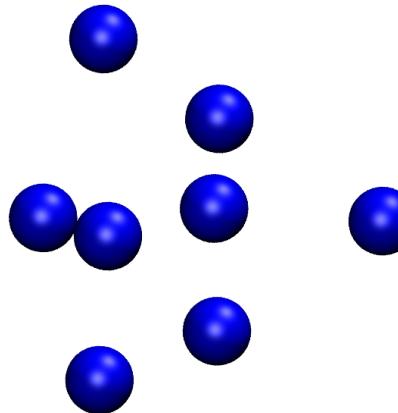
lj\_09\_Cu\_AFTER\_DFT



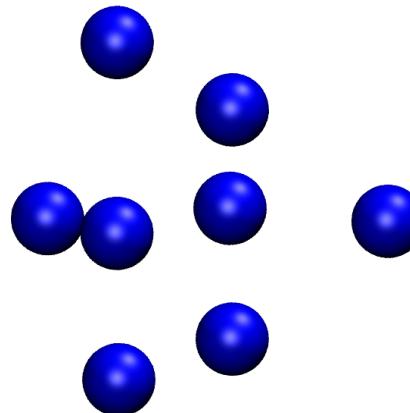
Different

# ClustersNi Número 82

Molecule A G\_08\_Ni



Molecule B G\_08\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1351.65	-0.00419552	0.0117528
-0.00419552	1351.64	-0.0031736
0.0117528	-0.0031736	1351.66

Inertia Tensor - Molecule B

1190.24	6.60641	-0.89759
6.60641	1168.04	3.23374
-0.89759	3.23374	1191.18

EingenVectors - Molecule A

-0.508502	-0.847012	0.154908
0.668029	-0.501581	-0.549685
0.543288	-0.176033	0.820884

EingenVectors - Molecule B

-0.262972	0.955871	-0.130979
-0.0175286	0.131002	0.991227
-0.964644	-0.262961	0.0176947

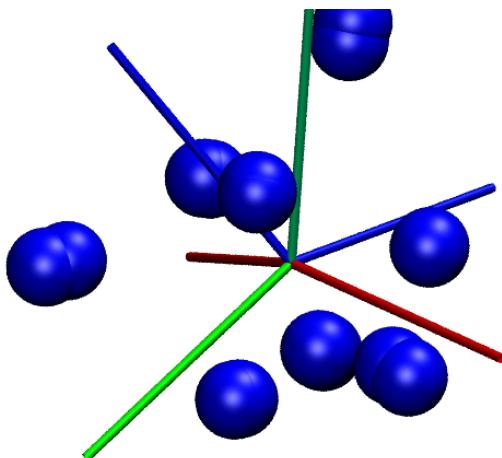
EingenValues - Molecule A

1351.64	1351.64	1351.67
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EingenValues - Molecule B

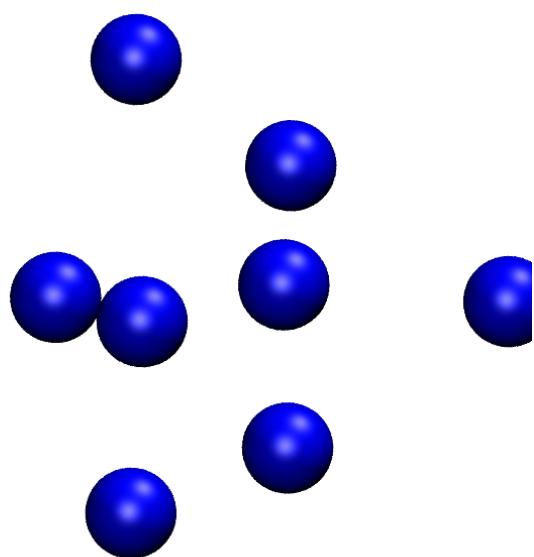
1165.78	1191.63	1192.06
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Different



ClustersNi Número 83

Molecule A



Molecule B

G\_09\_Ni

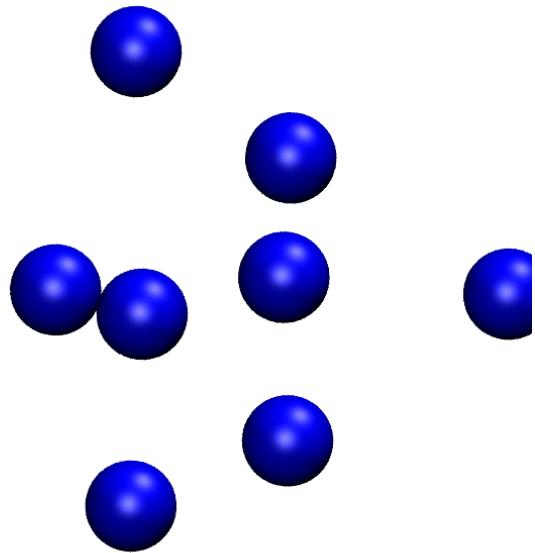
A cluster of 10 blue spheres arranged in three main horizontal rows. The top row has one sphere. The middle row has two spheres. The bottom row has five spheres, with the first two forming a small group, the next two forming another small group, and the last one being separate.

Different

ClustersNi Número 84

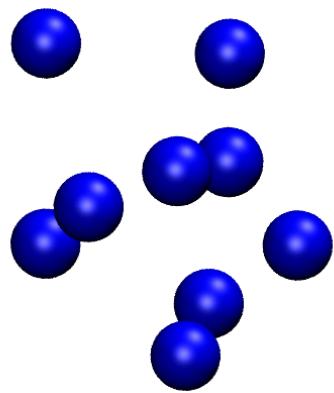
Molecule A

G\_08\_Ni



Molecule B

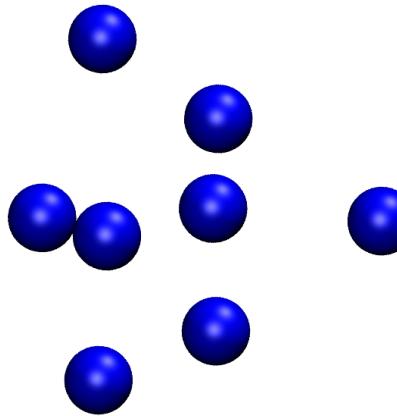
G\_09\_Ni\_AFTER\_DFT



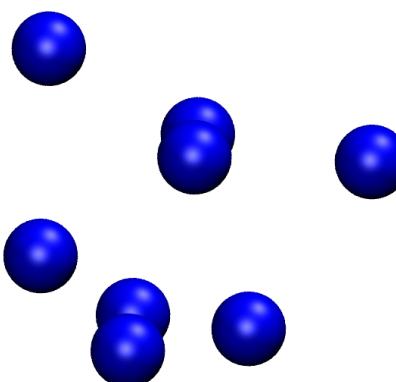
Different

# ClustersNi Número 85

Molecule A G\_08\_Ni



Molecule B SC\_08\_Ni



Inertia Tensor - Molecule A

1351.65	-0.00419552	0.0117528
-0.00419552	1351.64	-0.0031736
0.0117528	-0.0031736	1351.66

Inertia Tensor - Molecule B

1167.79	-0.00280809	0.01009
-0.00280809	1167.78	0.00700655
0.01009	0.00700655	1167.79

EingenVectors - Molecule A

-0.508502	-0.847012	0.154908
0.668029	-0.501581	-0.549685
0.543288	-0.176033	0.820884

EingenVectors - Molecule B

0.395943	0.735527	-0.549753
-0.57735	0.664947	0.473828
0.71407	0.129791	0.687938

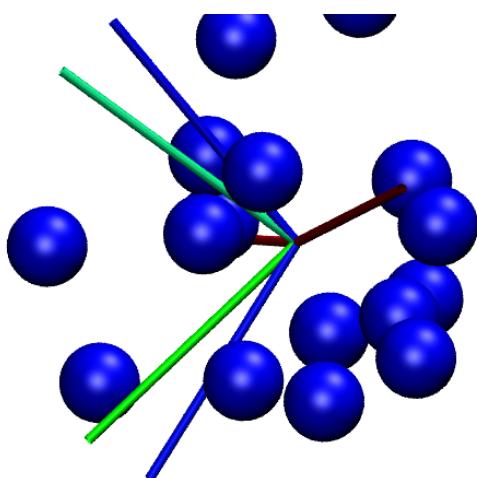
EingenValues - Molecule A

1351.64	1351.64	1351.67
---------	---------	---------

EingenValues - Molecule B

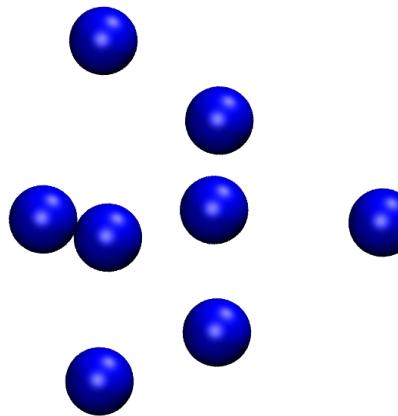
1167.77	1167.79	1167.8
---------	---------	--------

Different

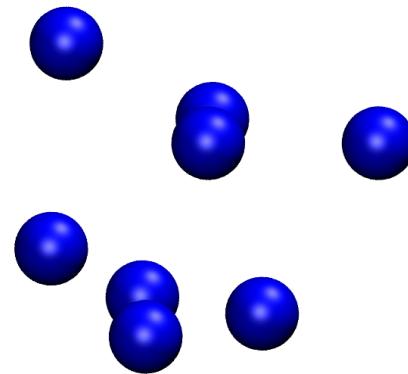


# ClustersNi Número 86

Molecule A G\_08\_Ni



Molecule B SC\_08\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1351.65	-0.00419552	0.0117528
-0.00419552	1351.64	-0.0031736
0.0117528	-0.0031736	1351.66

Inertia Tensor - Molecule B

1202.23	-22.8163	-12.5979
-22.8163	1197.22	1.92415
-12.5979	1.92415	1155.53

EingenVectors - Molecule A

-0.508502	-0.847012	0.154908
0.668029	-0.501581	-0.549685
0.543288	-0.176033	0.820884

EingenVectors - Molecule B

0.285716	0.10352	0.952707
0.595734	0.759527	-0.261189
-0.750645	0.642185	0.155339

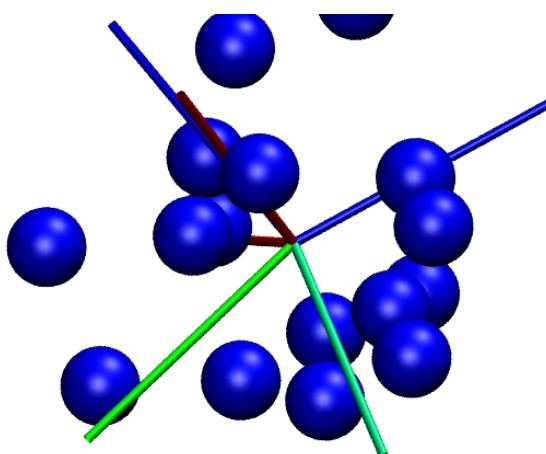
EingenValues - Molecule A

1351.64	1351.64	1351.67
---------	---------	---------

EingenValues - Molecule B

1151.96	1178.67	1224.36
---------	---------	---------

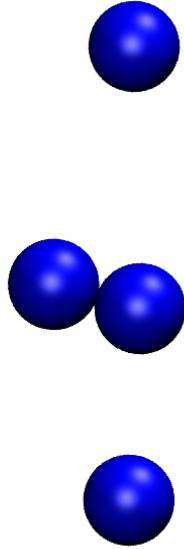
Different



ClustersNi Número 87

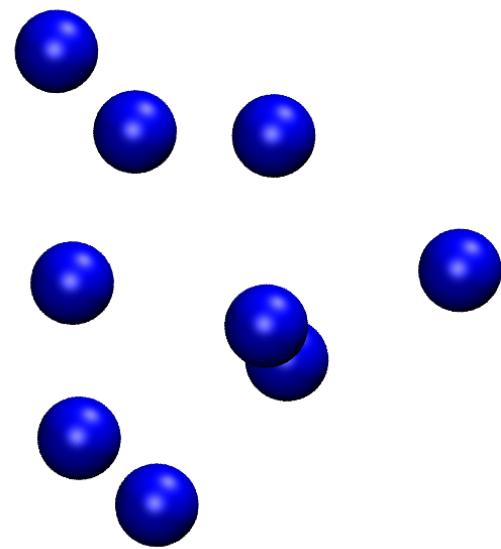
Molecule A

G\_08\_Ni



Molecule B

SC\_09\_Ni

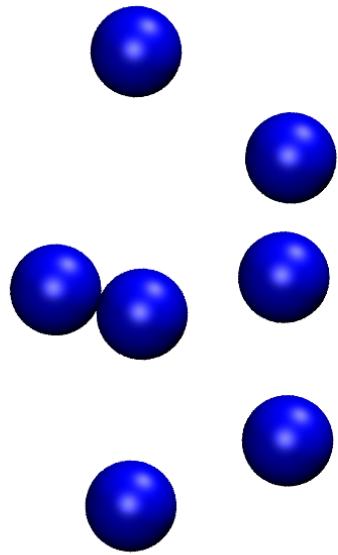


Different

ClustersNi Número 88

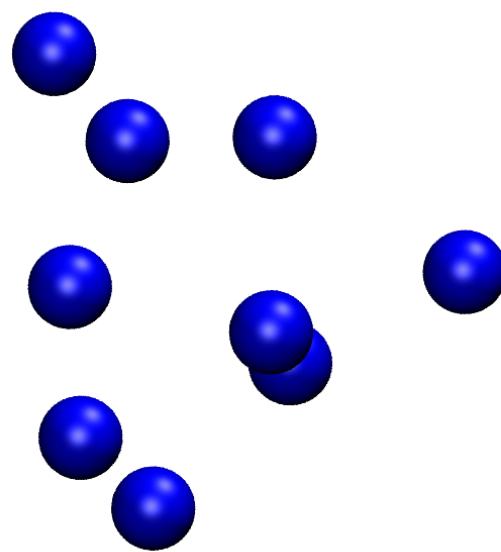
Molecule A

G\_08\_Ni



Molecule B

SC\_09\_Ni\_AFTER\_DFT

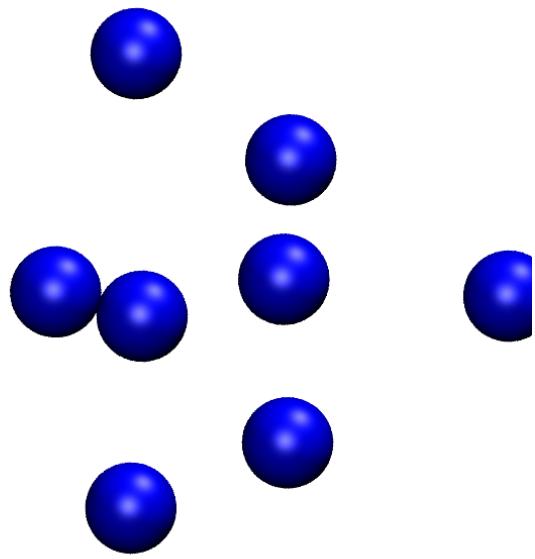


Different

ClustersNi Número 89

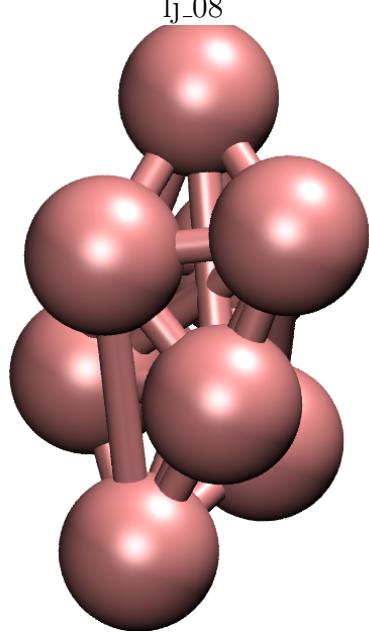
Molecule A

G\_08\_Ni



Molecule B

lj\_08

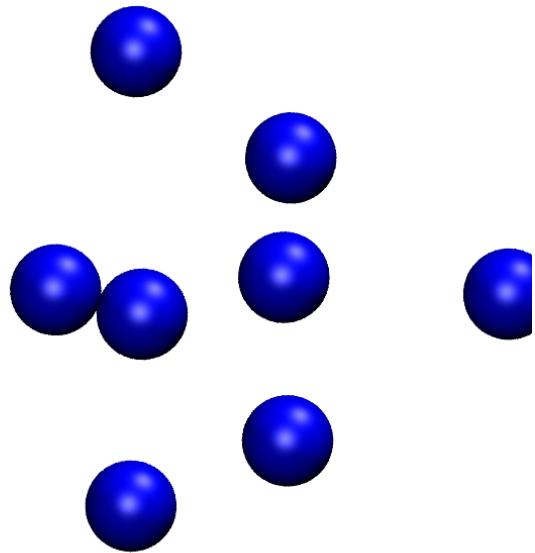


Different

ClustersNi Número 90

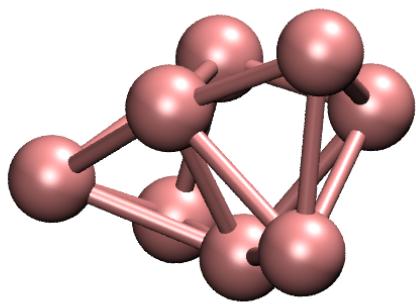
Molecule A

G\_08\_Ni



Molecule B

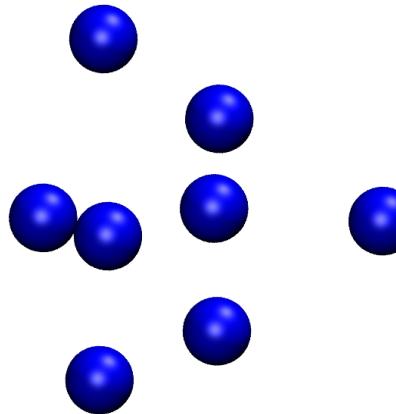
lj\_08\_Ni



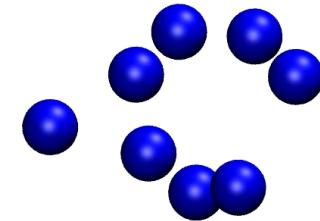
Different

# ClustersNi Número 91

Molecule A G\_08\_Ni



Molecule B lj\_08\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1351.65	-0.00419552	0.0117528
-0.00419552	1351.64	-0.0031736
0.0117528	-0.0031736	1351.66

Inertia Tensor - Molecule B

1461.29	-67.9001	-380.896
-67.9001	1626.58	-132.788
-380.896	-132.788	885.164

EingenVectors - Molecule A

-0.508502	-0.847012	0.154908
0.668029	-0.501581	-0.549685
0.543288	-0.176033	0.820884

EingenVectors - Molecule B

0.440314	0.154412	0.884466
-0.488448	-0.785372	0.380276
-0.753354	0.599456	0.270388

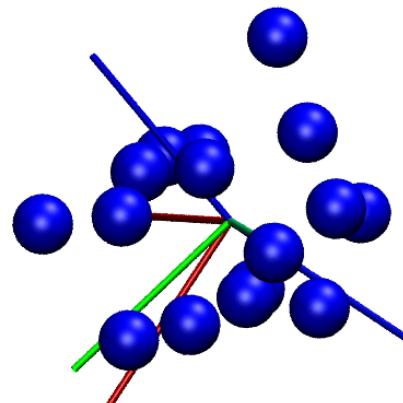
EingenValues - Molecule A

1351.64	1351.64	1351.67
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EingenValues - Molecule B

672.361	1648.65	1652.02
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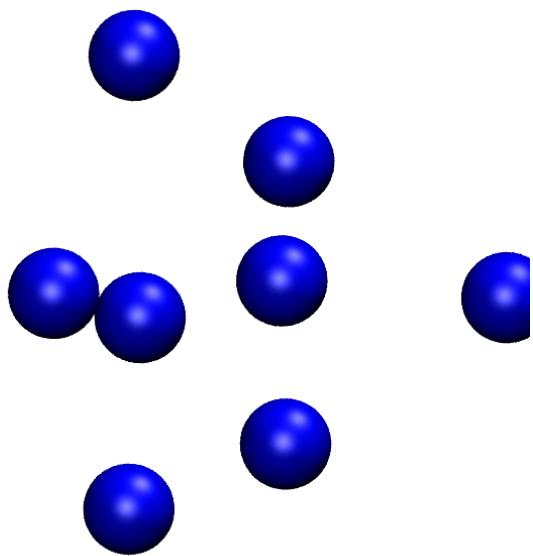
Different



ClustersNi Número 92

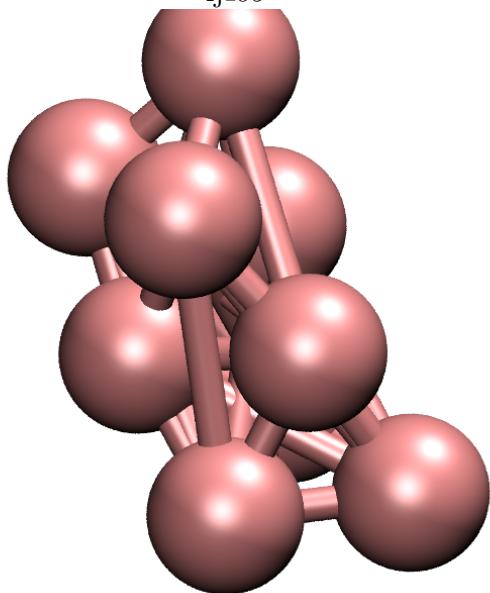
Molecule A

G\_08\_Ni



Molecule B

lj\_09

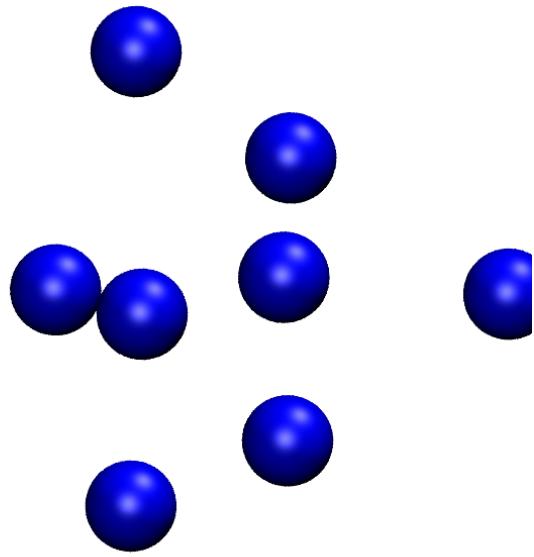


Different

ClustersNi Número 93

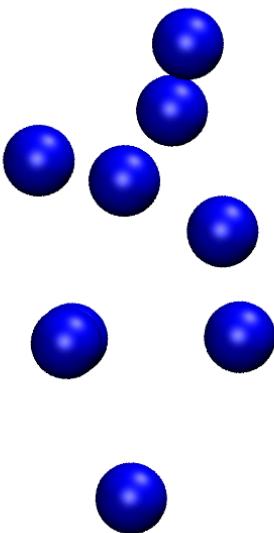
Molecule A

G\_08\_Ni



Molecule B

lj\_09\_Ni

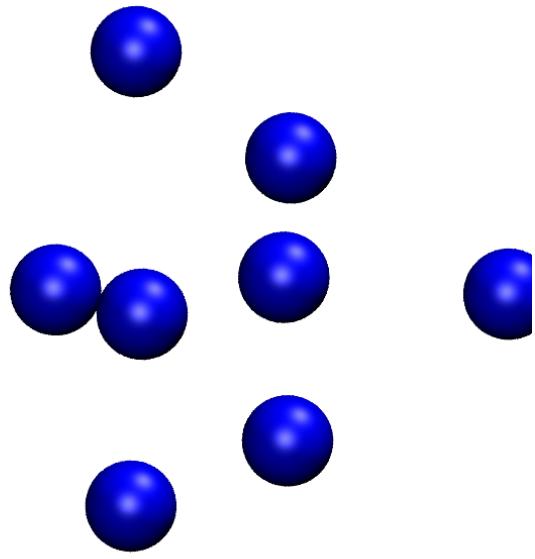


Different

ClustersNi Número 94

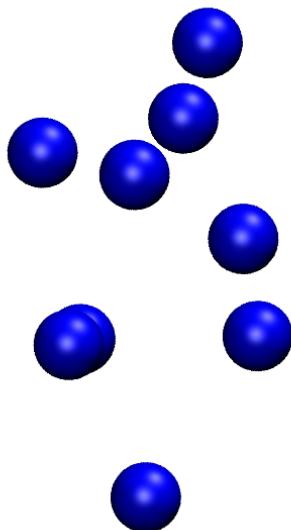
Molecule A

G\_08\_Ni



Molecule B

lj\_09\_Ni\_AFTER\_DFT

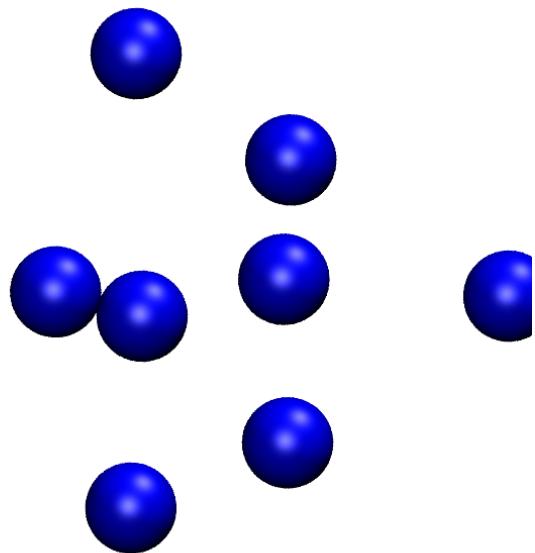


Different

ClustersNi Número 95

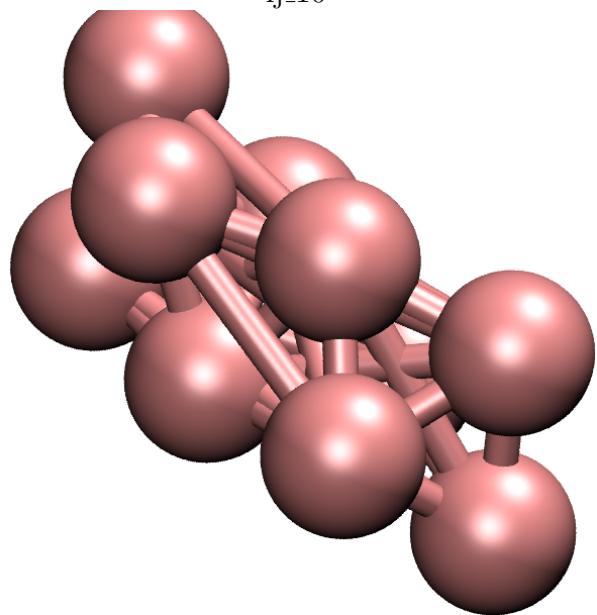
Molecule A

G\_08\_Ni



Molecule B

lj\_10

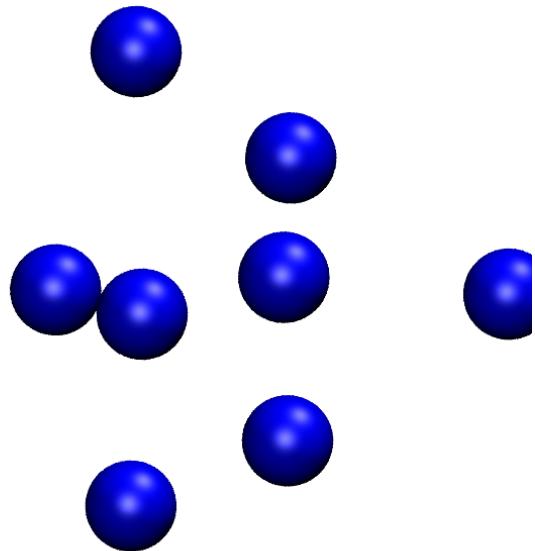


Different

ClustersNi Número 96

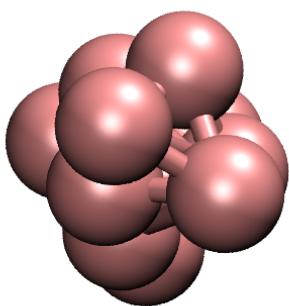
Molecule A

G\_08\_Ni



Molecule B

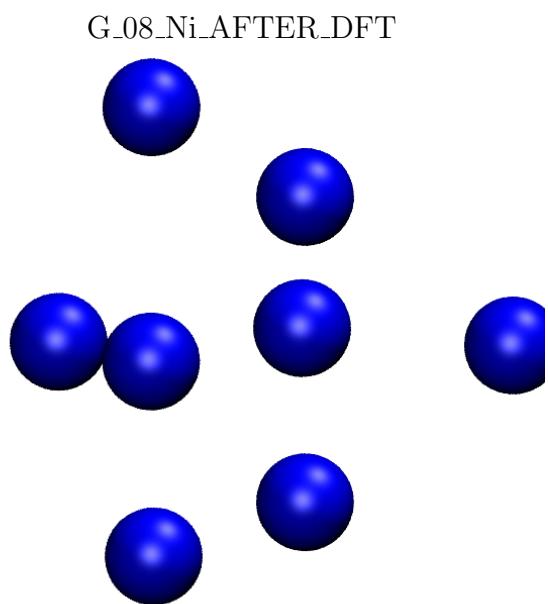
lj\_11



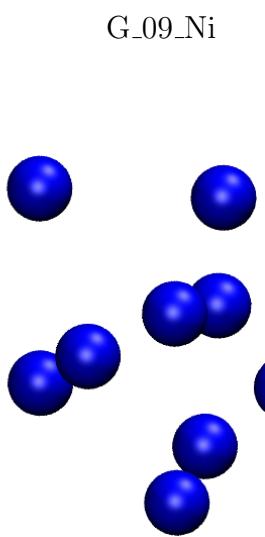
Different

ClustersNi Número 97

Molecule A



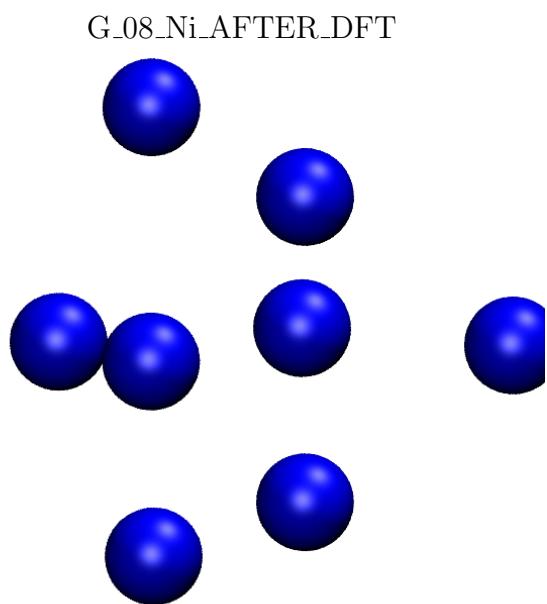
Molecule B



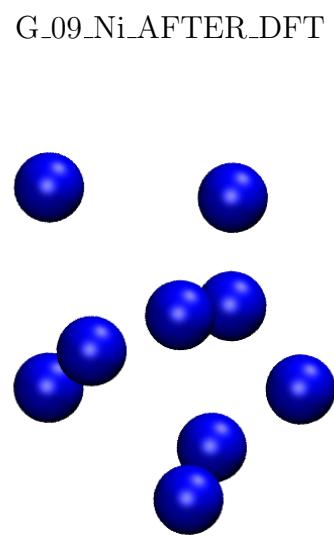
Different

ClustersNi Número 98

Molecule A



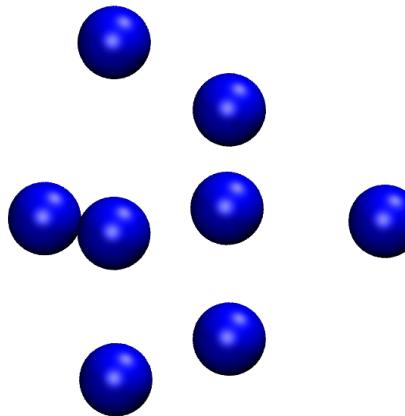
Molecule B



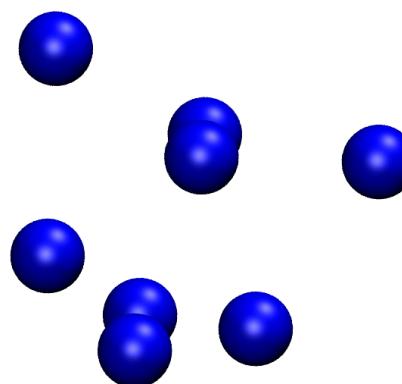
Different

# ClustersNi Número 99

Molecule A G\_08\_Ni\_AFTER\_DFT



Molecule B SC\_08\_Ni



Inertia Tensor - Molecule A

1190.24	6.60641	-0.89759
6.60641	1168.04	3.23374
-0.89759	3.23374	1191.18

Inertia Tensor - Molecule B

1167.79	-0.00280809	0.01009
-0.00280809	1167.78	0.00700655
0.01009	0.00700655	1167.79

EingenVectors - Molecule A

-0.262972	0.955871	-0.130979
-0.0175286	0.131002	0.991227
-0.964644	-0.262961	0.0176947

EingenVectors - Molecule B

0.395943	0.735527	-0.549753
-0.57735	0.664947	0.473828
0.71407	0.129791	0.687938

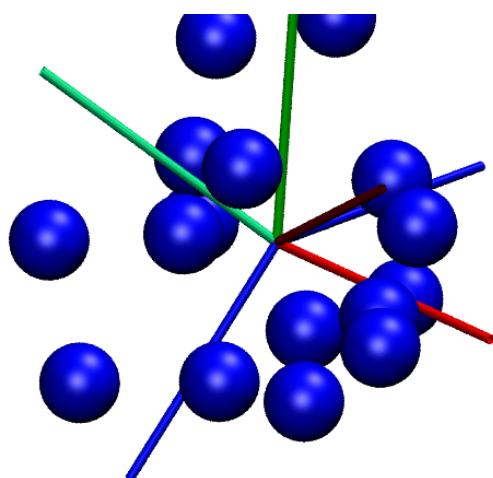
EingenValues - Molecule A

1165.78	1191.63	1192.06
---------	---------	---------

EingenValues - Molecule B

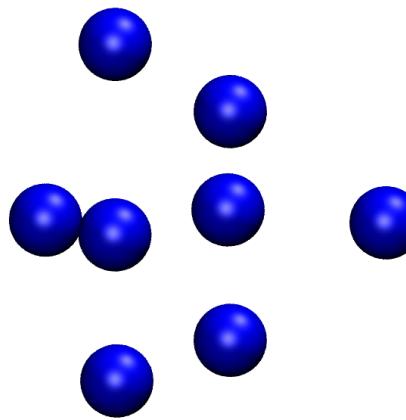
1167.77	1167.79	1167.8
---------	---------	--------

Different

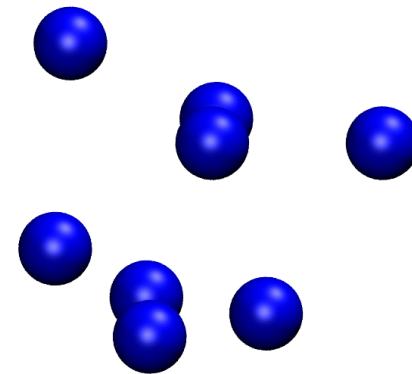


# ClustersNi Número 100

Molecule A G\_08\_Ni\_AFTER\_DFT



Molecule B SC\_08\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1190.24	6.60641	-0.89759
6.60641	1168.04	3.23374
-0.89759	3.23374	1191.18

Inertia Tensor - Molecule B

1202.23	-22.8163	-12.5979
-22.8163	1197.22	1.92415
-12.5979	1.92415	1155.53

EingenVectors - Molecule A

-0.262972	0.955871	-0.130979
-0.0175286	0.131002	0.991227
-0.964644	-0.262961	0.0176947

EingenVectors - Molecule B

0.285716	0.10352	0.952707
0.595734	0.759527	-0.261189
-0.750645	0.642185	0.155339

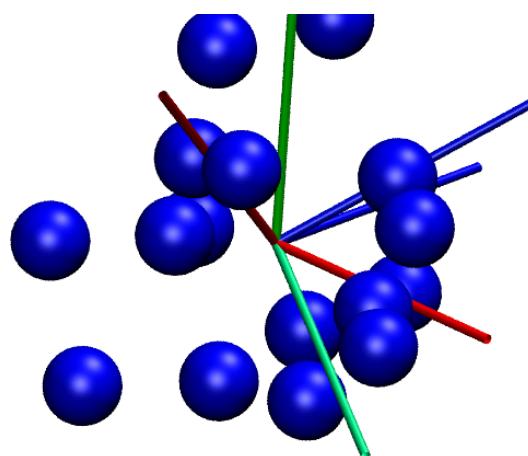
EingenValues - Molecule A

1165.78	1191.63	1192.06
---------	---------	---------

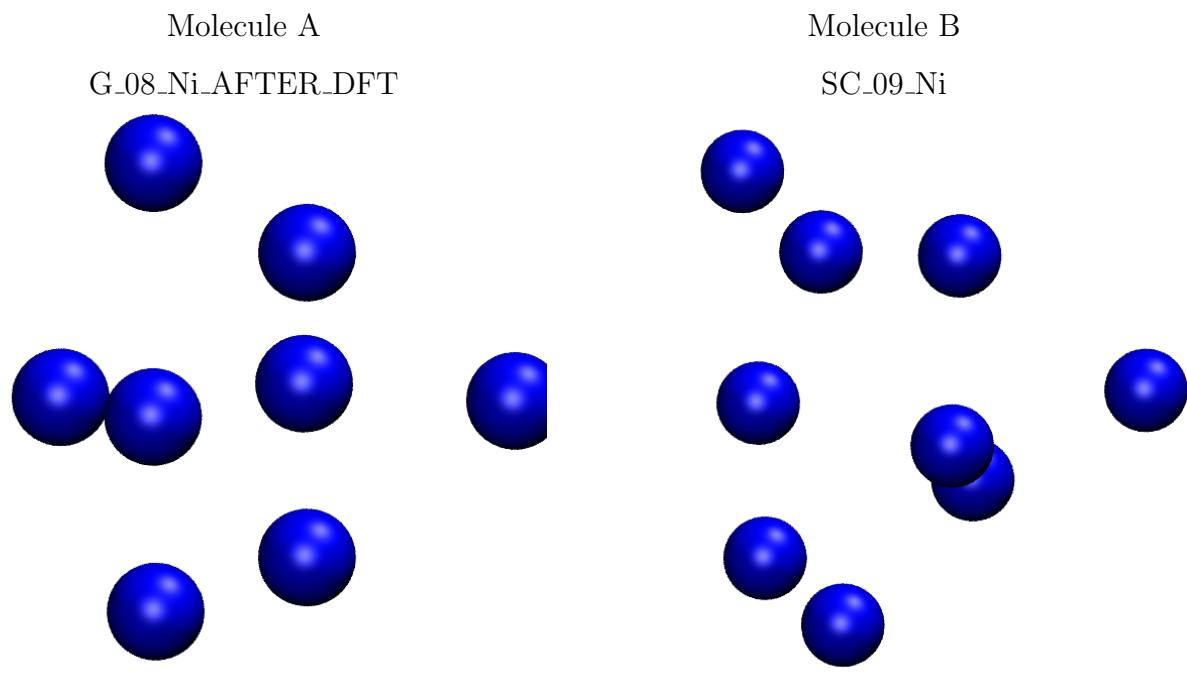
EingenValues - Molecule B

1151.96	1178.67	1224.36
---------	---------	---------

Different



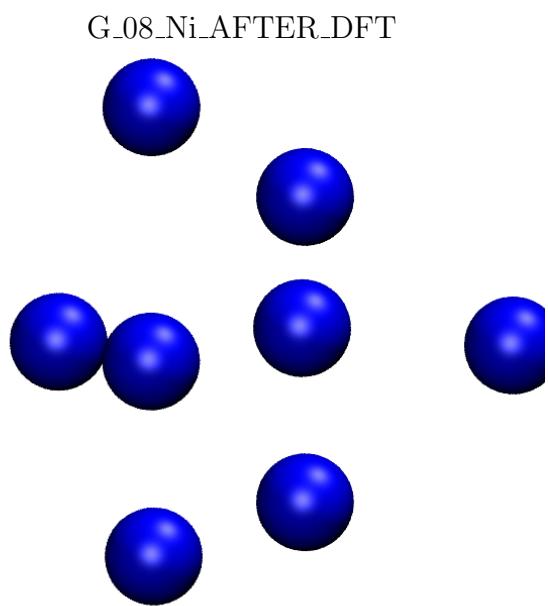
ClustersNi Número 101



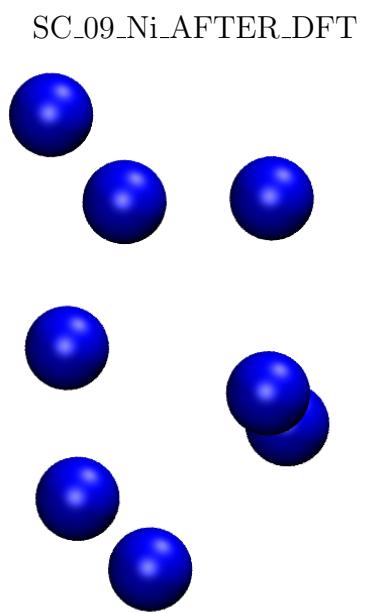
Different

ClustersNi Número 102

Molecule A



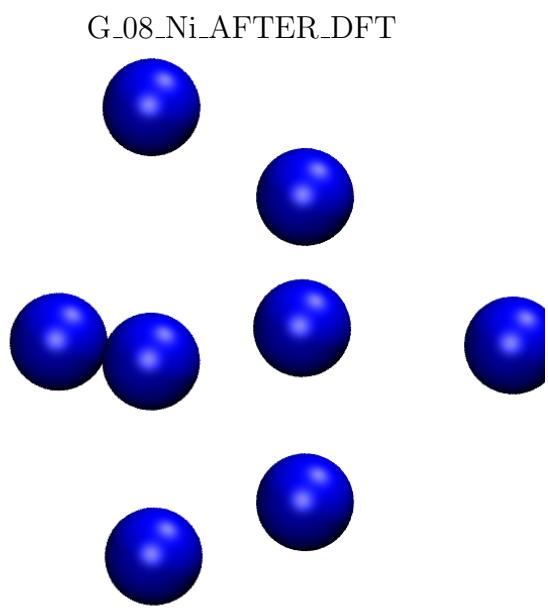
Molecule B



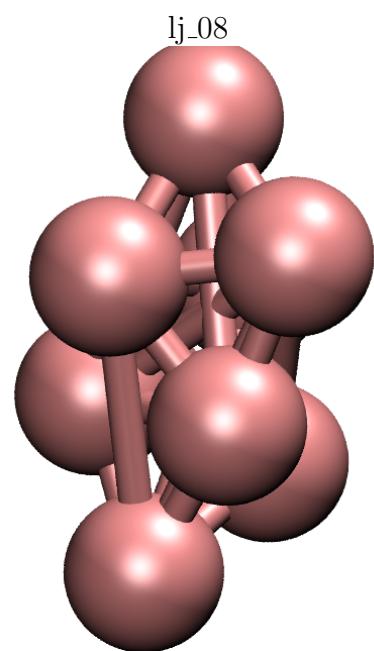
Different

ClustersNi Número 103

Molecule A



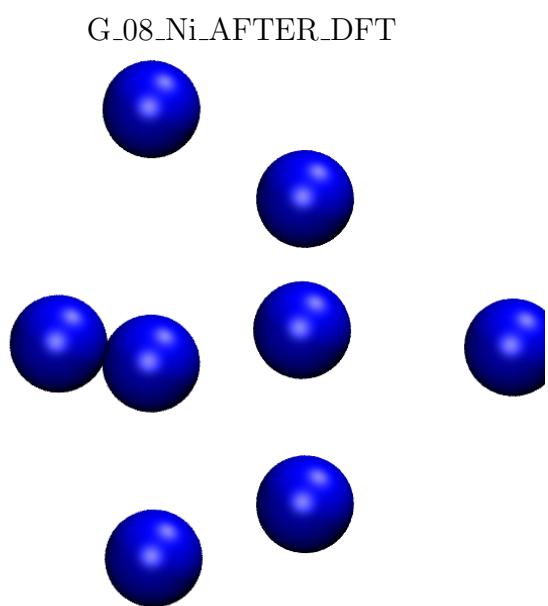
Molecule B



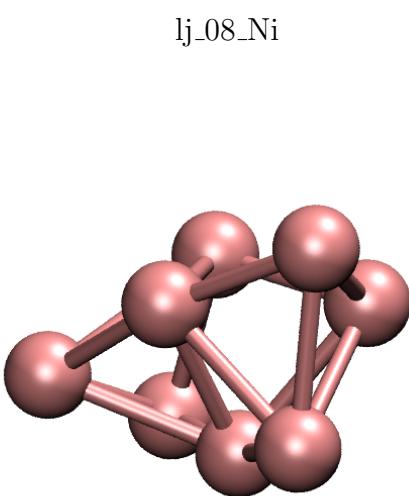
Different

ClustersNi Número 104

Molecule A



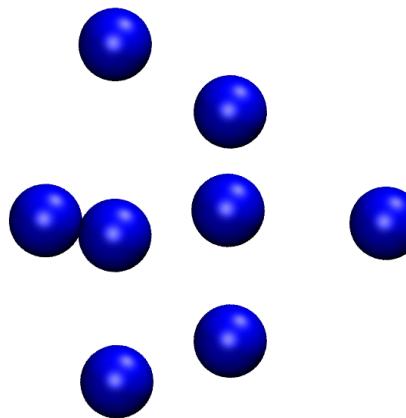
Molecule B



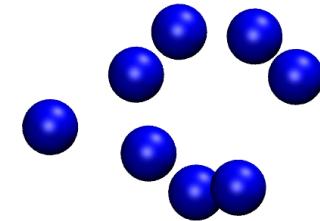
Different

# ClustersNi Número 105

Molecule A G\_08\_Ni\_AFTER\_DFT



Molecule B lj\_08\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1190.24	6.60641	-0.89759
6.60641	1168.04	3.23374
-0.89759	3.23374	1191.18

Inertia Tensor - Molecule B

1461.29	-67.9001	-380.896
-67.9001	1626.58	-132.788
-380.896	-132.788	885.164

EingenVectors - Molecule A

-0.262972	0.955871	-0.130979
-0.0175286	0.131002	0.991227
-0.964644	-0.262961	0.0176947

EingenVectors - Molecule B

0.440314	0.154412	0.884466
-0.488448	-0.785372	0.380276
-0.753354	0.599456	0.270388

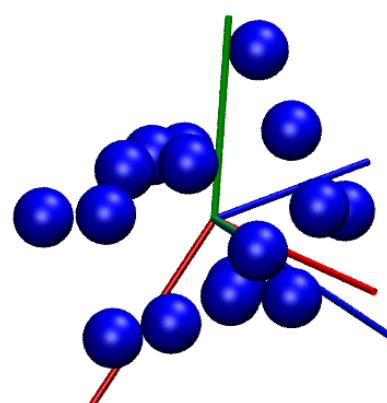
EingenValues - Molecule A

1165.78	1191.63	1192.06
---------	---------	---------

EingenValues - Molecule B

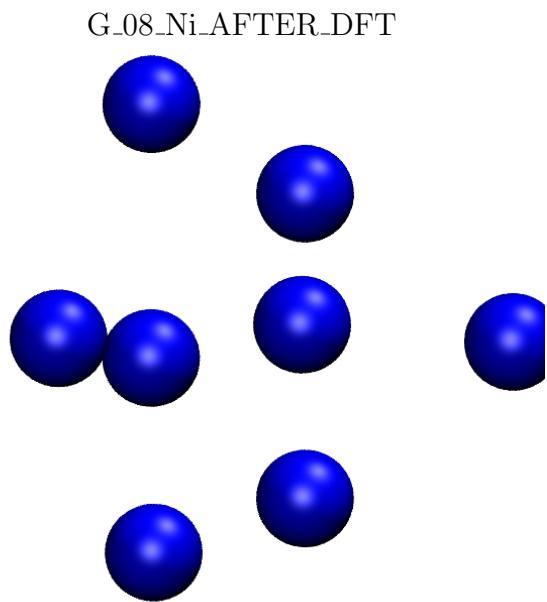
672.361	1648.65	1652.02
---------	---------	---------

Different

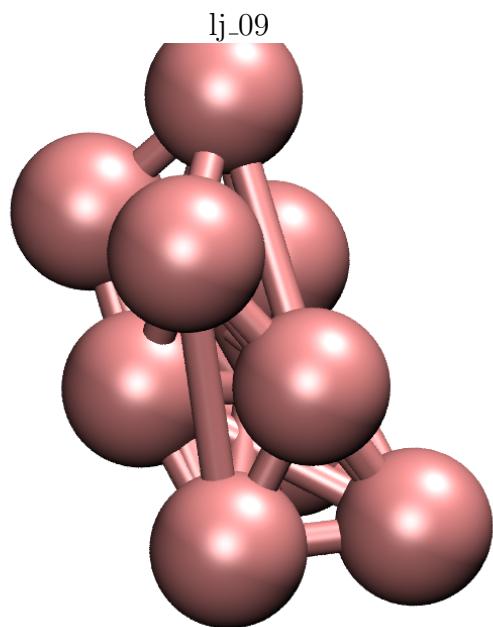


ClustersNi Número 106

Molecule A



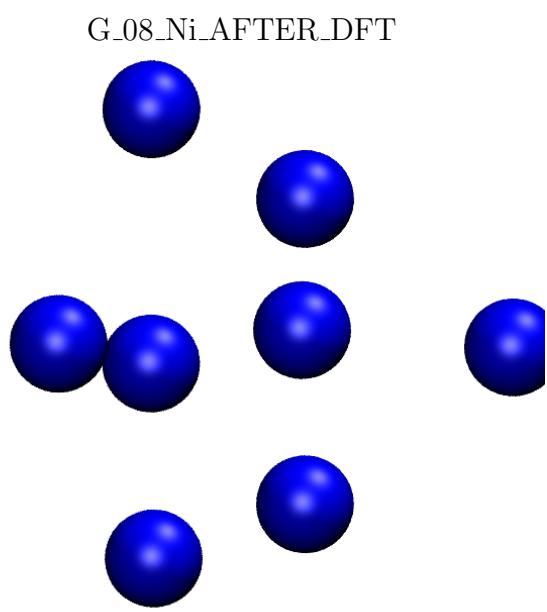
Molecule B



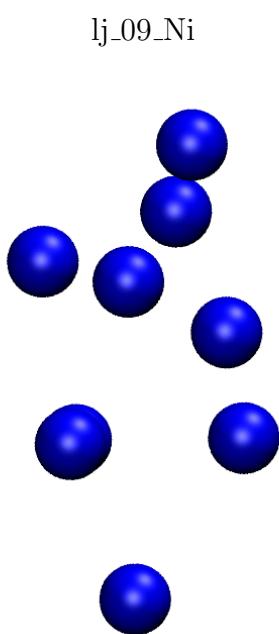
Different

ClustersNi Número 107

Molecule A



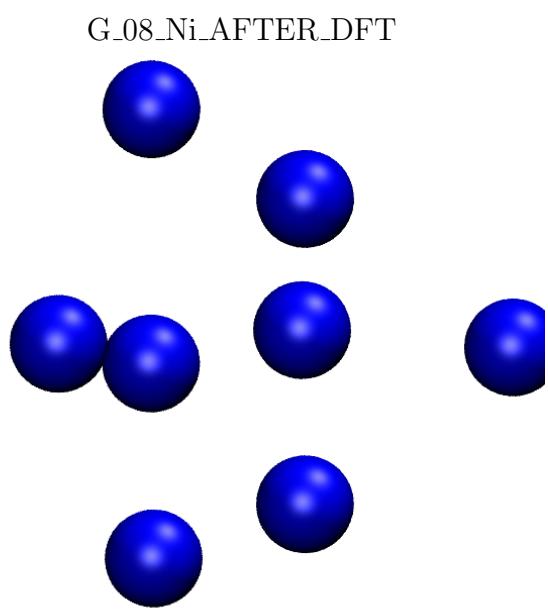
Molecule B



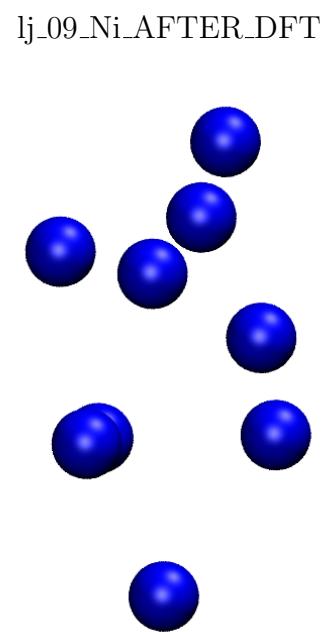
Different

ClustersNi Número 108

Molecule A



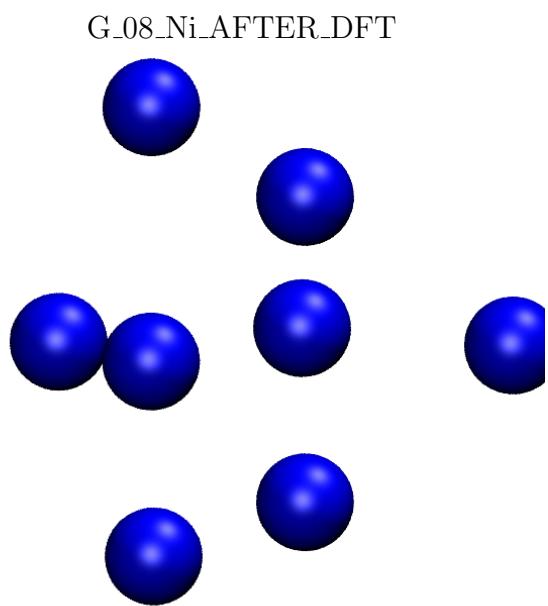
Molecule B



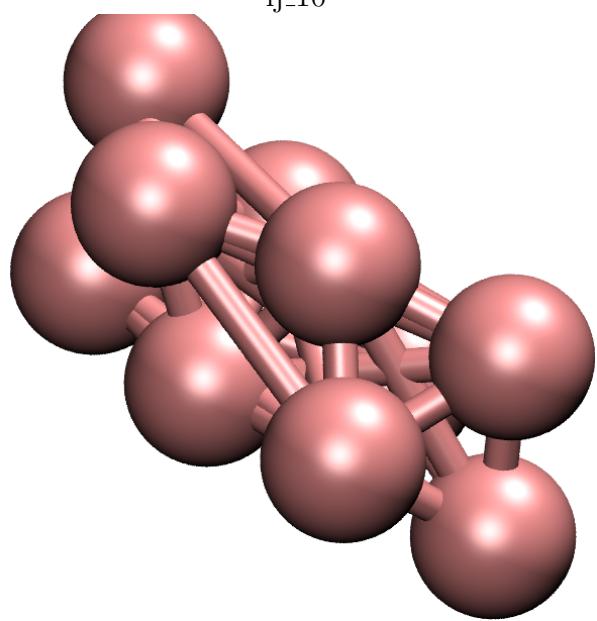
Different

ClustersNi Número 109

Molecule A



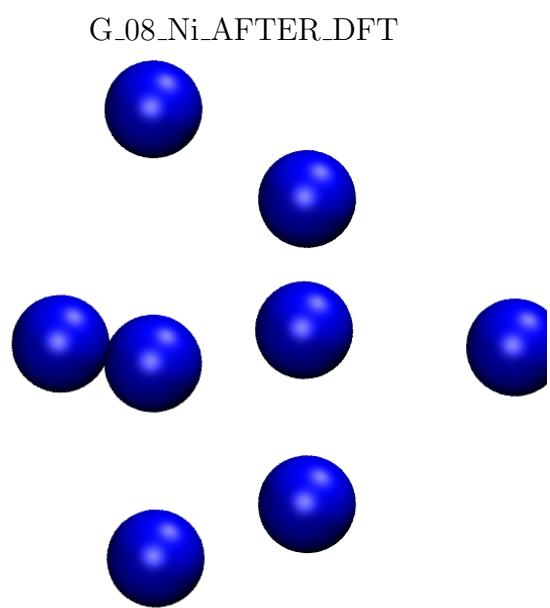
Molecule B



Different

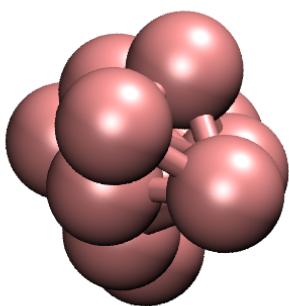
ClustersNi Número 110

Molecule A



Molecule B

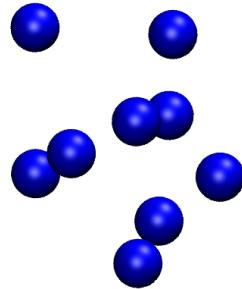
lj\_11



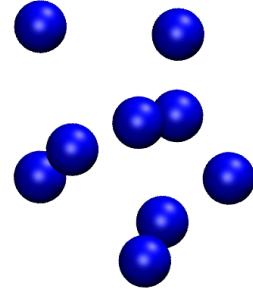
Different

# ClustersNi Número 111

Molecule A G\_09\_Ni



Molecule B G\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

2295.28	127.678	34.3162
127.678	2047.43	-608.198
34.3162	-608.198	1341.02

Inertia Tensor - Molecule B

2034.24	115.071	30.1504
115.071	1837.6	-545.965
30.1504	-545.965	1191.04

EingenVectors - Molecule A

0.0714239	-0.501716	-0.862078
-0.850908	0.420309	-0.315112
0.520436	0.756056	-0.396895

EingenVectors - Molecule B

0.0718467	-0.498105	-0.864135
-0.874868	0.3846	-0.29443
0.479003	0.777158	-0.408144

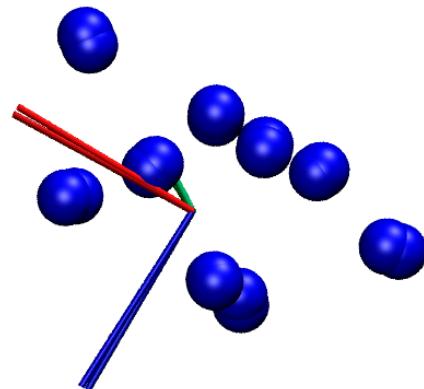
EingenValues - Molecule A

984.213	2244.92	2454.59
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EingenValues - Molecule B

873.833	1993.8	2195.25
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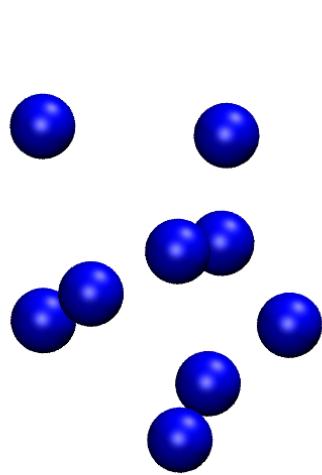
Different



ClustersNi Número 112

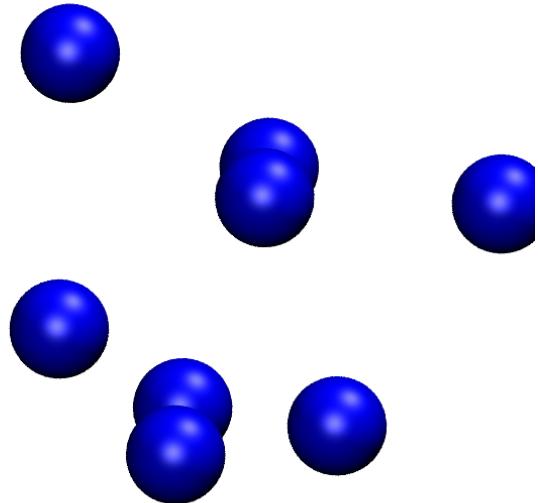
Molecule A

G\_09\_Ni



Molecule B

SC\_08\_Ni

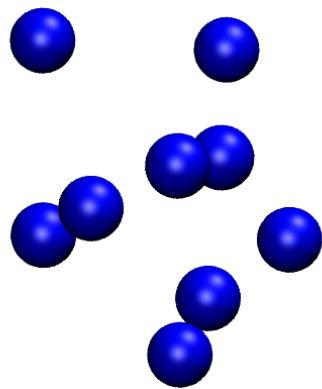


Different

ClustersNi Número 113

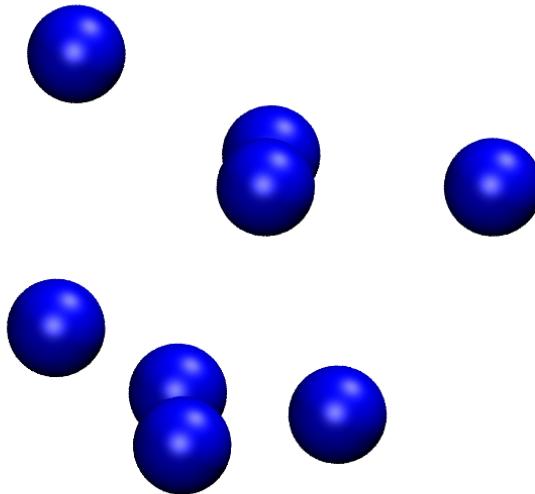
Molecule A

G\_09\_Ni



Molecule B

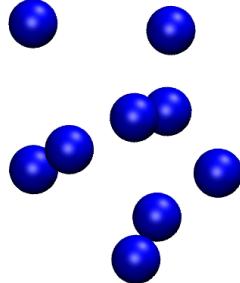
SC\_08\_Ni\_AFTER\_DFT



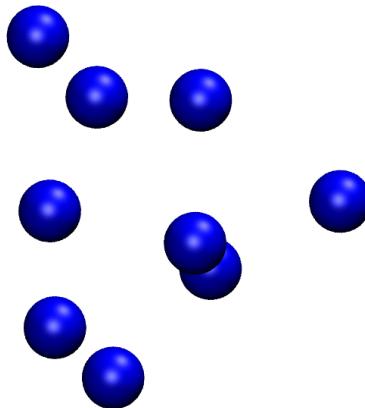
Different

# ClustersNi Número 114

Molecule A G\_09\_Ni



Molecule B SC\_09\_Ni



Inertia Tensor - Molecule A

2295.28	127.678	34.3162
127.678	2047.43	-608.198
34.3162	-608.198	1341.02

Inertia Tensor - Molecule B

1536.98	56.225	-101.457
56.225	1328.77	-222.686
-101.457	-222.686	1805.96

EingenVectors - Molecule A

0.0714239	-0.501716	-0.862078
-0.850908	0.420309	-0.315112
0.520436	0.756056	-0.396895

EingenVectors - Molecule B

0.0545275	-0.93243	-0.357212
-0.957676	0.0524255	-0.283033
-0.282636	-0.357527	0.890108

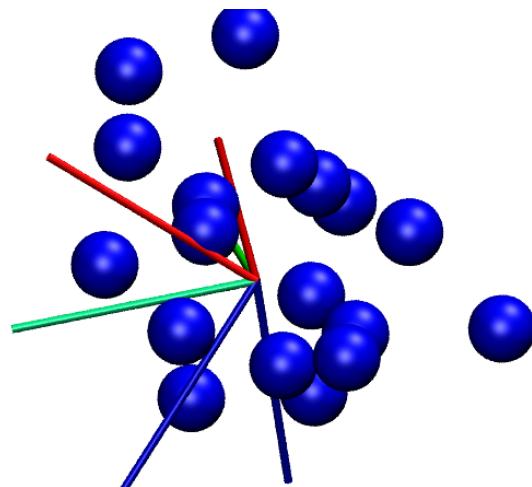
EingenValues - Molecule A

984.213	2244.92	2454.59
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EingenValues - Molecule B

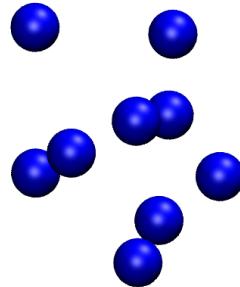
1240.17	1503.92	1927.62
---------	---------	---------

Different

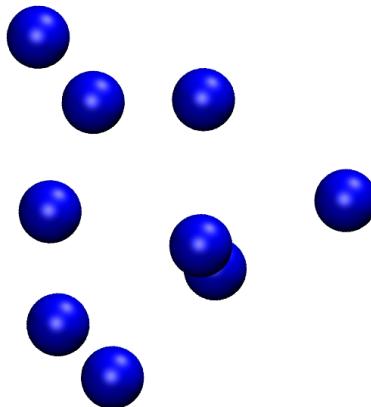


# ClustersNi Número 115

Molecule A G\_09\_Ni



Molecule B SC\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

2295.28	127.678	34.3162
127.678	2047.43	-608.198
34.3162	-608.198	1341.02

Inertia Tensor - Molecule B

1526.11	61.3141	-104.189
61.3141	1367.3	-214.394
-104.189	-214.394	1801.23

EingenVectors - Molecule A

0.0714239	-0.501716	-0.862078
-0.850908	0.420309	-0.315112
0.520436	0.756056	-0.396895

EingenVectors - Molecule B

0.0759984	-0.927891	-0.365024
-0.954757	0.0378395	-0.294969
-0.287511	-0.370927	0.883035

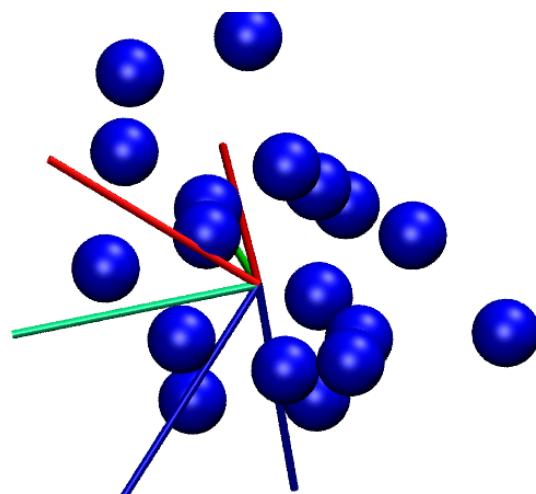
EingenValues - Molecule A

984.213	2244.92	2454.59
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EingenValues - Molecule B

1277.93	1491.49	1925.21
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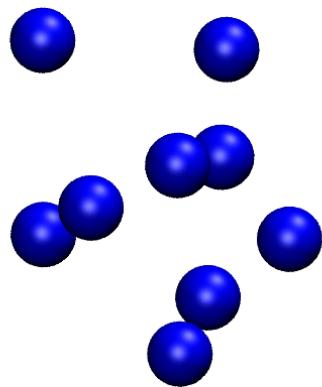
Different



ClustersNi Número 116

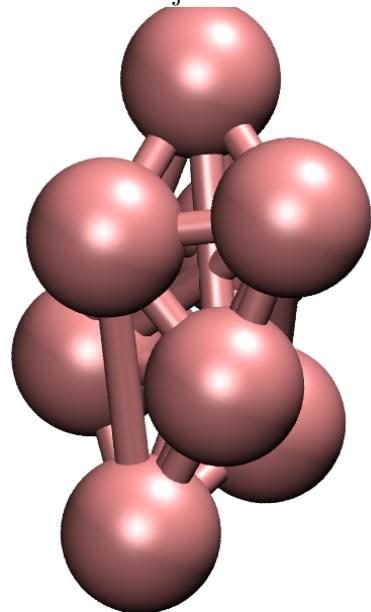
Molecule A

G\_09\_Ni



Molecule B

lj\_08

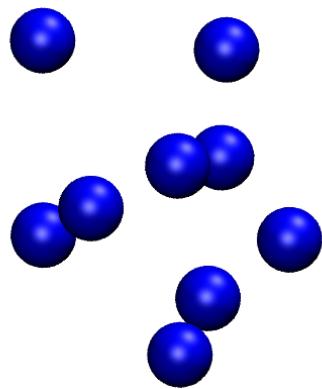


Different

ClustersNi Número 117

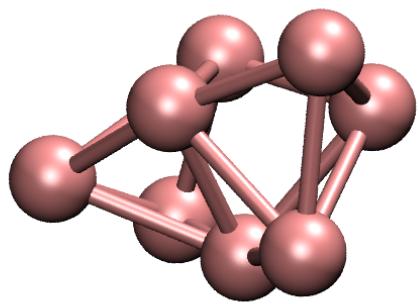
Molecule A

G\_09\_Ni



Molecule B

lj\_08\_Ni

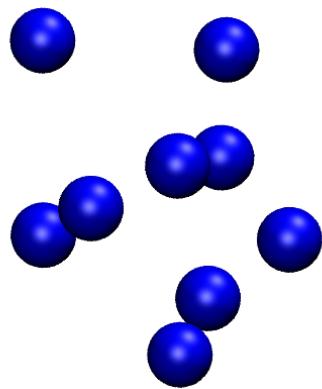


Different

ClustersNi Número 118

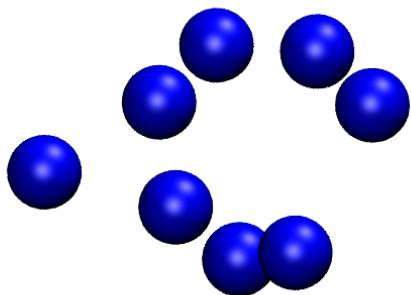
Molecule A

G\_09\_Ni



Molecule B

lj\_08\_Ni\_AFTER\_DFT

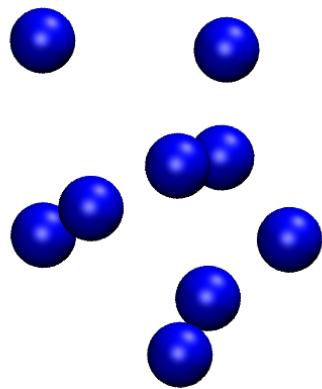


Different

ClustersNi Número 119

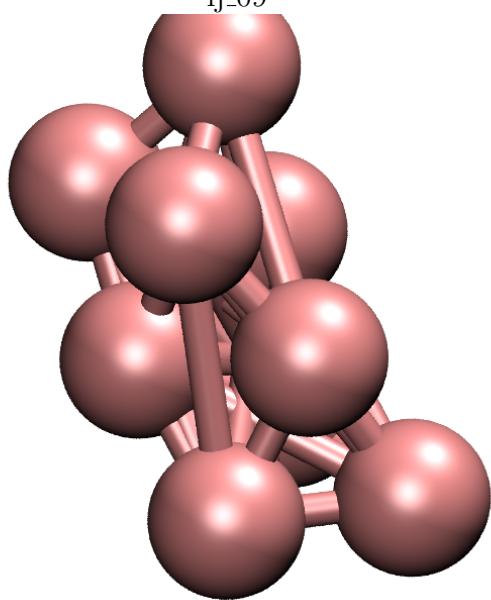
Molecule A

G\_09\_Ni



Molecule B

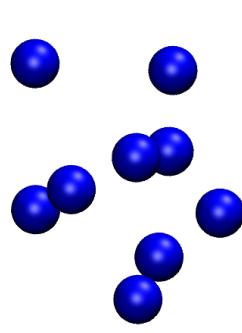
lj\_09



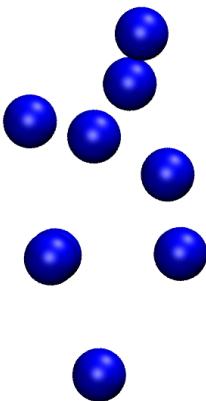
Different

# ClustersNi Número 120

Molecule A G\_09\_Ni



Molecule B lj\_09\_Ni



Inertia Tensor - Molecule A

2295.28	127.678	34.3162
127.678	2047.43	-608.198
34.3162	-608.198	1341.02

Inertia Tensor - Molecule B

2099.87	-92.0868	87.5491
-92.0868	1185.59	628.538
87.5491	628.538	1533.16

EingenVectors - Molecule A

0.0714239	-0.501716	-0.862078
-0.850908	0.420309	-0.315112
0.520436	0.756056	-0.396895

EingenVectors - Molecule B

-0.0896058	-0.791993	0.603919
0.134366	-0.610428	-0.780592
-0.986872	-0.0112006	-0.161115

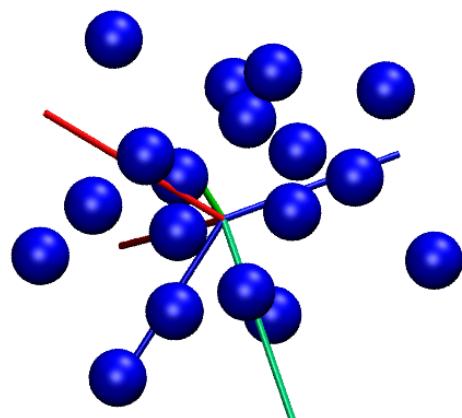
EingenValues - Molecule A

984.213	2244.92	2454.59
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EingenValues - Molecule B

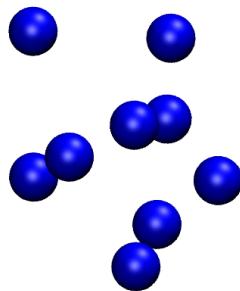
695.893	2009.61	2113.12
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Different

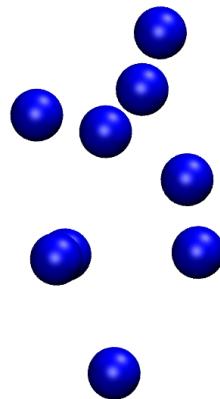


# ClustersNi Número 121

Molecule A G\_09\_Ni



Molecule B lj\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

2295.28	127.678	34.3162
127.678	2047.43	-608.198
34.3162	-608.198	1341.02

Inertia Tensor - Molecule B

2192.28	-89.3917	85.1517
-89.3917	1303.55	619.274
85.1517	619.274	1643.51

EigenVectors - Molecule A

0.0714239	-0.501716	-0.862078
-0.850908	0.420309	-0.315112
0.520436	0.756056	-0.396895

EigenVectors - Molecule B

-0.0891023	-0.791474	0.604673
0.147893	-0.610872	-0.777794
-0.984981	-0.0201236	-0.171483

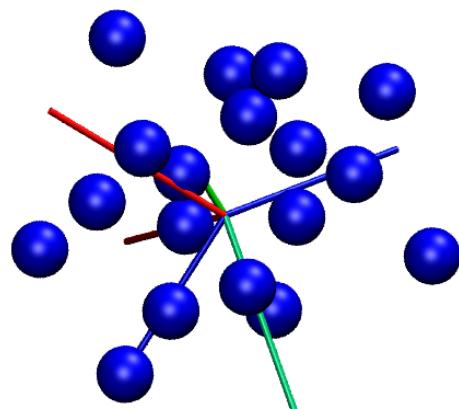
EigenValues - Molecule A

984.213	2244.92	2454.59
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EigenValues - Molecule B

820.373	2113.69	2205.28
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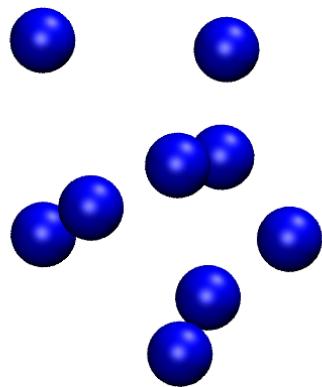
Different



ClustersNi Número 122

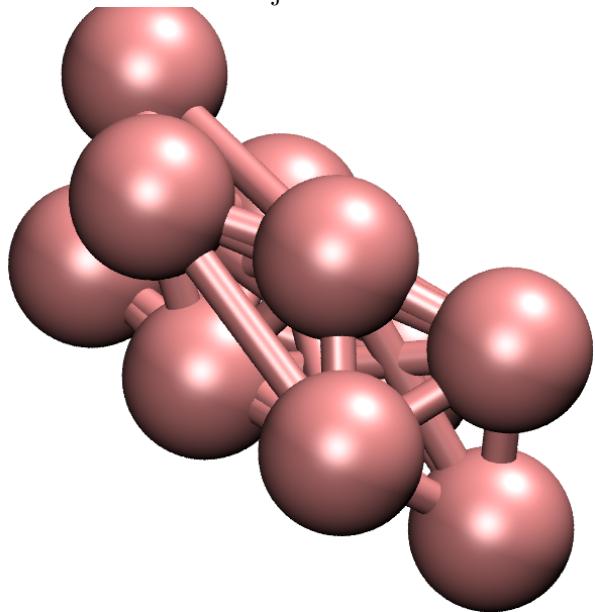
Molecule A

G\_09\_Ni



Molecule B

lj\_10

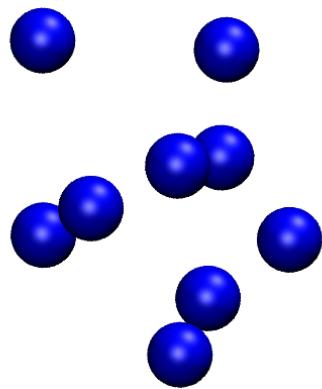


Different

ClustersNi Número 123

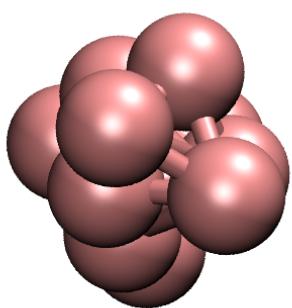
Molecule A

G\_09\_Ni



Molecule B

lj\_11

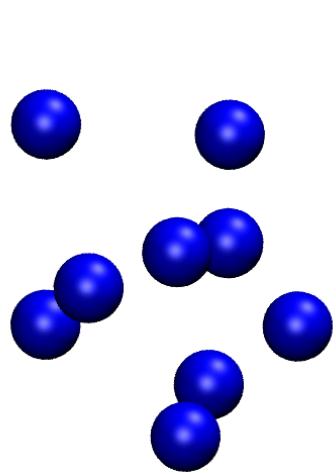


Different

ClustersNi Número 124

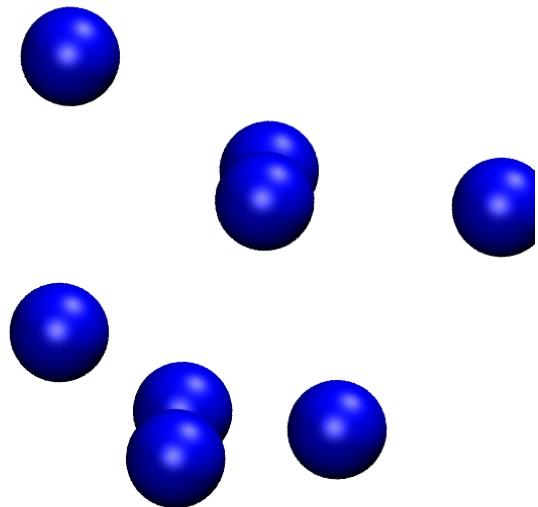
Molecule A

G\_09\_Ni\_AFTER\_DFT



Molecule B

SC\_08\_Ni

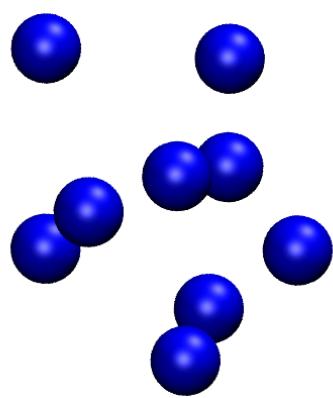


Different

ClustersNi Número 125

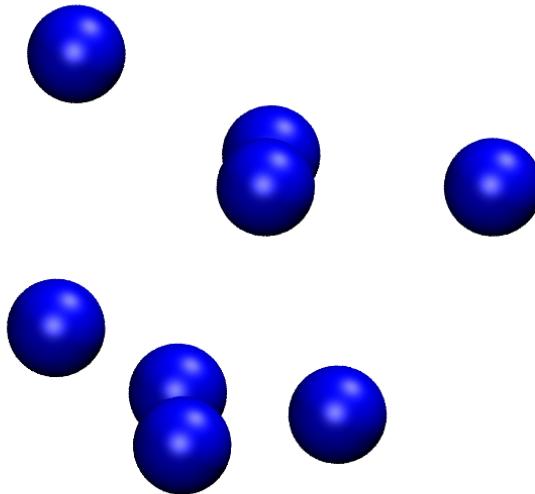
Molecule A

G\_09\_Ni\_AFTER\_DFT



Molecule B

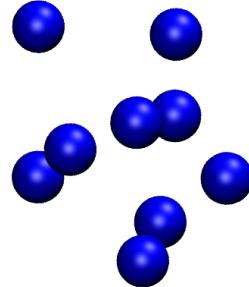
SC\_08\_Ni\_AFTER\_DFT



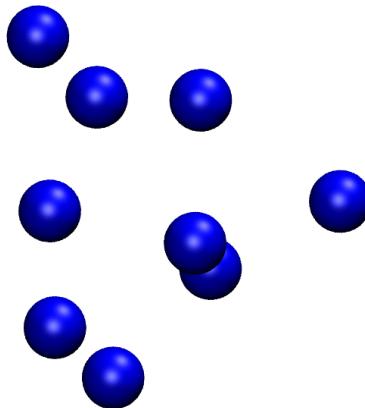
Different

# ClustersNi Número 126

Molecule A G\_09\_Ni\_AFTER\_DFT



Molecule B SC\_09\_Ni



Inertia Tensor - Molecule A

2034.24	115.071	30.1504
115.071	1837.6	-545.965
30.1504	-545.965	1191.04

Inertia Tensor - Molecule B

1536.98	56.225	-101.457
56.225	1328.77	-222.686
-101.457	-222.686	1805.96

EingenVectors - Molecule A

0.0718467	-0.498105	-0.864135
-0.874868	0.3846	-0.29443
0.479003	0.777158	-0.408144

EingenVectors - Molecule B

0.0545275	-0.93243	-0.357212
-0.957676	0.0524255	-0.283033
-0.282636	-0.357527	0.890108

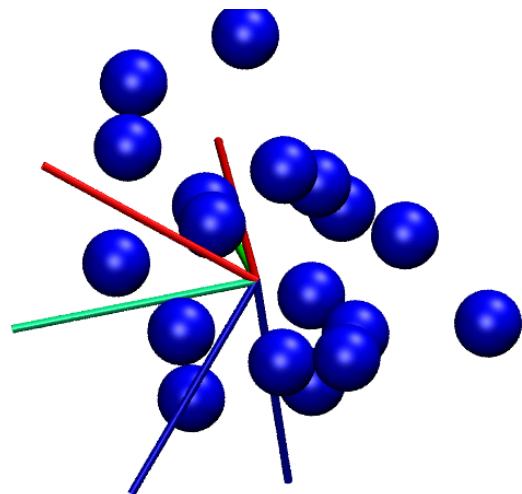
EingenValues - Molecule A

873.833	1993.8	2195.25
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EingenValues - Molecule B

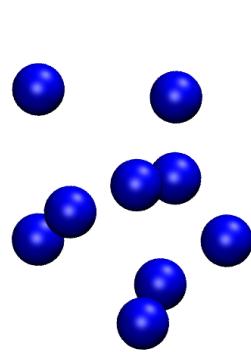
1240.17	1503.92	1927.62
---------	---------	---------

Different

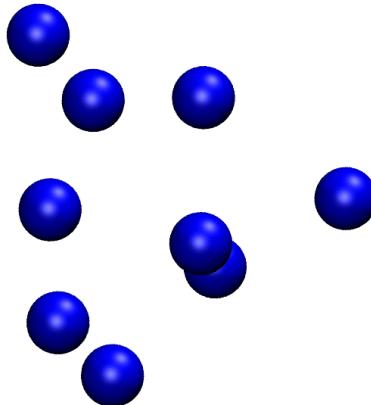


# ClustersNi Número 127

Molecule A G\_09\_Ni\_AFTER\_DFT



Molecule B SC\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

2034.24	115.071	30.1504
115.071	1837.6	-545.965
30.1504	-545.965	1191.04

Inertia Tensor - Molecule B

1526.11	61.3141	-104.189
61.3141	1367.3	-214.394
-104.189	-214.394	1801.23

EingenVectors - Molecule A

0.0718467	-0.498105	-0.864135
-0.874868	0.3846	-0.29443
0.479003	0.777158	-0.408144

EingenVectors - Molecule B

0.0759984	-0.927891	-0.365024
-0.954757	0.0378395	-0.294969
-0.287511	-0.370927	0.883035

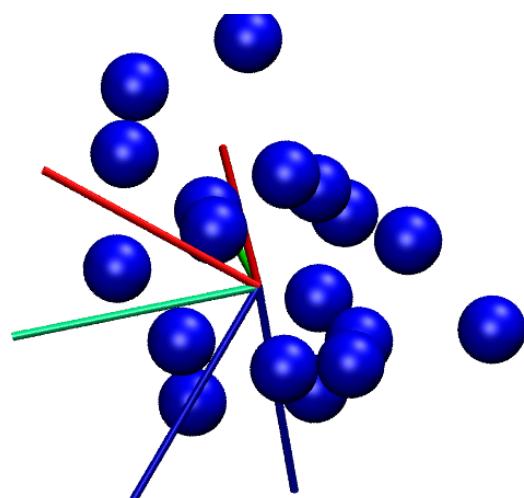
EingenValues - Molecule A

873.833	1993.8	2195.25
---------	--------	---------

EingenValues - Molecule B

1277.93	1491.49	1925.21
---------	---------	---------

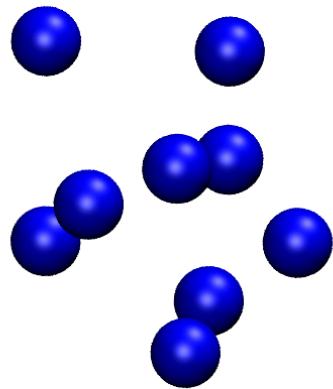
Different



ClustersNi Número 128

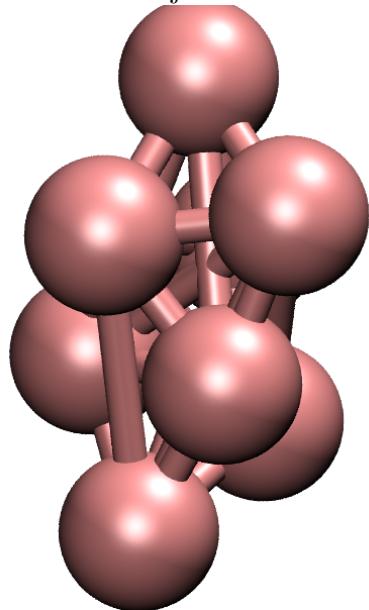
Molecule A

G\_09\_Ni\_AFTER\_DFT



Molecule B

lj\_08

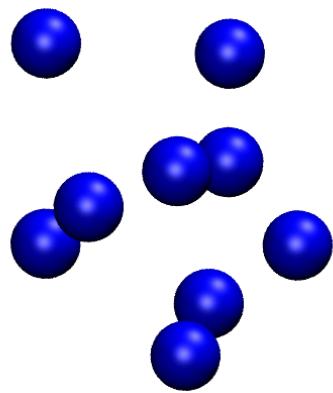


Different

ClustersNi Número 129

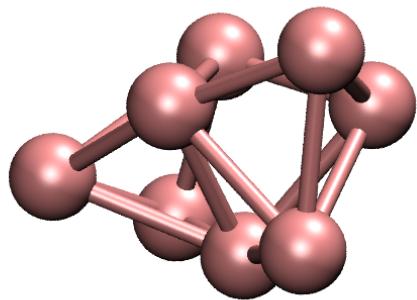
Molecule A

G\_09\_Ni\_AFTER\_DFT



Molecule B

lj\_08\_Ni

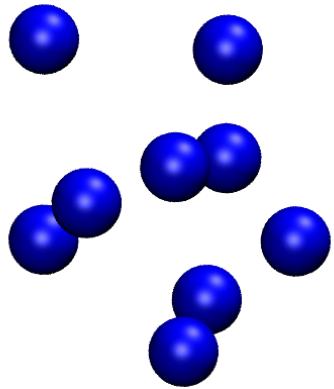


Different

ClustersNi Número 130

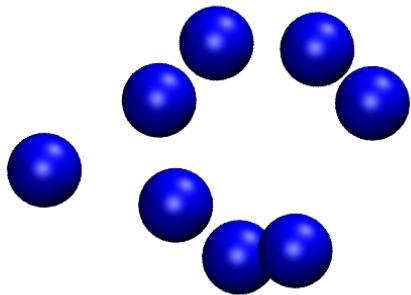
Molecule A

G\_09\_Ni\_AFTER\_DFT



Molecule B

lj\_08\_Ni\_AFTER\_DFT

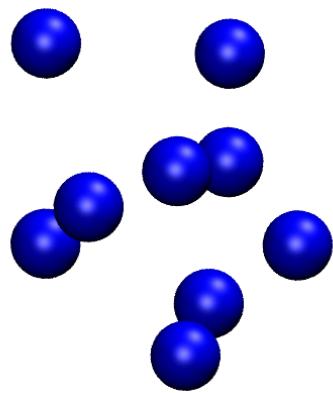


Different

ClustersNi Número 131

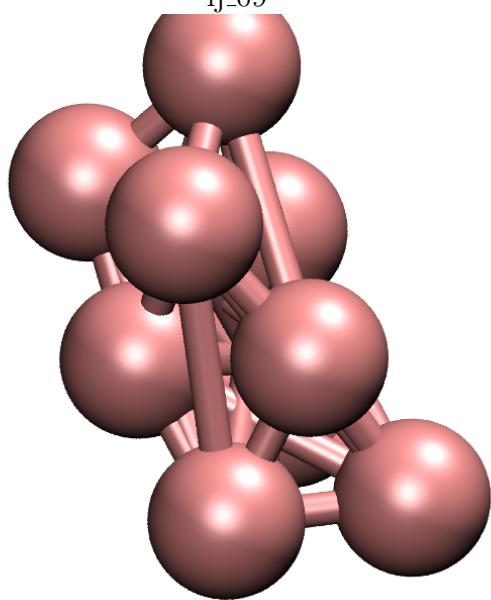
Molecule A

G\_09\_Ni\_AFTER\_DFT



Molecule B

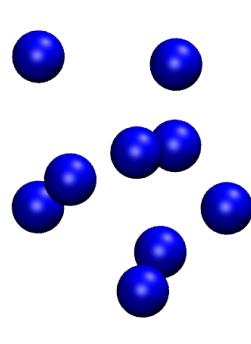
lj\_09



Different

# ClustersNi Número 132

Molecule A G\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

2034.24	115.071	30.1504
115.071	1837.6	-545.965
30.1504	-545.965	1191.04

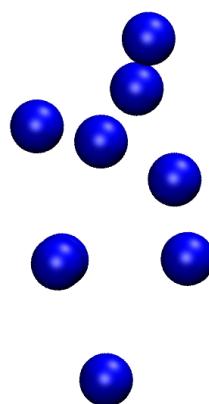
EingenVectors - Molecule A

0.0718467	-0.498105	-0.864135
-0.874868	0.3846	-0.29443
0.479003	0.777158	-0.408144

EingenValues - Molecule A

873.833	1993.8	2195.25
---------	--------	---------

Molecule B lj\_09\_Ni



Inertia Tensor - Molecule B

2099.87	-92.0868	87.5491
-92.0868	1185.59	628.538
87.5491	628.538	1533.16

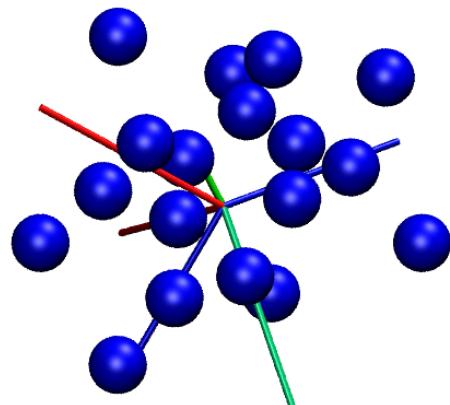
EingenVectors - Molecule B

-0.0896058	-0.791993	0.603919
0.134366	-0.610428	-0.780592
-0.986872	-0.0112006	-0.161115

EingenValues - Molecule B

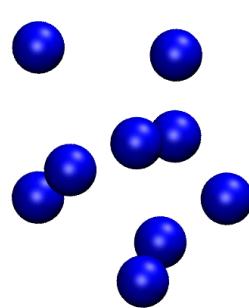
695.893	2009.61	2113.12
---------	---------	---------

Different

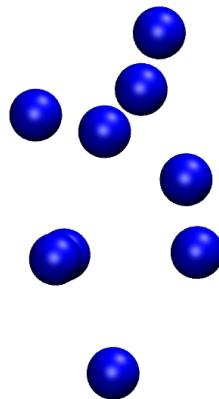


# ClustersNi Número 133

Molecule A G\_09\_Ni\_AFTER\_DFT



Molecule B lj\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

2034.24	115.071	30.1504
115.071	1837.6	-545.965
30.1504	-545.965	1191.04

Inertia Tensor - Molecule B

2192.28	-89.3917	85.1517
-89.3917	1303.55	619.274
85.1517	619.274	1643.51

EigenVectors - Molecule A

0.0718467	-0.498105	-0.864135
-0.874868	0.3846	-0.29443
0.479003	0.777158	-0.408144

EigenVectors - Molecule B

-0.0891023	-0.791474	0.604673
0.147893	-0.610872	-0.777794
-0.984981	-0.0201236	-0.171483

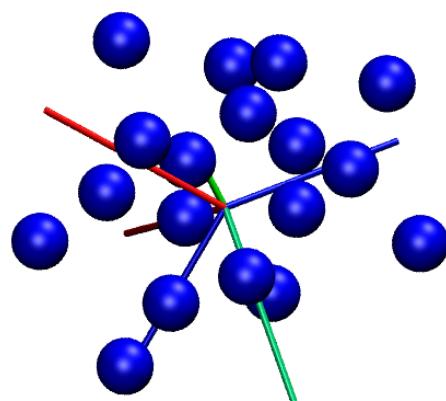
EigenValues - Molecule A

873.833	1993.8	2195.25
---------	--------	---------

EigenValues - Molecule B

820.373	2113.69	2205.28
---------	---------	---------

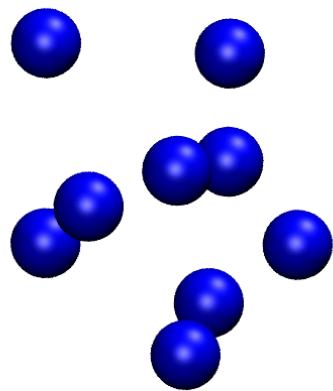
Different



ClustersNi Número 134

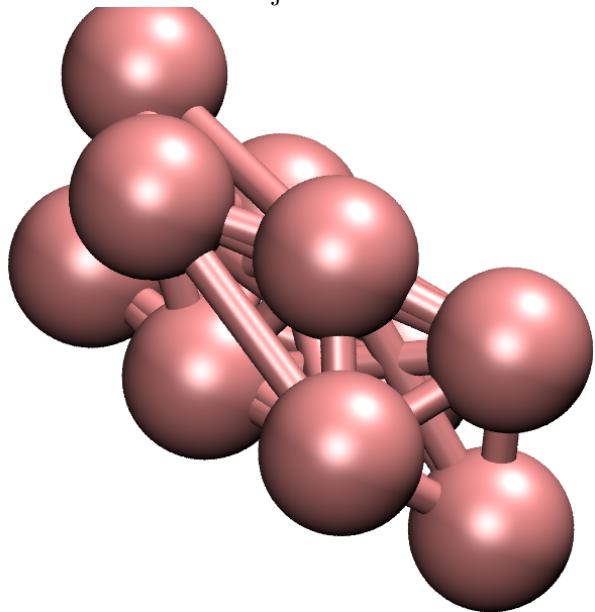
Molecule A

G\_09\_Ni\_AFTER\_DFT



Molecule B

lj\_10

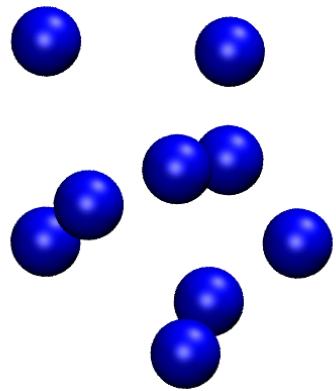


Different

ClustersNi Número 135

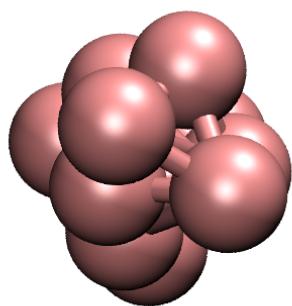
Molecule A

G\_09\_Ni\_AFTER\_DFT



Molecule B

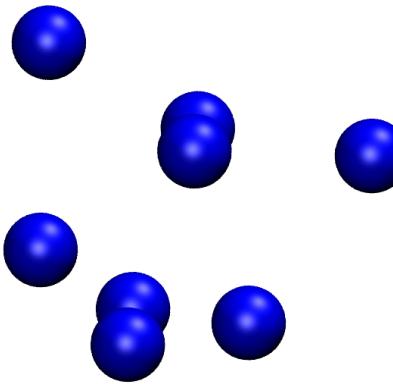
lj\_11



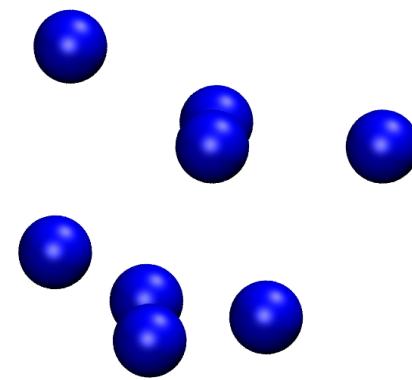
Different

# ClustersNi Número 136

Molecule A SC\_08\_Ni



Molecule B SC\_08\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1167.79	-0.00280809	0.01009
-0.00280809	1167.78	0.00700655
0.01009	0.00700655	1167.79

Inertia Tensor - Molecule B

1202.23	-22.8163	-12.5979
-22.8163	1197.22	1.92415
-12.5979	1.92415	1155.53

EingenVectors - Molecule A

0.395943	0.735527	-0.549753
-0.57735	0.664947	0.473828
0.71407	0.129791	0.687938

EingenVectors - Molecule B

0.285716	0.10352	0.952707
0.595734	0.759527	-0.261189
-0.750645	0.642185	0.155339

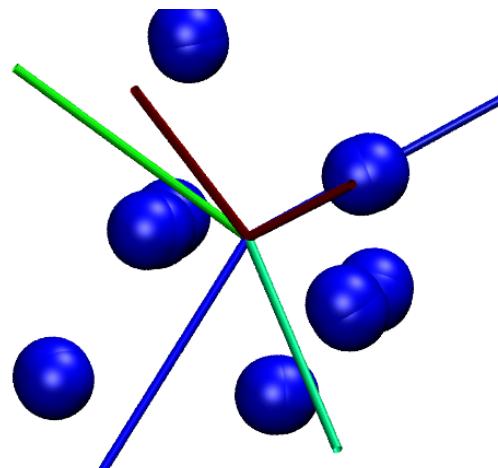
EingenValues - Molecule A

1167.77	1167.79	1167.8
---------	---------	--------

EingenValues - Molecule B

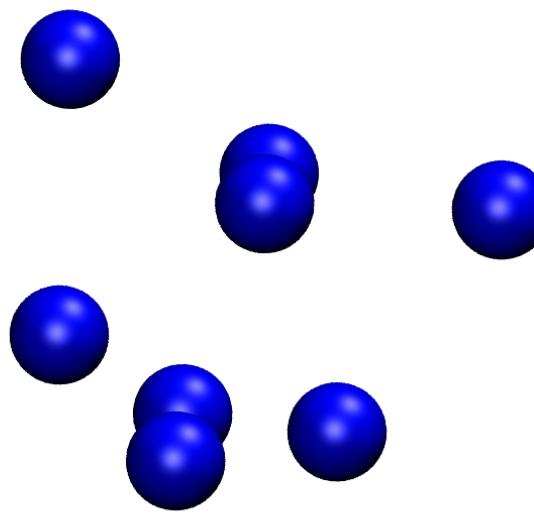
1151.96	1178.67	1224.36
---------	---------	---------

Different



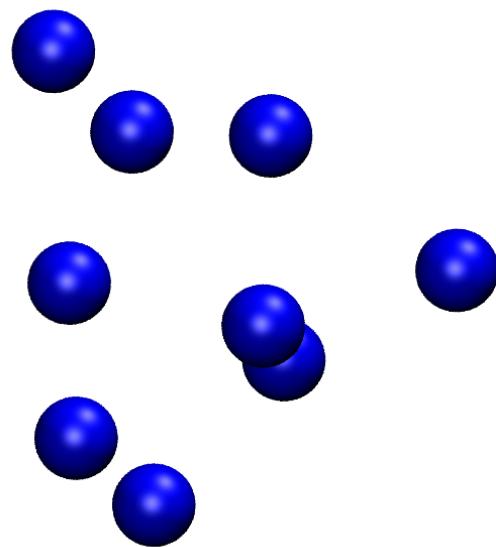
ClustersNi Número 137

Molecule A



SC\_08\_Ni

Molecule B



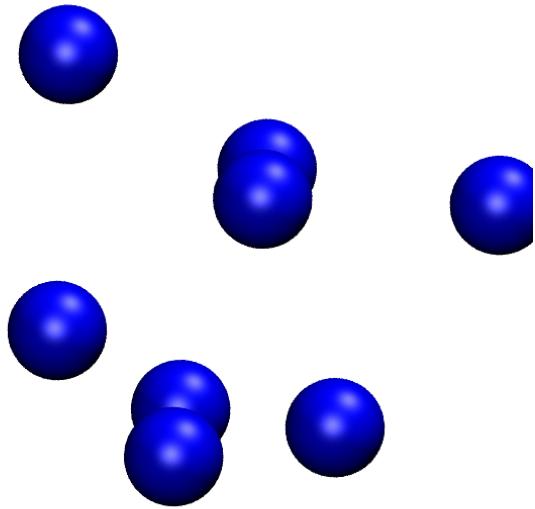
SC\_09\_Ni

Different

ClustersNi Número 138

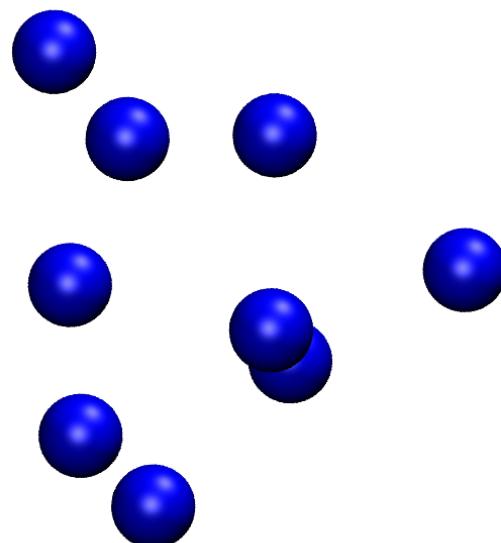
Molecule A

SC\_08\_Ni



Molecule B

SC\_09\_Ni\_AFTER\_DFT

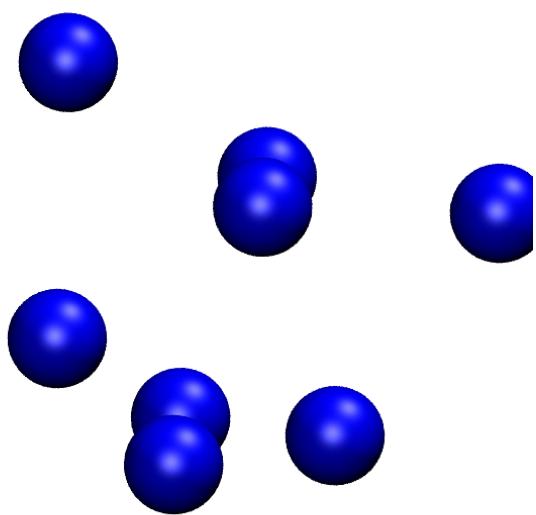


Different

ClustersNi Número 139

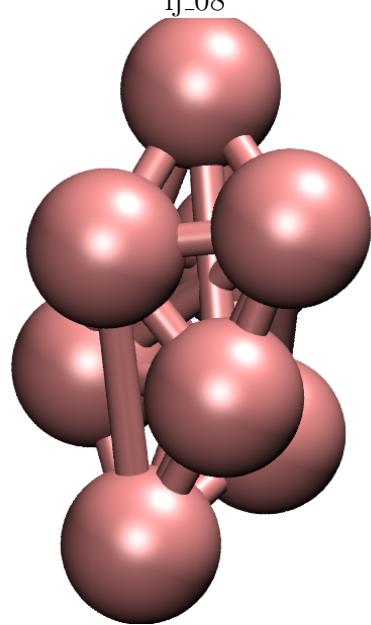
Molecule A

SC\_08\_Ni



Molecule B

lj\_08

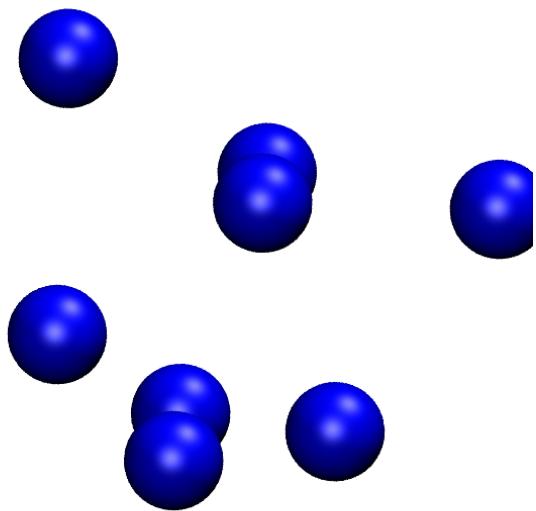


Different

ClustersNi Número 140

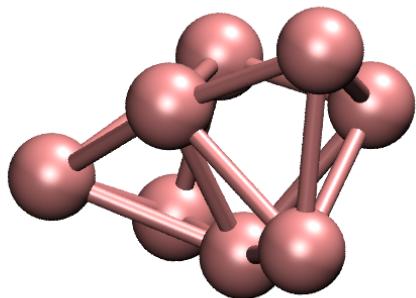
Molecule A

SC\_08\_Ni



Molecule B

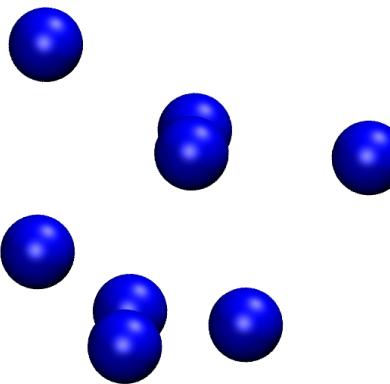
lj\_08\_Ni



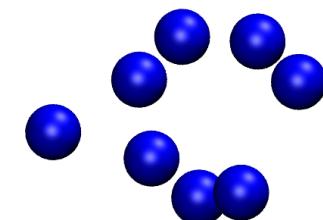
Different

# ClustersNi Número 141

Molecule A SC\_08\_Ni



Molecule B lj\_08\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1167.79	-0.00280809	0.01009
-0.00280809	1167.78	0.00700655
0.01009	0.00700655	1167.79

Inertia Tensor - Molecule B

1461.29	-67.9001	-380.896
-67.9001	1626.58	-132.788
-380.896	-132.788	885.164

EigenVectors - Molecule A

0.395943	0.735527	-0.549753
-0.57735	0.664947	0.473828
0.71407	0.129791	0.687938

EigenVectors - Molecule B

0.440314	0.154412	0.884466
-0.488448	-0.785372	0.380276
-0.753354	0.599456	0.270388

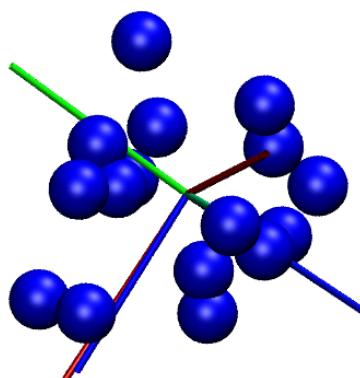
EigenValues - Molecule A

1167.77	1167.79	1167.8
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EigenValues - Molecule B

672.361	1648.65	1652.02
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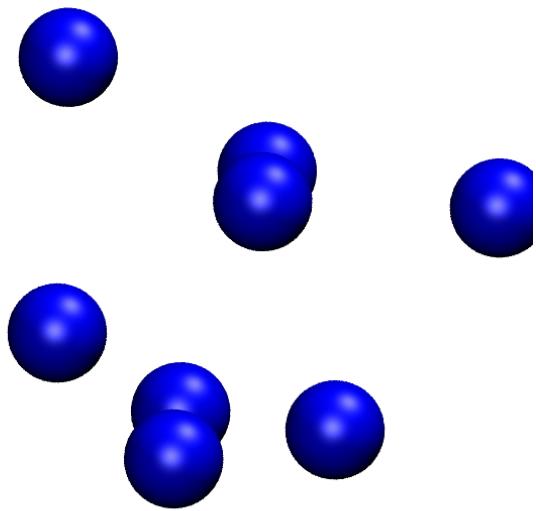
Different



ClustersNi Número 142

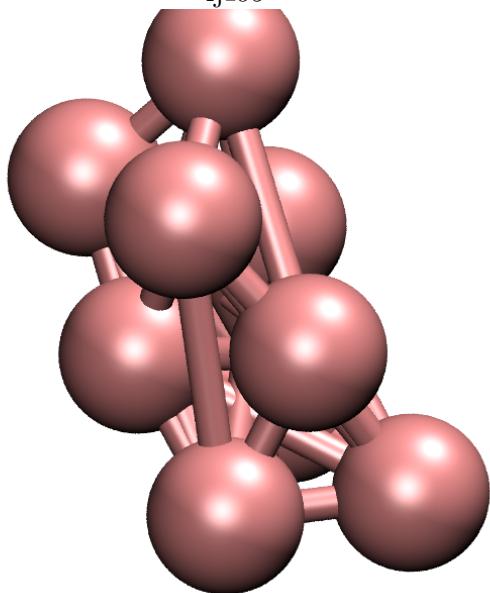
Molecule A

SC\_08\_Ni



Molecule B

lj\_09

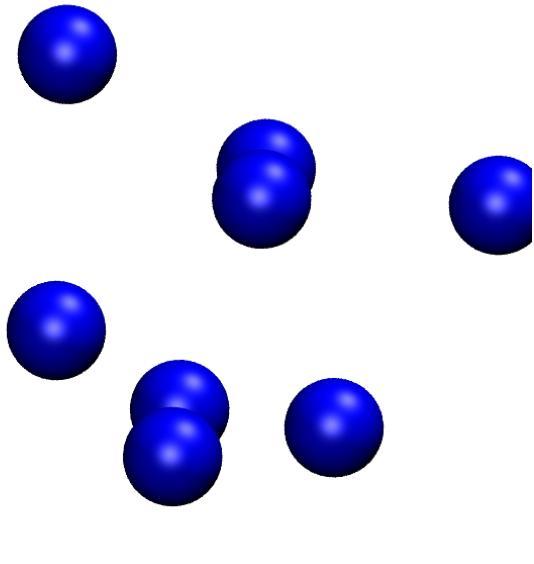


Different

ClustersNi Número 143

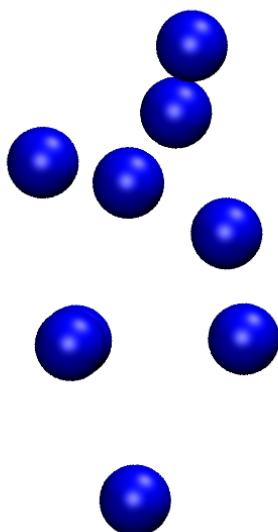
Molecule A

SC\_08\_Ni



Molecule B

lj\_09\_Ni

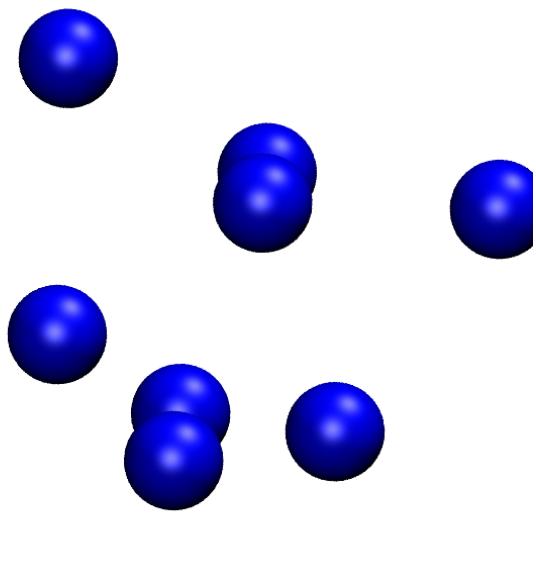


Different

ClustersNi Número 144

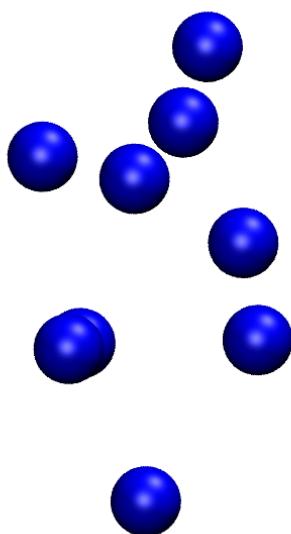
Molecule A

SC\_08\_Ni



Molecule B

lj\_09\_Ni\_AFTER\_DFT

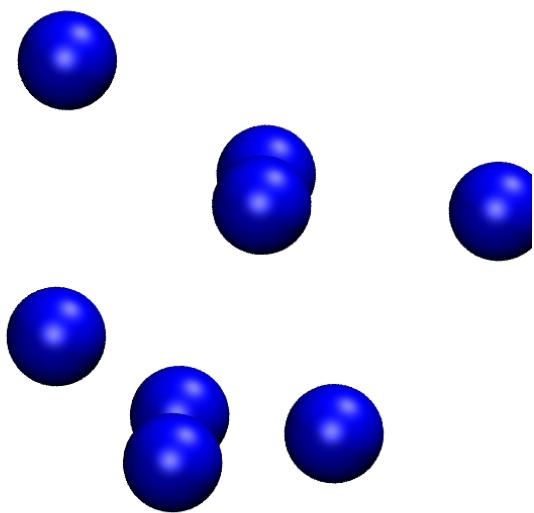


Different

ClustersNi Número 145

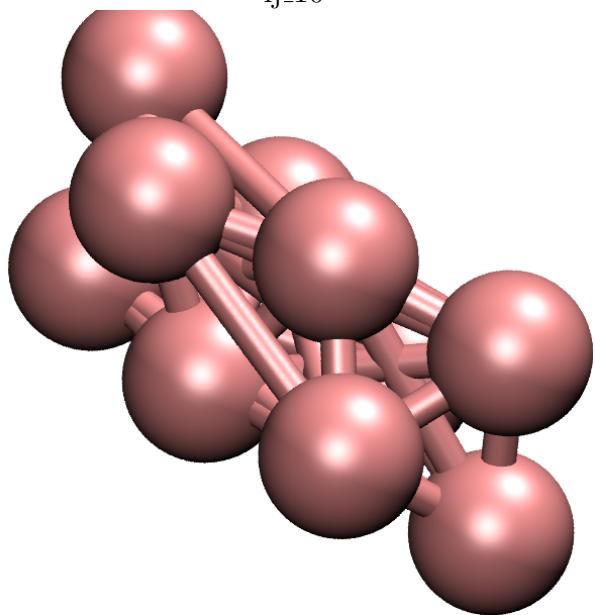
Molecule A

SC\_08\_Ni



Molecule B

lj\_10

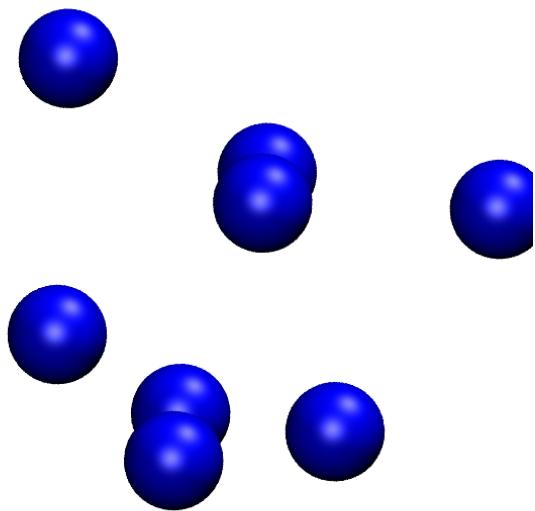


Different

ClustersNi Número 146

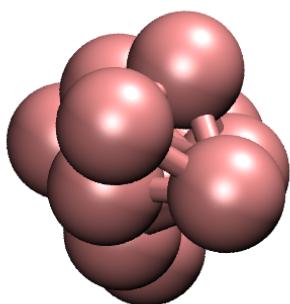
Molecule A

SC\_08\_Ni



Molecule B

lj\_11

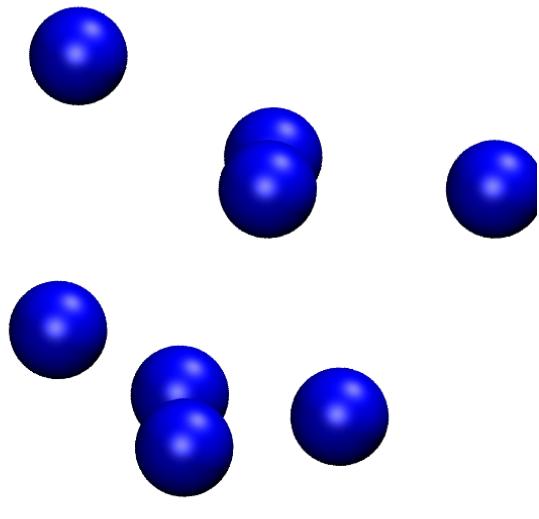


Different

ClustersNi Número 147

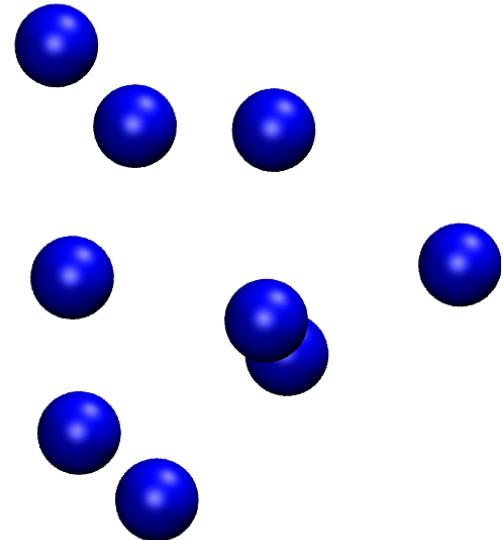
Molecule A

SC\_08\_Ni\_AFTER\_DFT



Molecule B

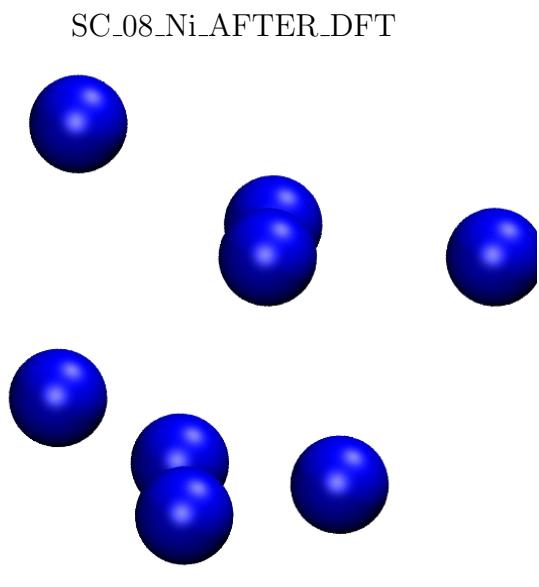
SC\_09\_Ni



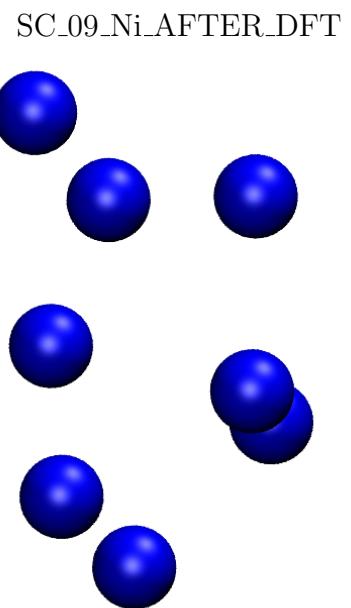
Different

ClustersNi Número 148

Molecule A



Molecule B

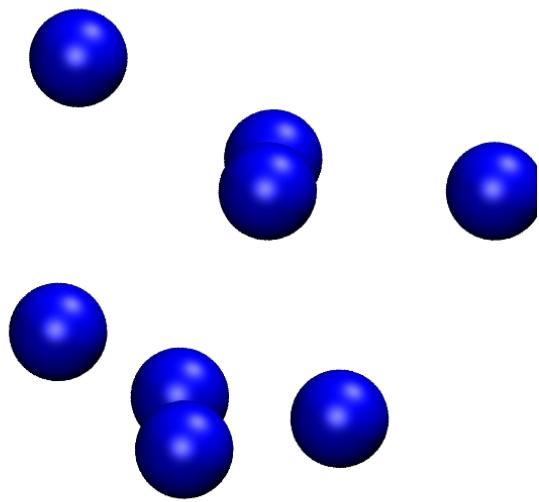


Different

ClustersNi Número 149

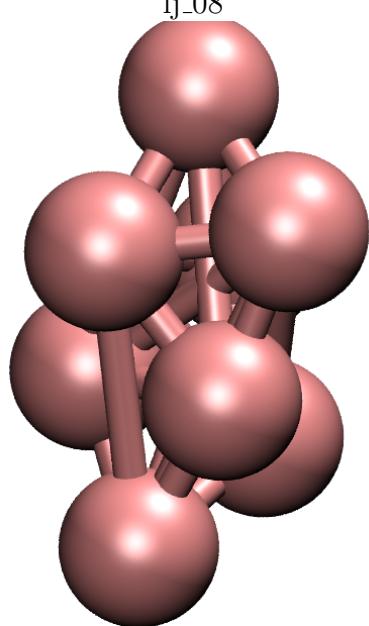
Molecule A

SC\_08\_Ni\_AFTER\_DFT



Molecule B

lj\_08

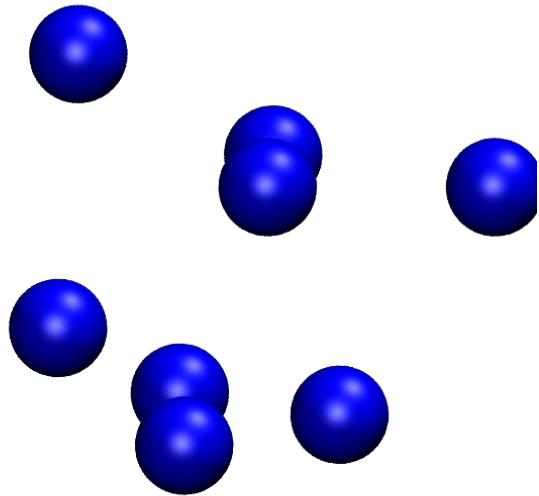


Different

ClustersNi Número 150

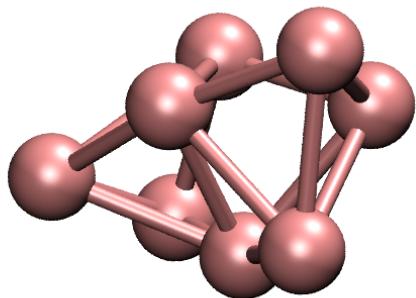
Molecule A

SC\_08\_Ni\_AFTER\_DFT



Molecule B

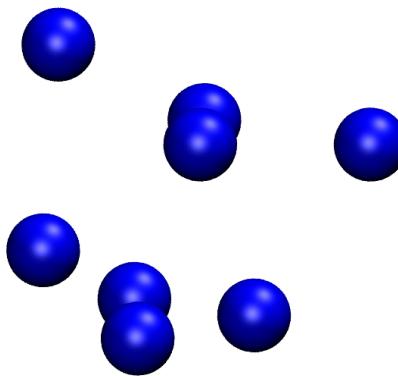
lj\_08\_Ni



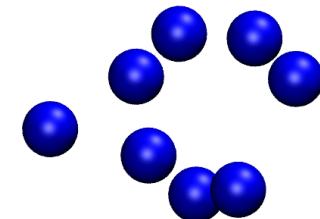
Different

# ClustersNi Número 151

Molecule A SC\_08\_Ni\_AFTER\_DFT



Molecule B lj\_08\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1202.23	-22.8163	-12.5979
-22.8163	1197.22	1.92415
-12.5979	1.92415	1155.53

Inertia Tensor - Molecule B

1461.29	-67.9001	-380.896
-67.9001	1626.58	-132.788
-380.896	-132.788	885.164

EigenVectors - Molecule A

0.285716	0.10352	0.952707
0.595734	0.759527	-0.261189
-0.750645	0.642185	0.155339

EigenVectors - Molecule B

0.440314	0.154412	0.884466
-0.488448	-0.785372	0.380276
-0.753354	0.599456	0.270388

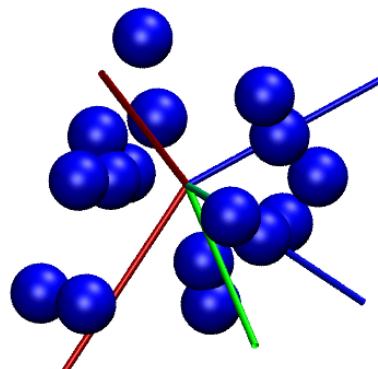
EigenValues - Molecule A

1151.96	1178.67	1224.36
---------	---------	---------

EigenValues - Molecule B

672.361	1648.65	1652.02
---------	---------	---------

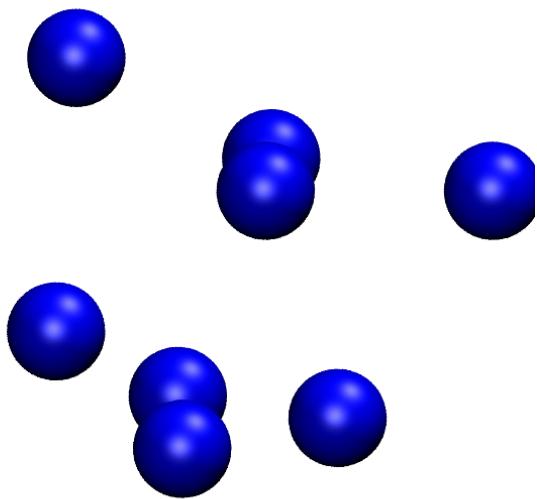
Different



ClustersNi Número 152

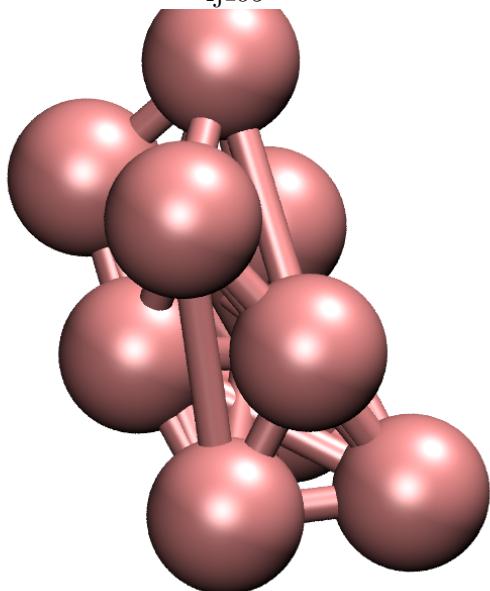
Molecule A

SC\_08\_Ni\_AFTER\_DFT



Molecule B

lj\_09

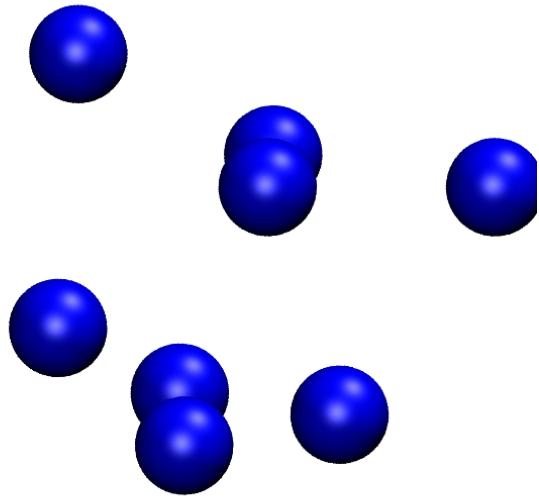


Different

ClustersNi Número 153

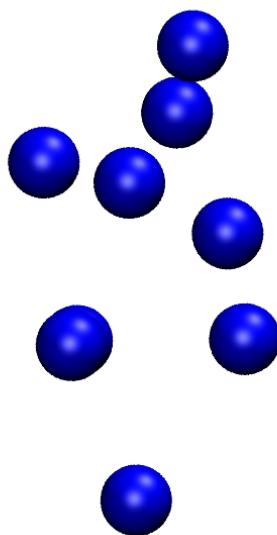
Molecule A

SC\_08\_Ni\_AFTER\_DFT



Molecule B

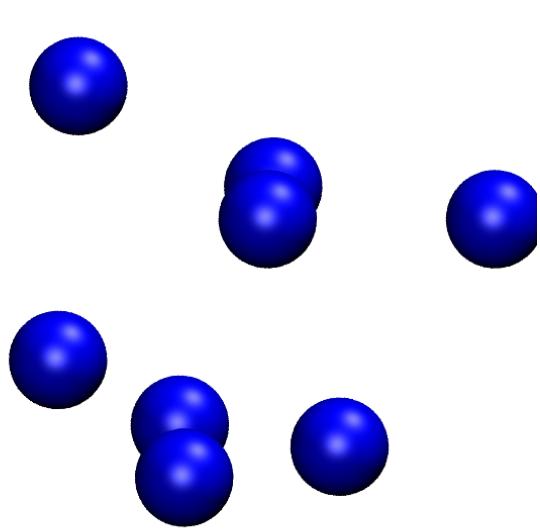
lj\_09\_Ni



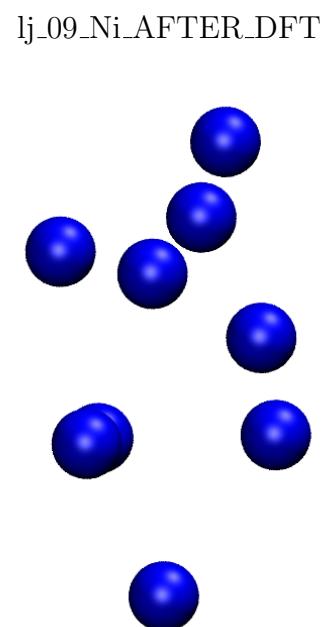
Different

ClustersNi Número 154

Molecule A



Molecule B

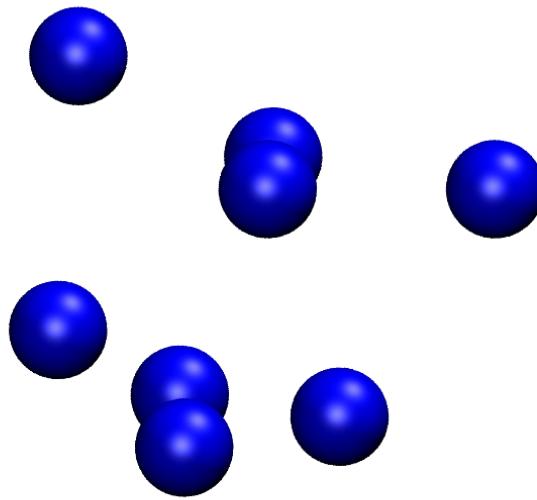


Different

ClustersNi Número 155

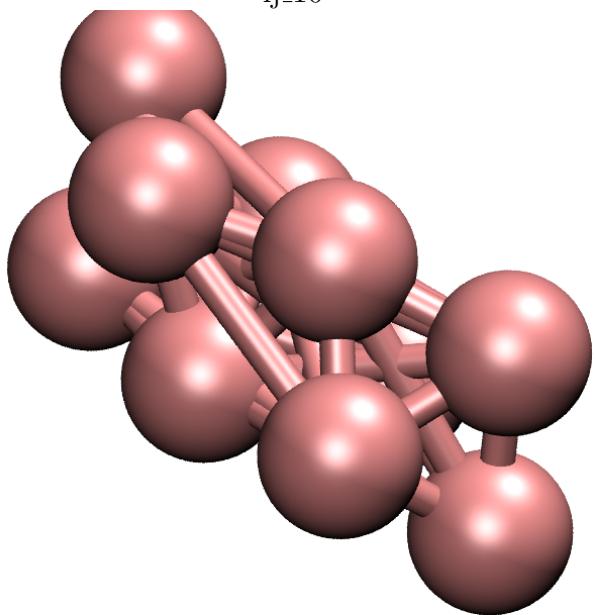
Molecule A

SC\_08\_Ni\_AFTER\_DFT



Molecule B

lj\_10

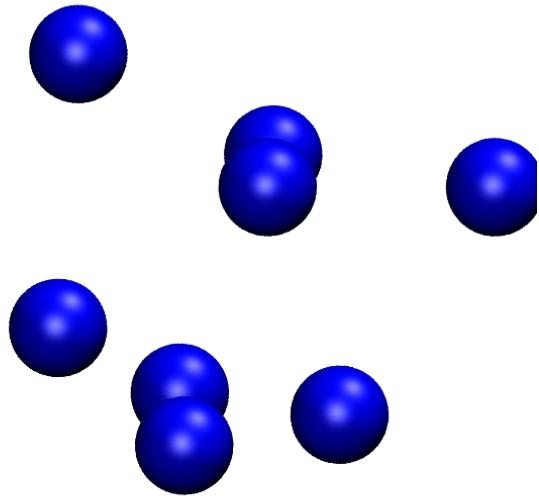


Different

ClustersNi Número 156

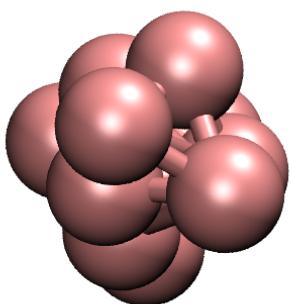
Molecule A

SC\_08\_Ni\_AFTER\_DFT



Molecule B

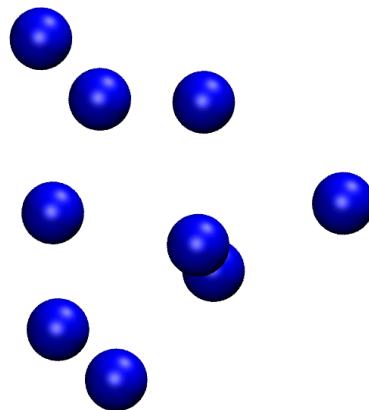
lj\_11



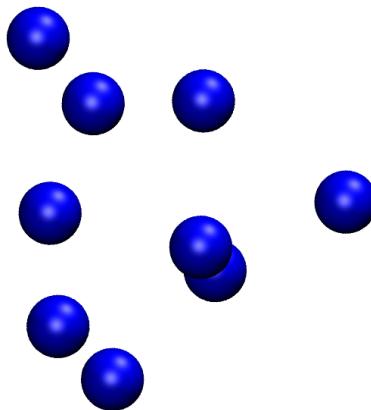
Different

# ClustersNi Número 157

Molecule A SC\_09\_Ni



Molecule B SC\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1536.98	56.225	-101.457
56.225	1328.77	-222.686
-101.457	-222.686	1805.96

Inertia Tensor - Molecule B

1526.11	61.3141	-104.189
61.3141	1367.3	-214.394
-104.189	-214.394	1801.23

EingenVectors - Molecule A

0.0545275	-0.93243	-0.357212
-0.957676	0.0524255	-0.283033
-0.282636	-0.357527	0.890108

EingenVectors - Molecule B

0.0759984	-0.927891	-0.365024
-0.954757	0.0378395	-0.294969
-0.287511	-0.370927	0.883035

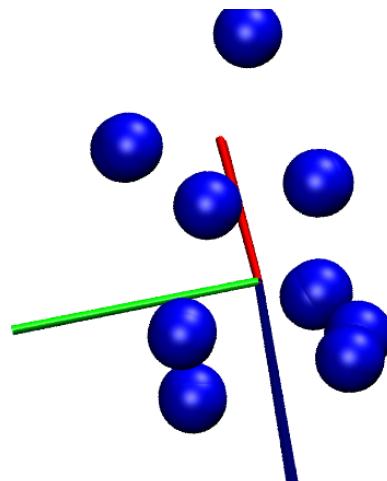
EingenValues - Molecule A

1240.17	1503.92	1927.62
---------	---------	---------

EingenValues - Molecule B

1277.93	1491.49	1925.21
---------	---------	---------

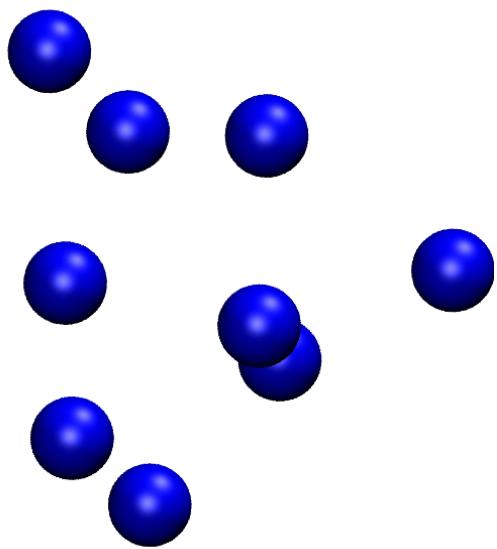
Different



ClustersNi Número 158

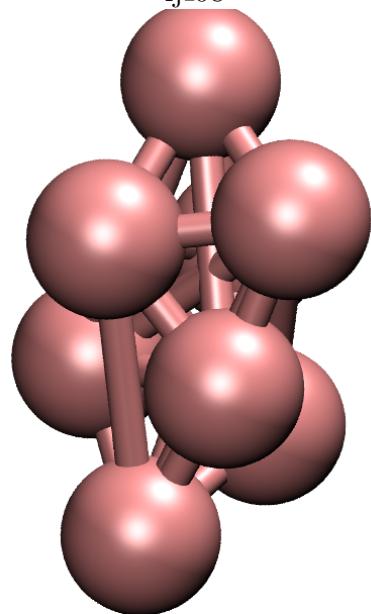
Molecule A

SC\_09\_Ni



Molecule B

lj\_08

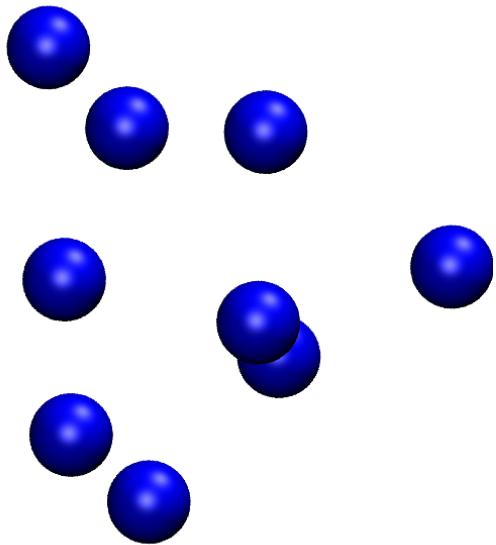


Different

ClustersNi Número 159

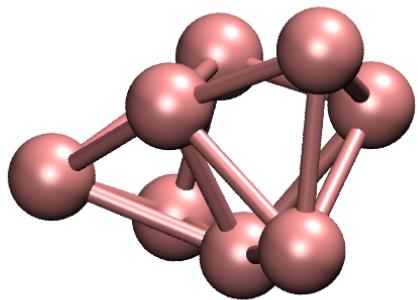
Molecule A

SC\_09\_Ni



Molecule B

lj\_08\_Ni

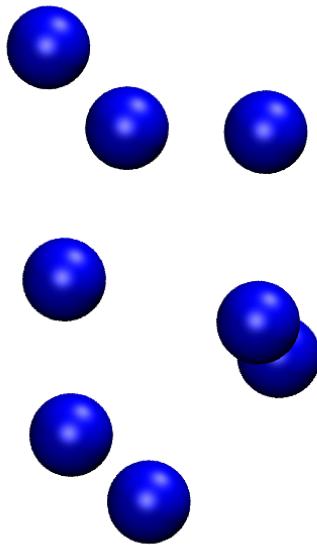


Different

ClustersNi Número 160

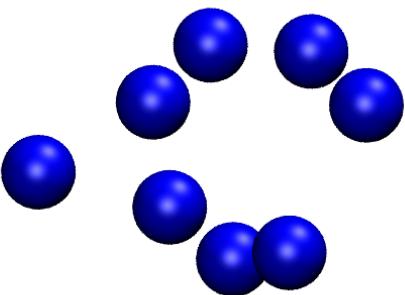
Molecule A

SC\_09\_Ni



Molecule B

lj\_08\_Ni\_AFTER\_DFT

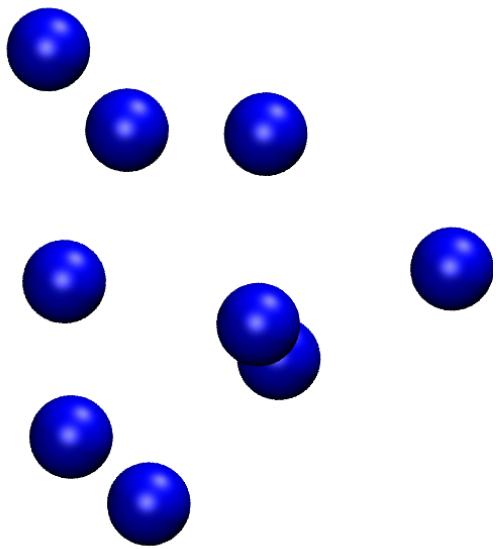


Different

ClustersNi Número 161

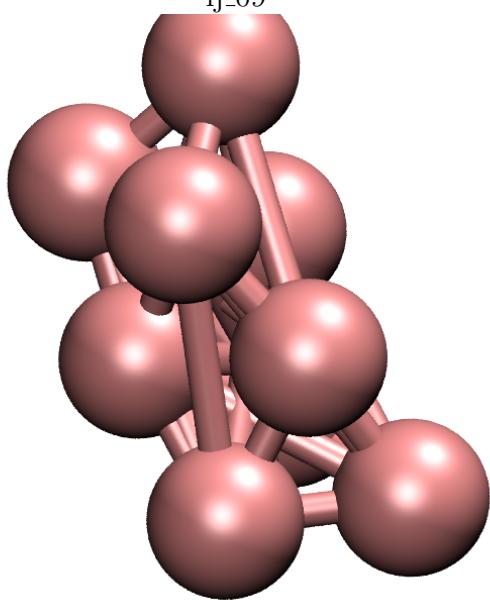
Molecule A

SC\_09\_Ni



Molecule B

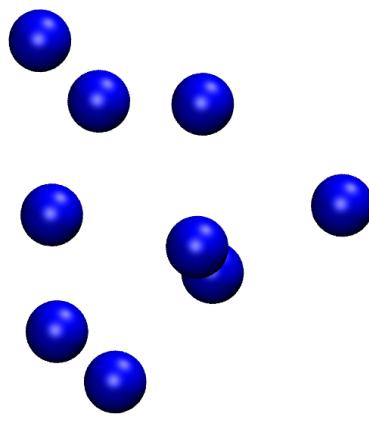
lj\_09



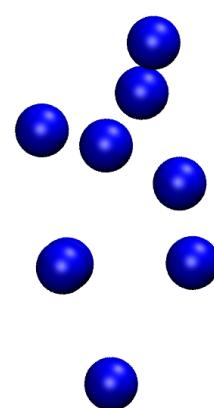
Different

# ClustersNi Número 162

Molecule A SC\_09\_Ni



Molecule B lj\_09\_Ni



Inertia Tensor - Molecule A

1536.98	56.225	-101.457
56.225	1328.77	-222.686
-101.457	-222.686	1805.96

Inertia Tensor - Molecule B

2099.87	-92.0868	87.5491
-92.0868	1185.59	628.538
87.5491	628.538	1533.16

EingenVectors - Molecule A

0.0545275	-0.93243	-0.357212
-0.957676	0.0524255	-0.283033
-0.282636	-0.357527	0.890108

EingenVectors - Molecule B

-0.0896058	-0.791993	0.603919
0.134366	-0.610428	-0.780592
-0.986872	-0.0112006	-0.161115

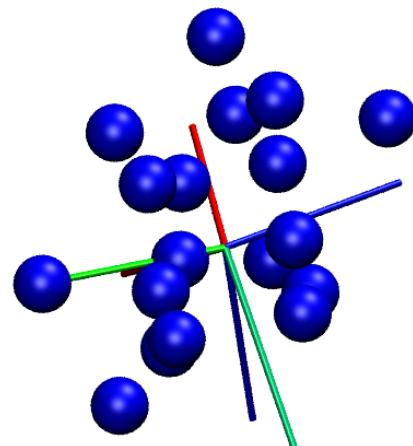
EingenValues - Molecule A

1240.17	1503.92	1927.62
---------	---------	---------

EingenValues - Molecule B

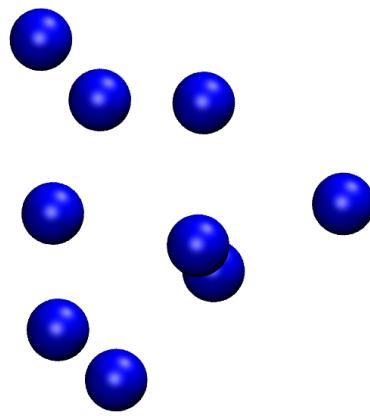
695.893	2009.61	2113.12
---------	---------	---------

Different

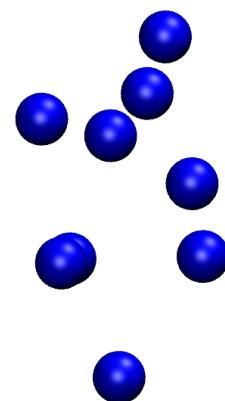


# ClustersNi Número 163

Molecule A SC\_09\_Ni



Molecule B lj\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1536.98	56.225	-101.457
56.225	1328.77	-222.686
-101.457	-222.686	1805.96

Inertia Tensor - Molecule B

2192.28	-89.3917	85.1517
-89.3917	1303.55	619.274
85.1517	619.274	1643.51

EigenVectors - Molecule A

0.0545275	-0.93243	-0.357212
-0.957676	0.0524255	-0.283033
-0.282636	-0.357527	0.890108

EigenVectors - Molecule B

-0.0891023	-0.791474	0.604673
0.147893	-0.610872	-0.777794
-0.984981	-0.0201236	-0.171483

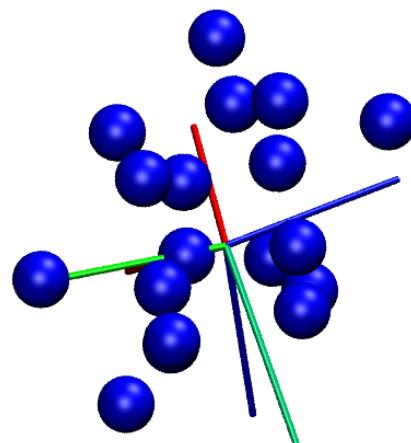
EigenValues - Molecule A

1240.17	1503.92	1927.62
---------	---------	---------

EigenValues - Molecule B

820.373	2113.69	2205.28
---------	---------	---------

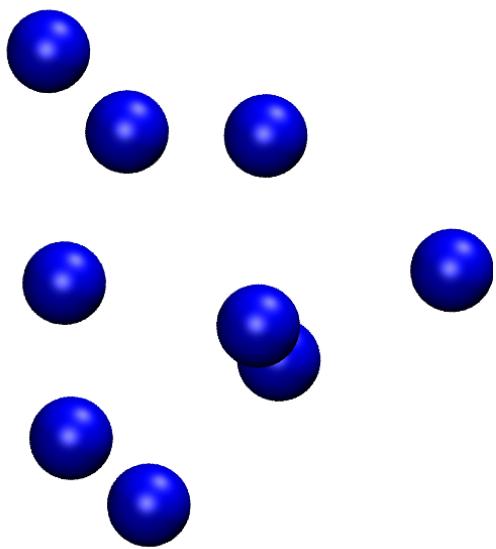
Different



ClustersNi Número 164

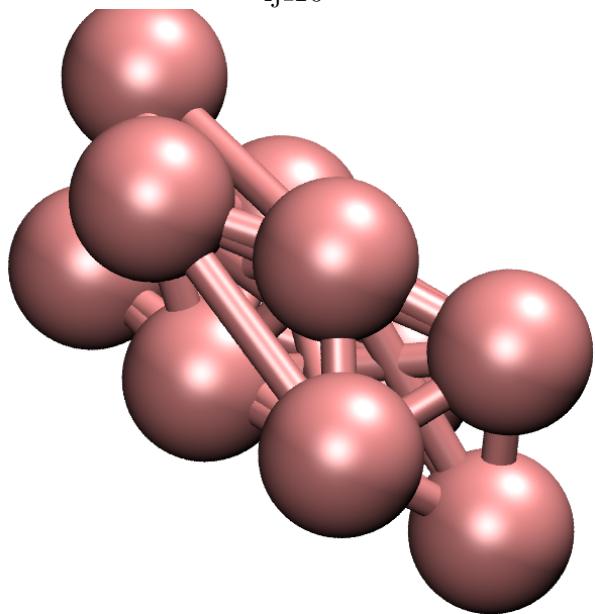
Molecule A

SC\_09\_Ni



Molecule B

lj\_10

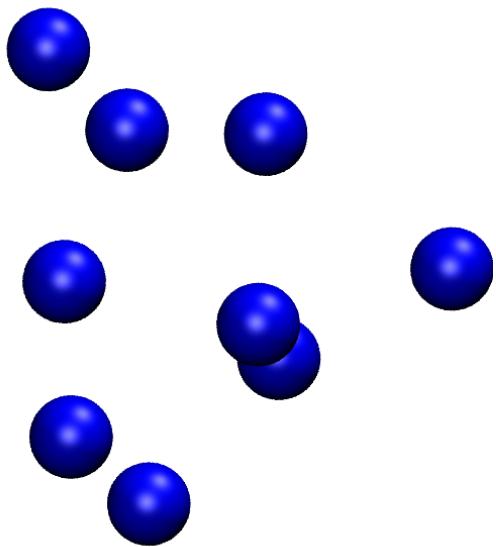


Different

ClustersNi Número 165

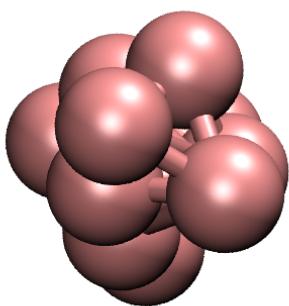
Molecule A

SC\_09\_Ni



Molecule B

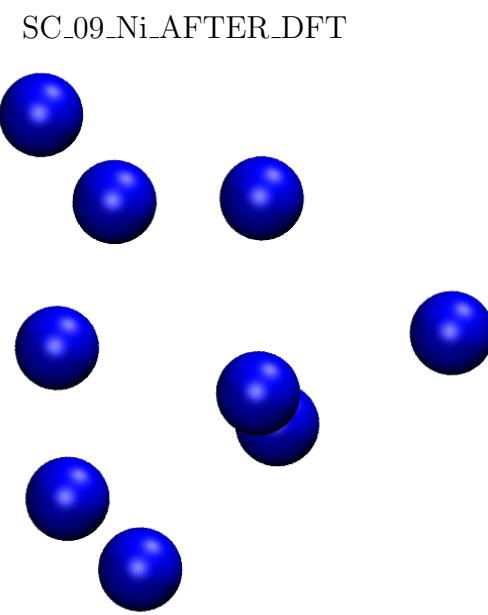
lj\_11



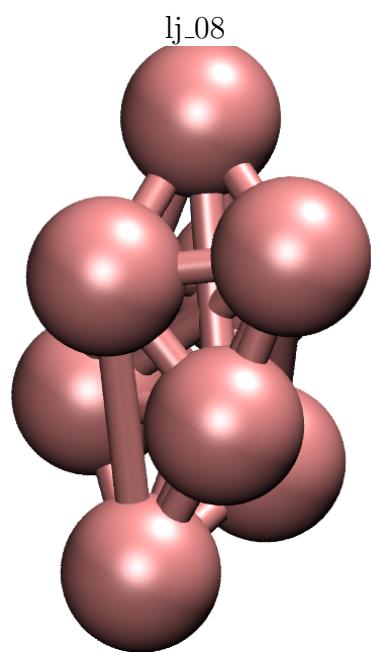
Different

ClustersNi Número 166

Molecule A



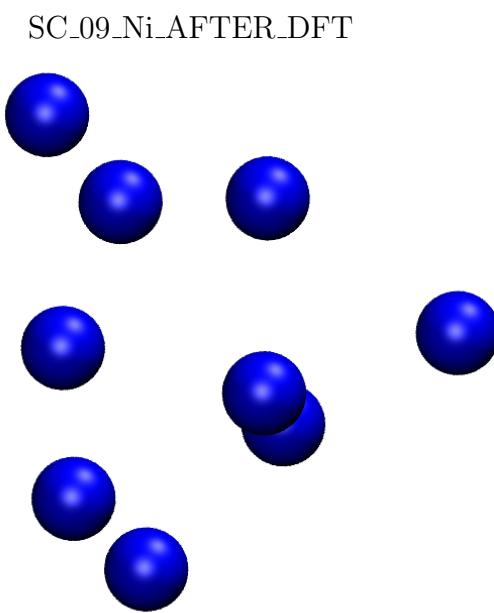
Molecule B



Different

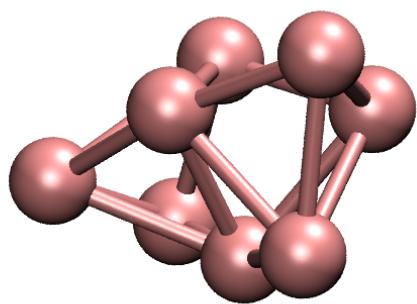
ClustersNi Número 167

Molecule A



Molecule B

lj\_08\_Ni

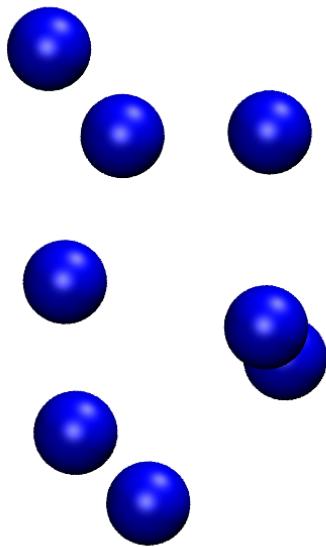


Different

ClustersNi Número 168

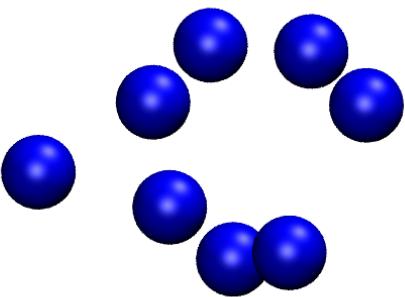
Molecule A

SC\_09\_Ni\_AFTER\_DFT



Molecule B

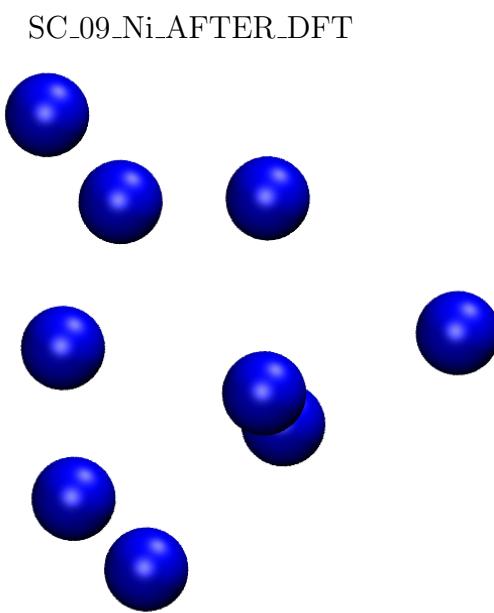
lj\_08\_Ni\_AFTER\_DFT



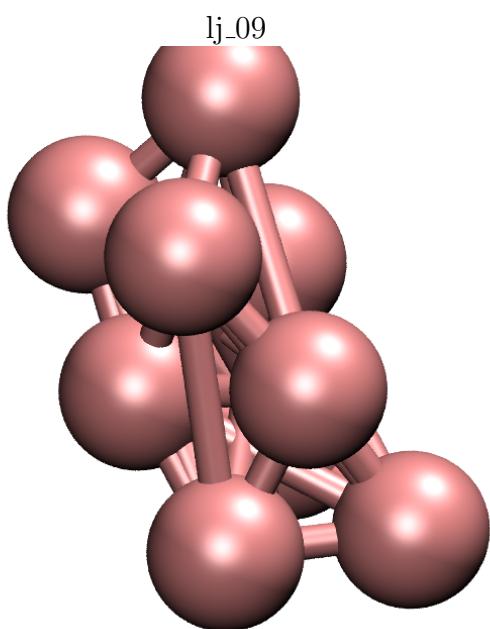
Different

ClustersNi Número 169

Molecule A



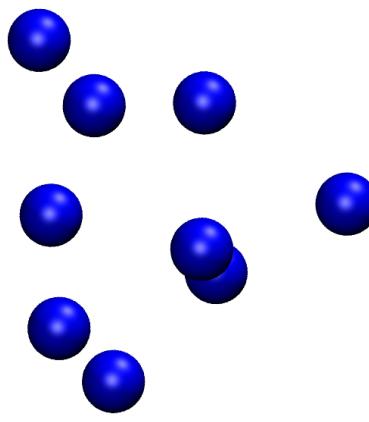
Molecule B



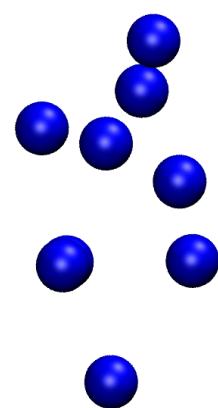
Different

# ClustersNi Número 170

Molecule A SC\_09\_Ni\_AFTER\_DFT



Molecule B lj\_09\_Ni



Inertia Tensor - Molecule A

1526.11	61.3141	-104.189
61.3141	1367.3	-214.394
-104.189	-214.394	1801.23

Inertia Tensor - Molecule B

2099.87	-92.0868	87.5491
-92.0868	1185.59	628.538
87.5491	628.538	1533.16

EingenVectors - Molecule A

0.0759984	-0.927891	-0.365024
-0.954757	0.0378395	-0.294969
-0.287511	-0.370927	0.883035

EingenVectors - Molecule B

-0.0896058	-0.791993	0.603919
0.134366	-0.610428	-0.780592
-0.986872	-0.0112006	-0.161115

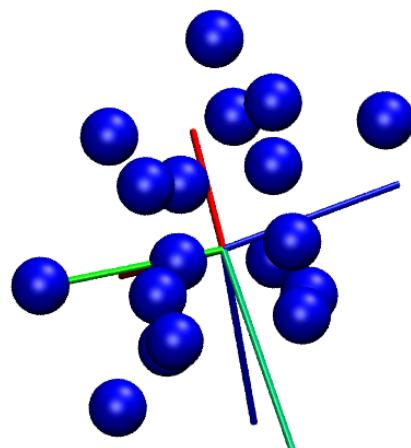
EingenValues - Molecule A

1277.93	1491.49	1925.21
---------	---------	---------

EingenValues - Molecule B

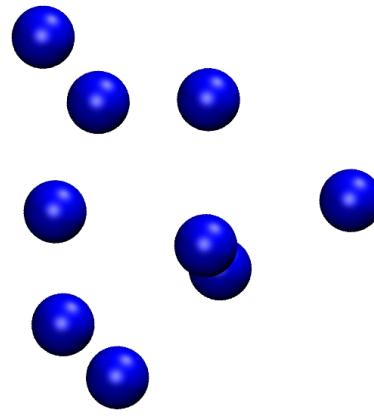
695.893	2009.61	2113.12
---------	---------	---------

Different

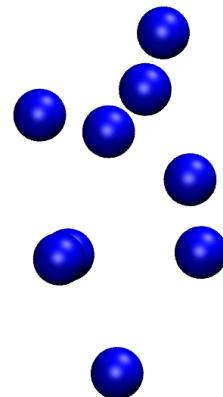


# ClustersNi Número 171

Molecule A SC\_09\_Ni\_AFTER\_DFT



Molecule B lj\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

1526.11	61.3141	-104.189
61.3141	1367.3	-214.394
-104.189	-214.394	1801.23

Inertia Tensor - Molecule B

2192.28	-89.3917	85.1517
-89.3917	1303.55	619.274
85.1517	619.274	1643.51

EigenVectors - Molecule A

0.0759984	-0.927891	-0.365024
-0.954757	0.0378395	-0.294969
-0.287511	-0.370927	0.883035

EigenVectors - Molecule B

-0.0891023	-0.791474	0.604673
0.147893	-0.610872	-0.777794
-0.984981	-0.0201236	-0.171483

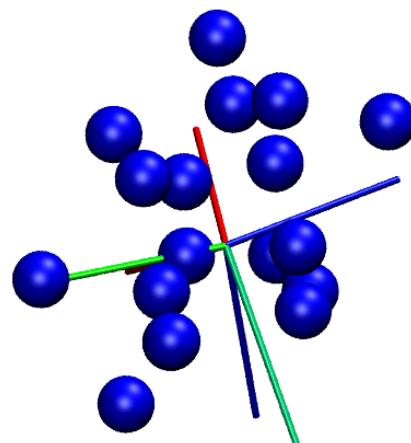
EigenValues - Molecule A

1277.93	1491.49	1925.21
---------	---------	---------

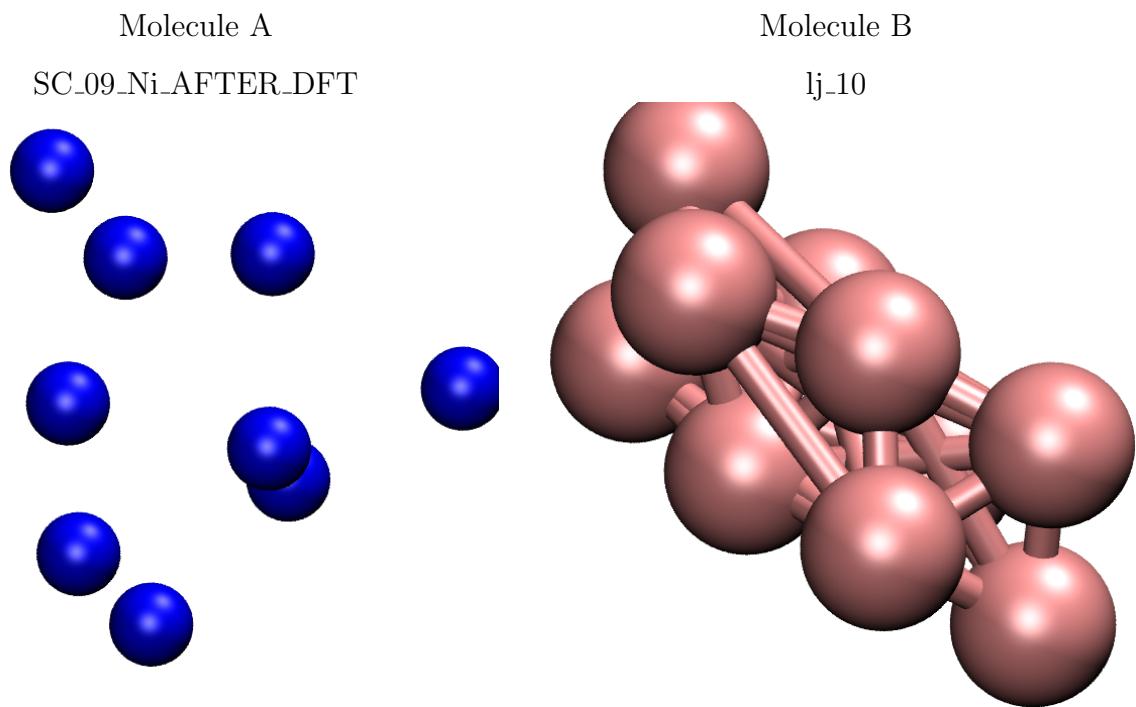
EigenValues - Molecule B

820.373	2113.69	2205.28
---------	---------	---------

Different



ClustersNi Número 172

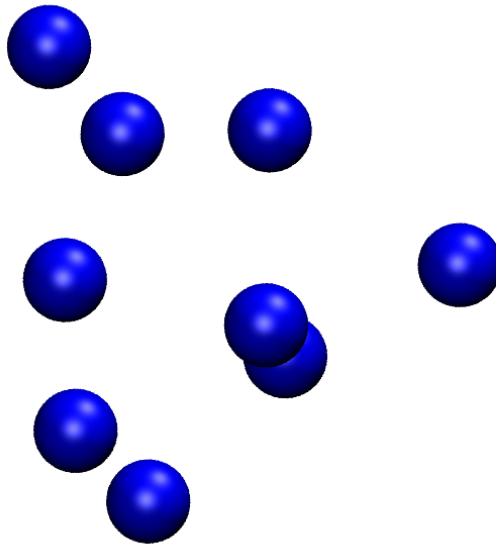


Different

ClustersNi Número 173

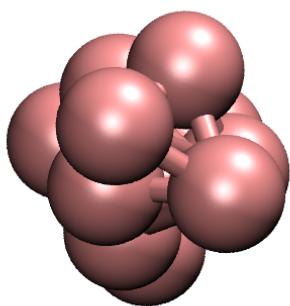
Molecule A

SC\_09\_Ni\_AFTER\_DFT



Molecule B

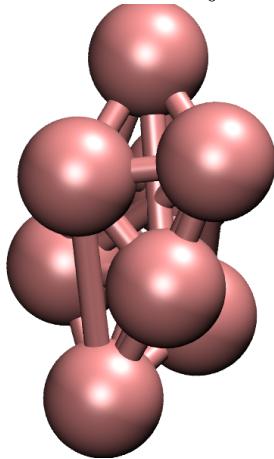
lj\_11



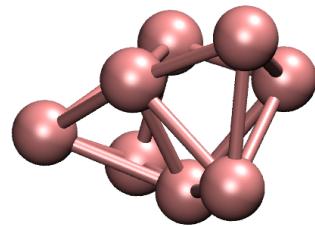
Different

# ClustersNi Número 174

Molecule A lj\_08



Molecule B lj\_08\_Ni



Inertia Tensor - Molecule A

261.999	-18.7437	-6.34405
-18.7437	120.16	-48.8007
-6.34405	-48.8007	248.357

Inertia Tensor - Molecule B

938.857	-52.894	-254.175
-52.894	1044.27	-104.28
-254.175	-104.28	556.076

EingenVectors - Molecule A

-0.122187	-0.940431	-0.31727
-0.991225	0.131869	-0.00913745
0.0504311	0.313369	-0.948291

EingenVectors - Molecule B

0.439206	0.180689	0.880028
-0.598991	-0.671163	0.43675
-0.669558	0.718952	0.186547

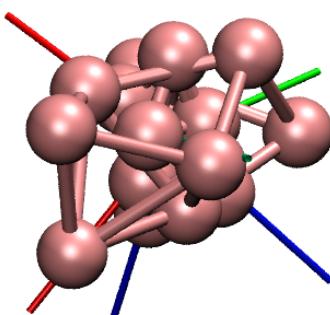
EingenValues - Molecule A

101.261	264.434	264.82
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EingenValues - Molecule B

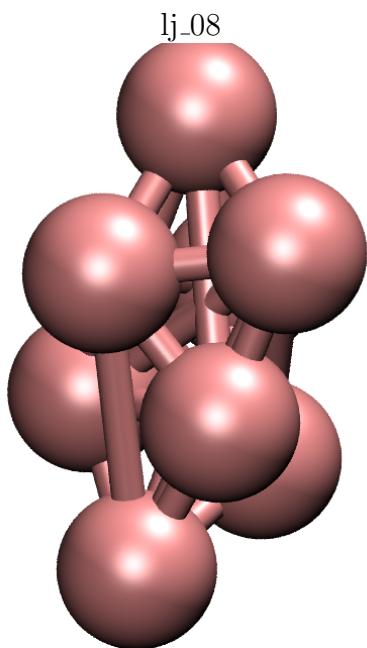
407.811	1064.92	1066.47
---------	---------	---------

Different

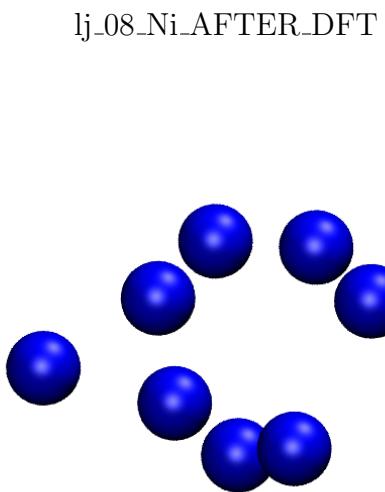


ClustersNi Número 175

Molecule A



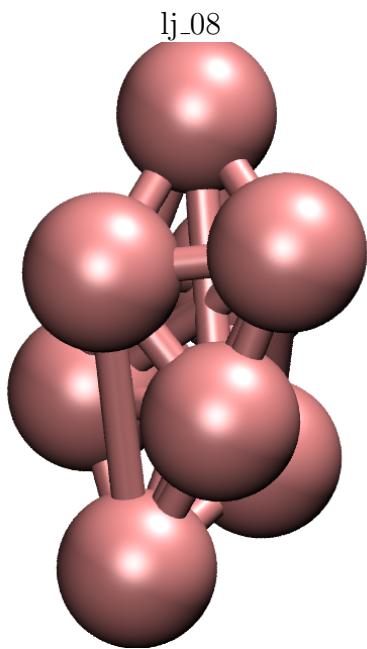
Molecule B



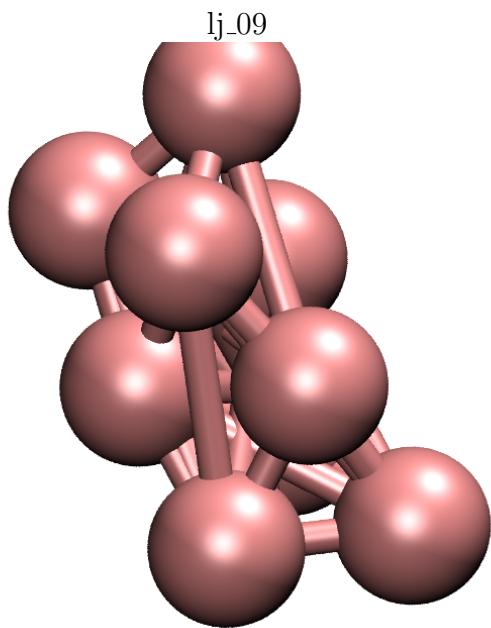
Different

ClustersNi Número 176

Molecule A



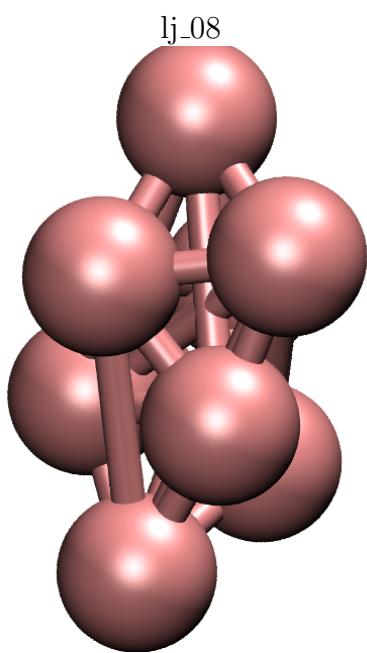
Molecule B



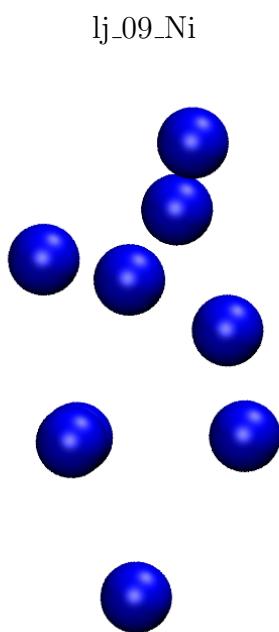
Different

ClustersNi Número 177

Molecule A



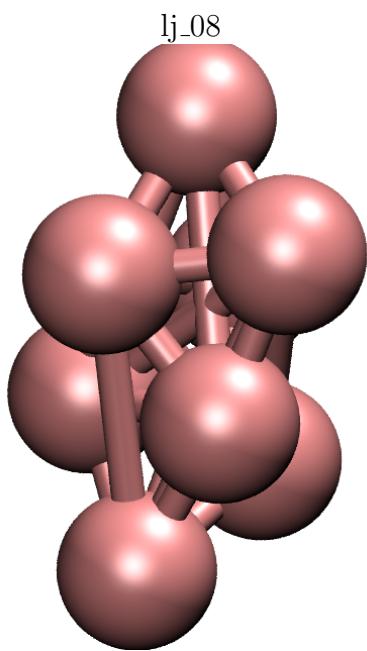
Molecule B



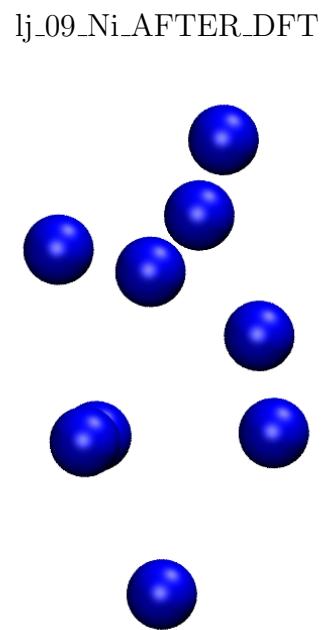
Different

ClustersNi Número 178

Molecule A



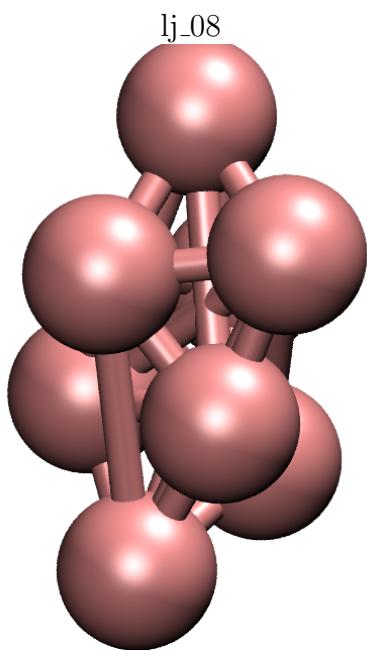
Molecule B



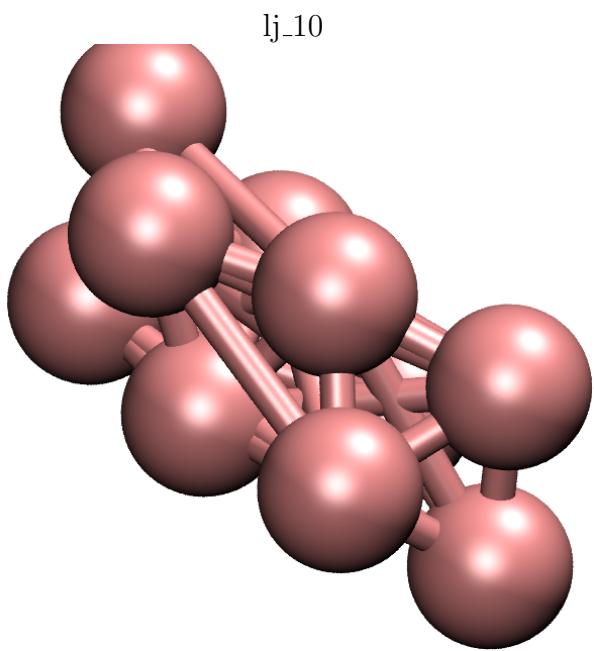
Different

ClustersNi Número 179

Molecule A



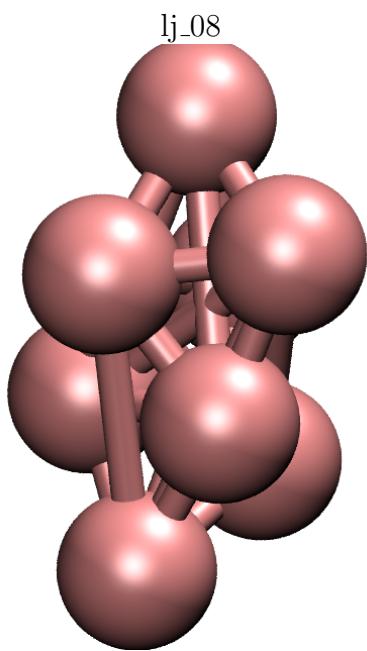
Molecule B



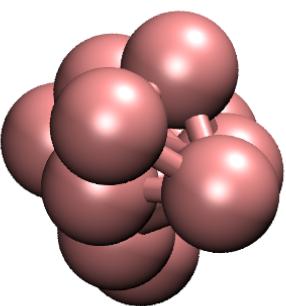
Different

ClustersNi Número 180

Molecule A



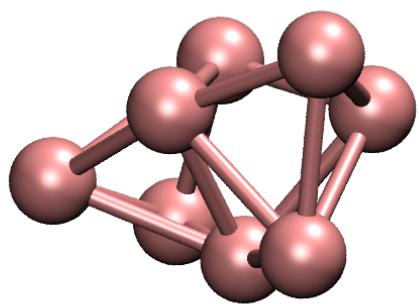
Molecule B



Different

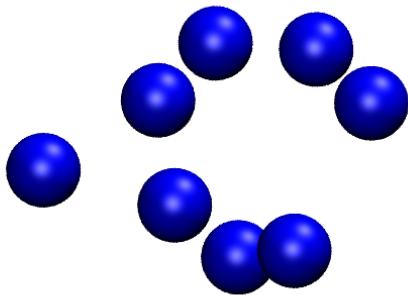
ClustersNi Número 181

Molecule A



Molecule B

lj\_08\_Ni\_AFTER\_DFT

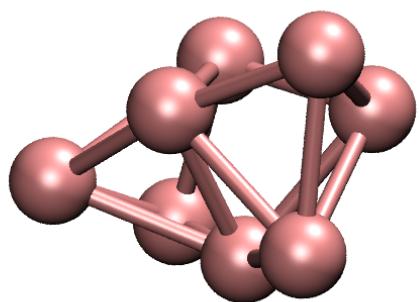


Different

ClustersNi Número 182

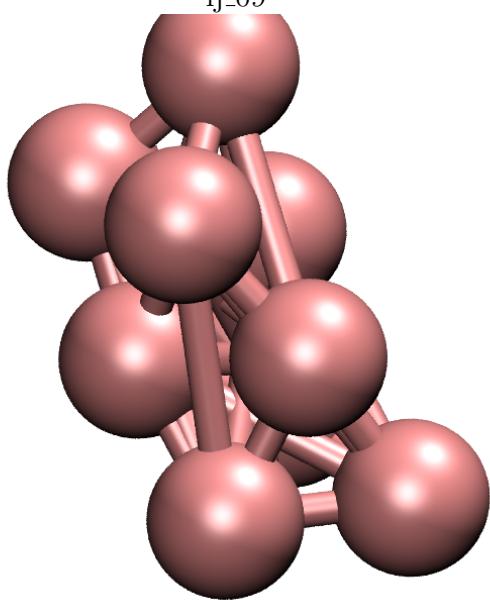
Molecule A

lj\_08\_Ni



Molecule B

lj\_09

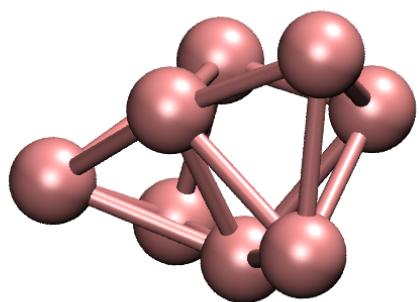


Different

ClustersNi Número 183

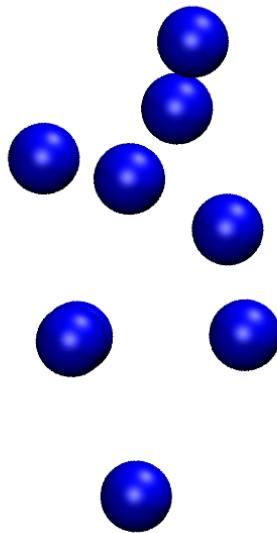
Molecule A

lj\_08\_Ni



Molecule B

lj\_09\_Ni

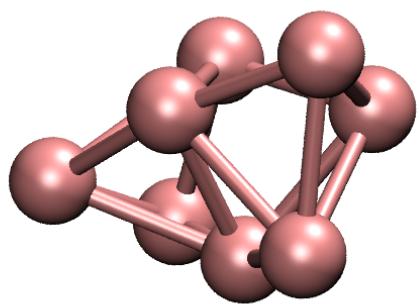


Different

ClustersNi Número 184

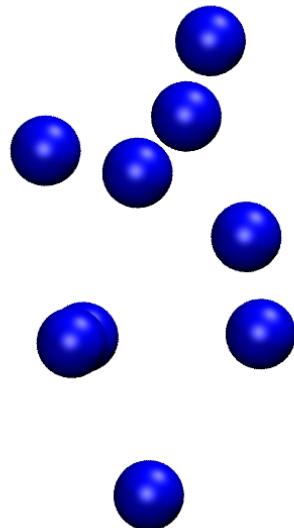
Molecule A

lj\_08\_Ni



Molecule B

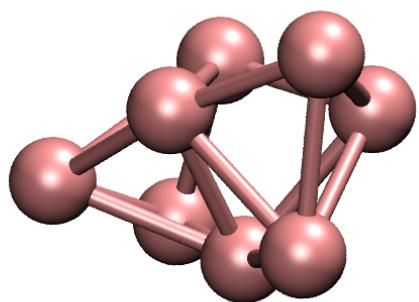
lj\_09\_Ni\_AFTER\_DFT



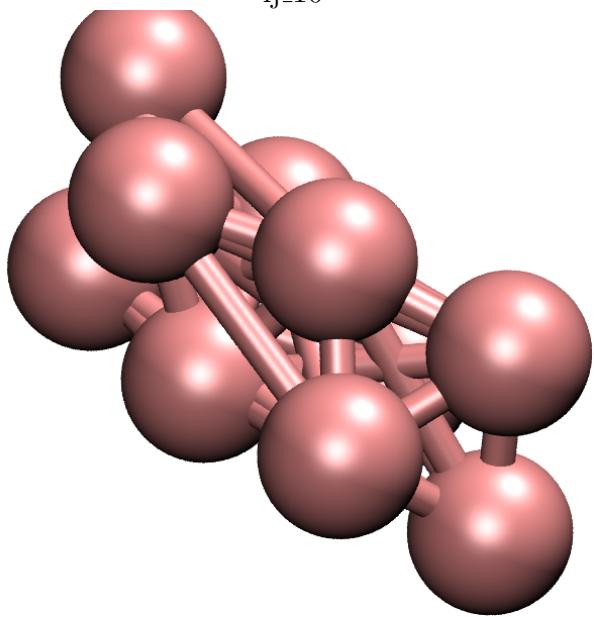
Different

ClustersNi Número 185

Molecule A



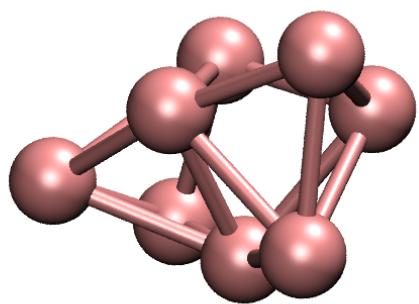
Molecule B



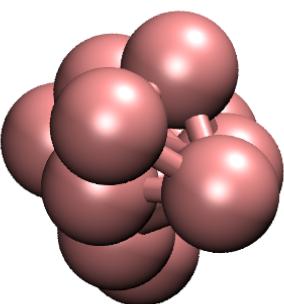
Different

ClustersNi Número 186

Molecule A



Molecule B

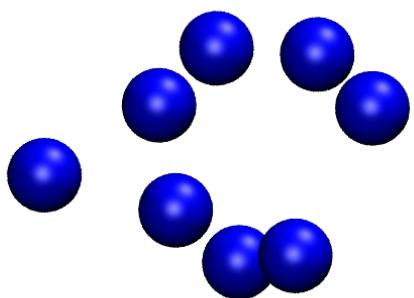


Different

ClustersNi Número 187

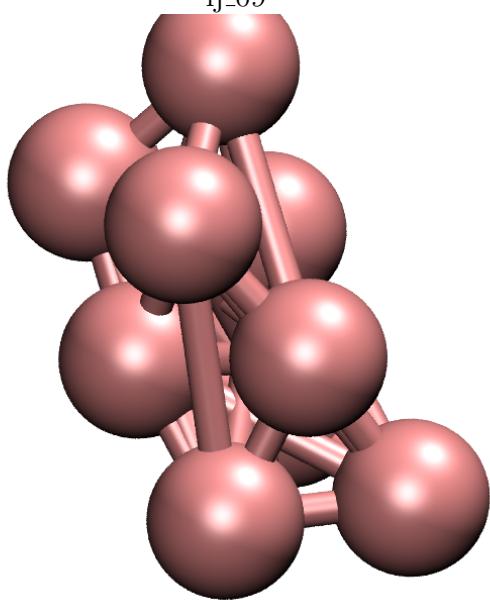
Molecule A

lj\_08\_Ni\_AFTER\_DFT



Molecule B

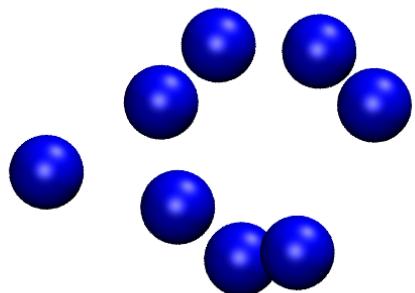
lj\_09



Different

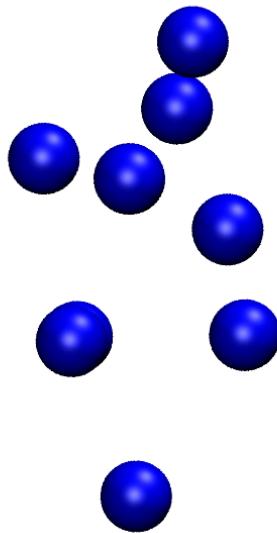
ClustersNi Número 188

Molecule A



Molecule B

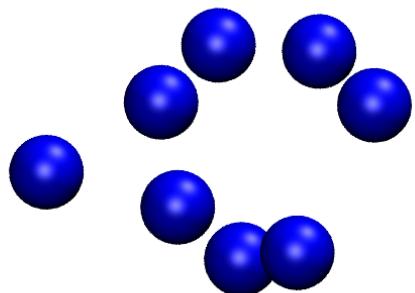
lj\_09\_Ni



Different

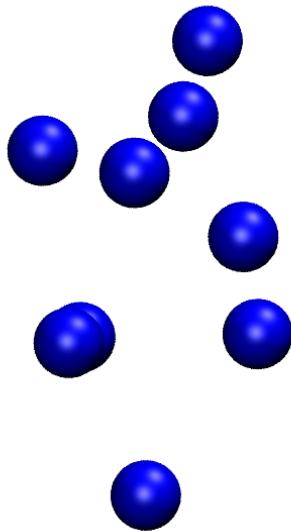
ClustersNi Número 189

Molecule A



Molecule B

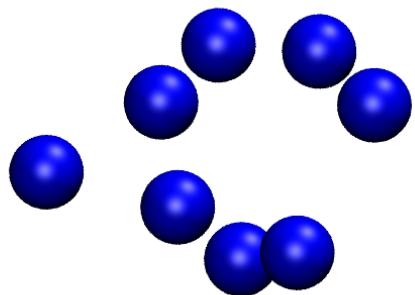
lj\_09\_Ni\_AFTER\_DFT



Different

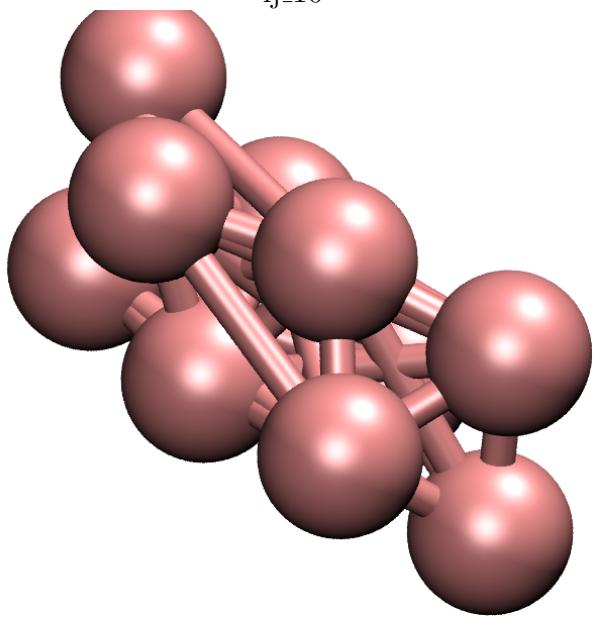
ClustersNi Número 190

Molecule A



Molecule B

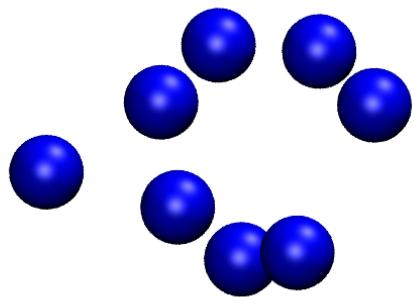
lj\_10



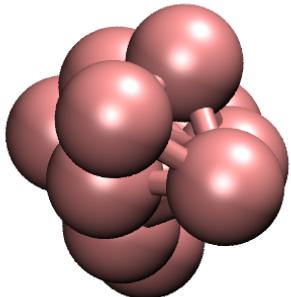
Different

ClustersNi Número 191

Molecule A



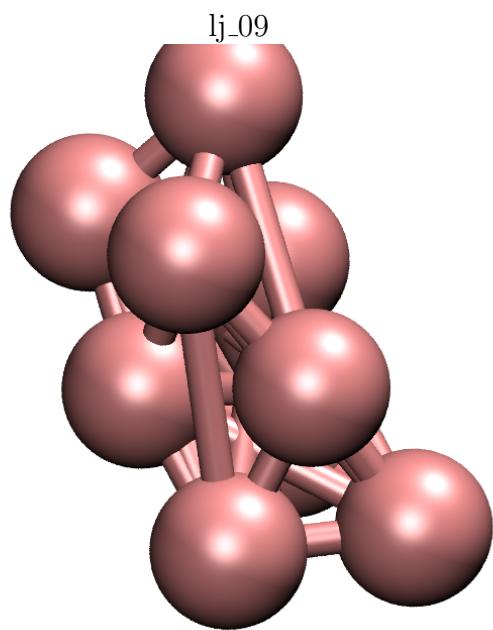
Molecule B



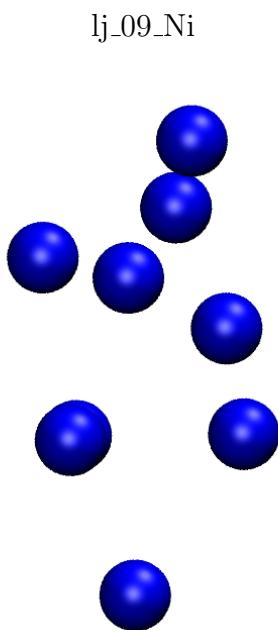
Different

ClustersNi Número 192

Molecule A



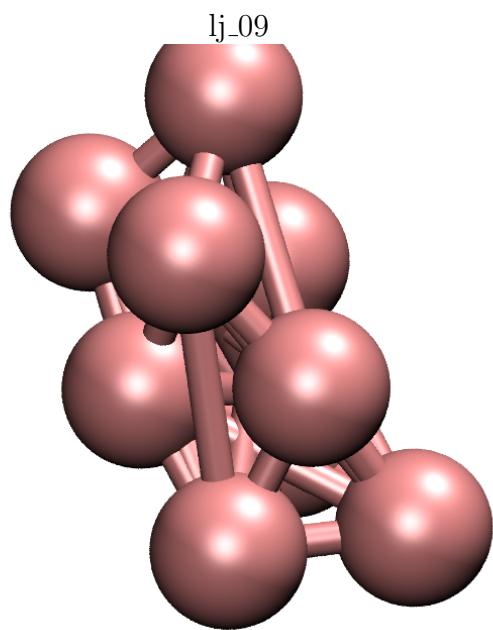
Molecule B



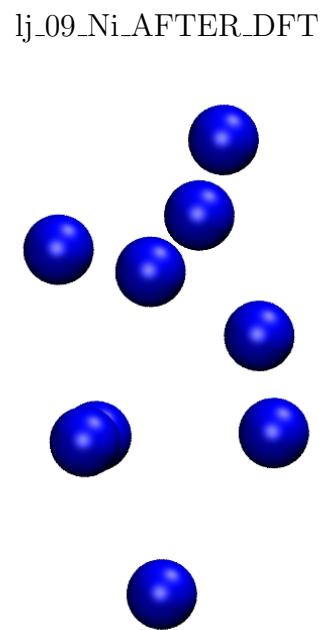
Different

ClustersNi Número 193

Molecule A



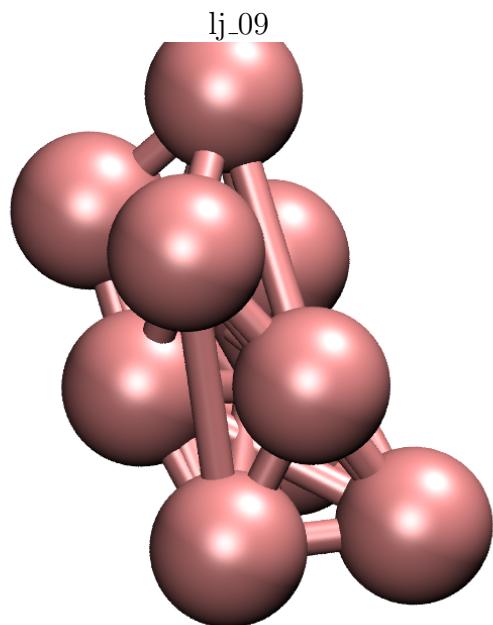
Molecule B



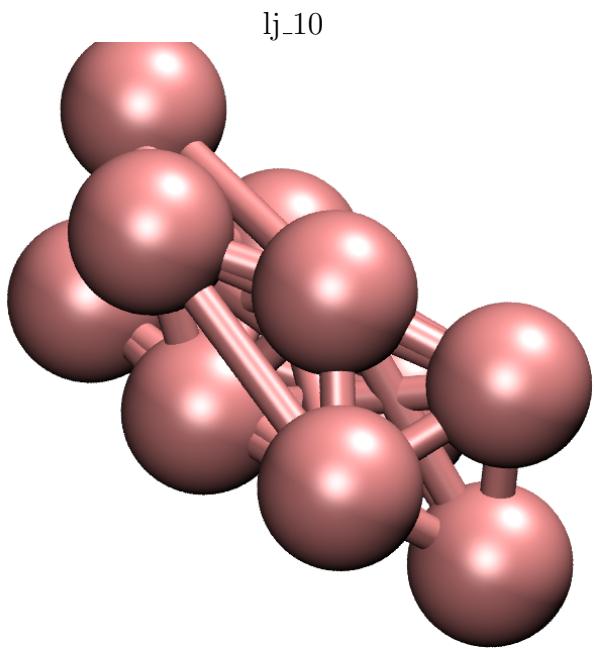
Different

ClustersNi Número 194

Molecule A



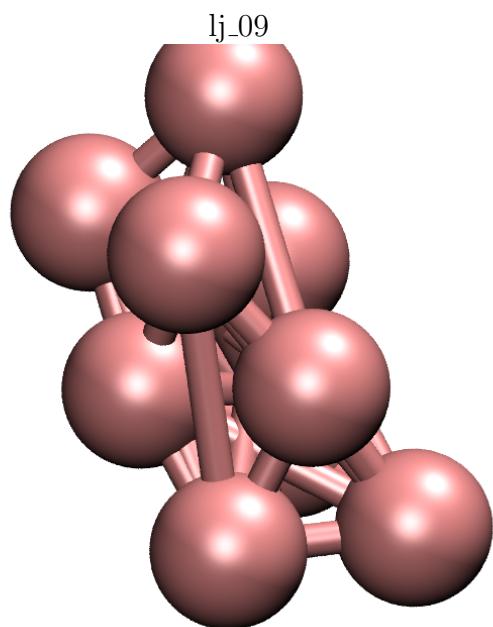
Molecule B



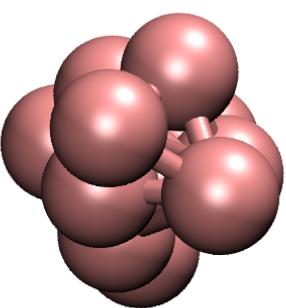
Different

ClustersNi Número 195

Molecule A



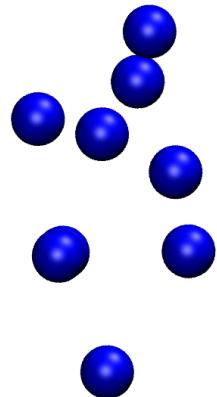
Molecule B



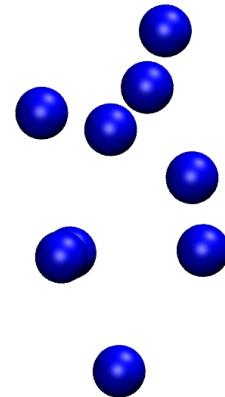
Different

# ClustersNi Número 196

Molecule A lj\_09\_Ni



Molecule B lj\_09\_Ni\_AFTER\_DFT



Inertia Tensor - Molecule A

2099.87	-92.0868	87.5491
-92.0868	1185.59	628.538
87.5491	628.538	1533.16

Inertia Tensor - Molecule B

2192.28	-89.3917	85.1517
-89.3917	1303.55	619.274
85.1517	619.274	1643.51

EingenVectors - Molecule A

-0.0896058	-0.791993	0.603919
0.134366	-0.610428	-0.780592
-0.986872	-0.0112006	-0.161115

EingenVectors - Molecule B

-0.0891023	-0.791474	0.604673
0.147893	-0.610872	-0.777794
-0.984981	-0.0201236	-0.171483

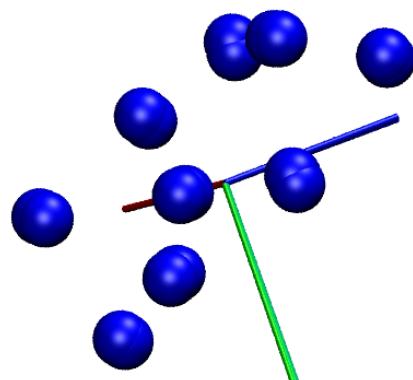
EingenValues - Molecule A

695.893	2009.61	2113.12
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EingenValues - Molecule B

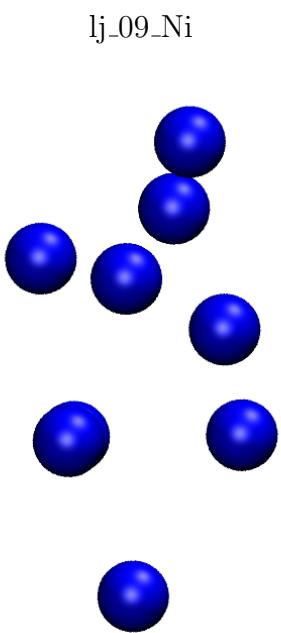
820.373	2113.69	2205.28
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Different



ClustersNi Número 197

Molecule A



Molecule B

lj\_10

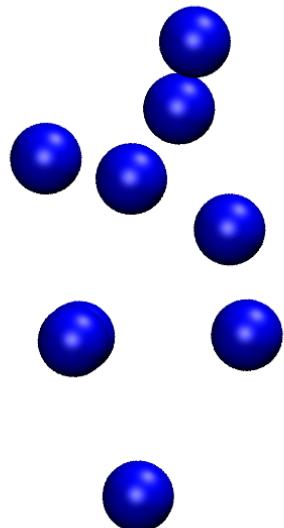
A 3D ball-and-stick model of a branched molecule. It consists of ten red spheres connected by multiple lines, forming a complex branched structure. This represents a more complex Ni cluster than Molecule A.

Different

ClustersNi Número 198

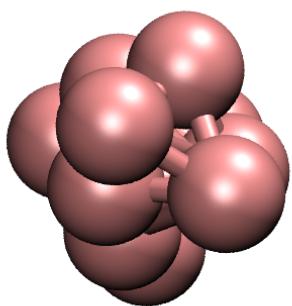
Molecule A

lj\_09\_Ni



Molecule B

lj\_11

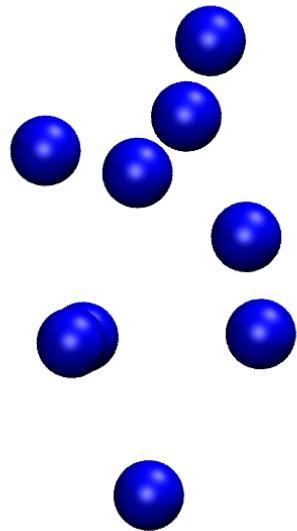


Different

ClustersNi Número 199

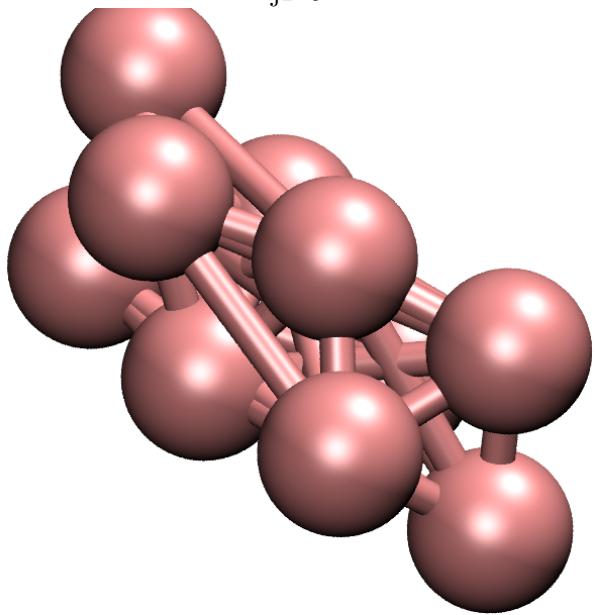
Molecule A

lj\_09\_Ni\_AFTER\_DFT



Molecule B

lj\_10

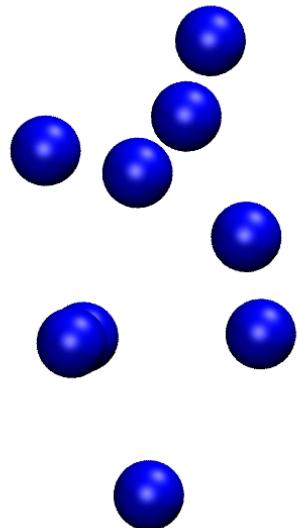


Different

ClustersNi Número 200

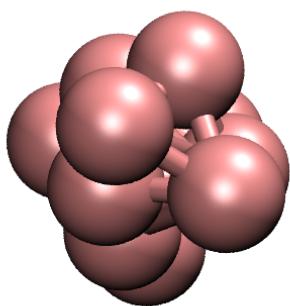
Molecule A

lj\_09\_Ni\_AFTER\_DFT



Molecule B

lj\_11

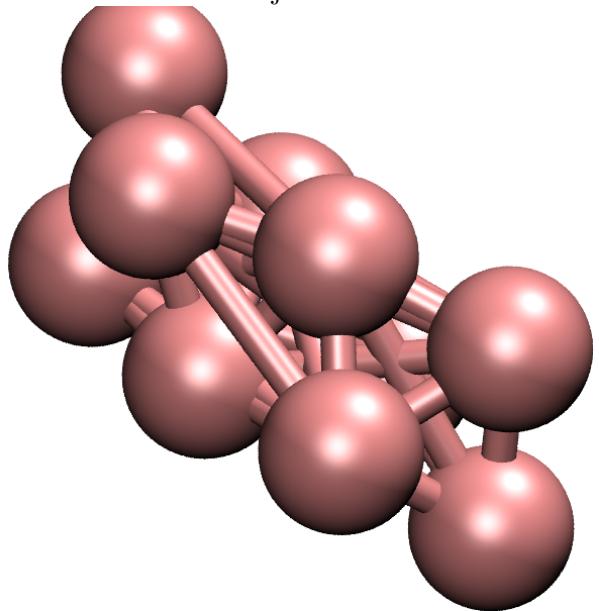


Different

ClustersNi Número 201

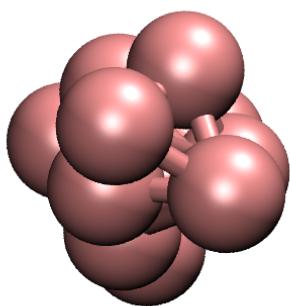
Molecule A

lj\_10



Molecule B

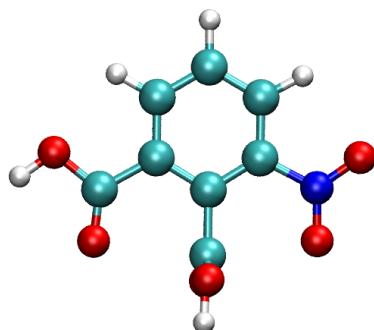
lj\_11



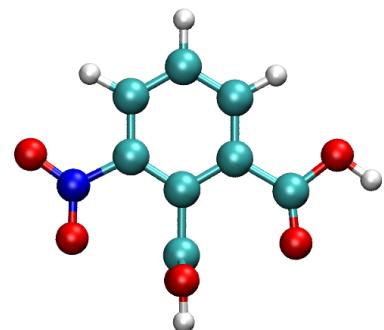
Different

FireTest Número 202

Molecule A 3NFAACa



Molecule B 3NFAACb



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

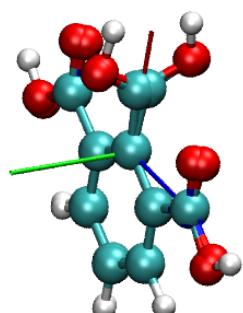
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

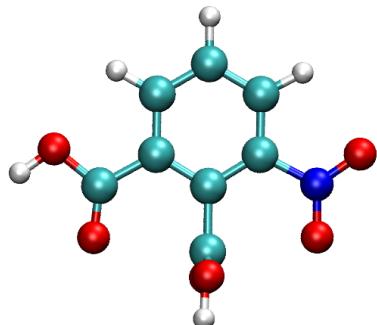
530.103	915.738	1361.08
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Equal

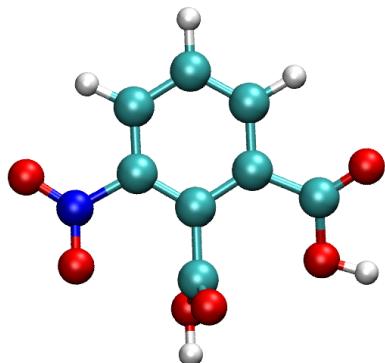


FireTest Número 203

Molecule A 3NFAACa



Molecule B 3NFAACCc



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

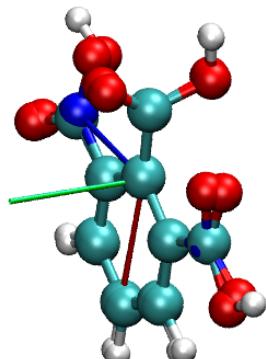
EingenValues - Molecule A

530.124	915.807	1361.14
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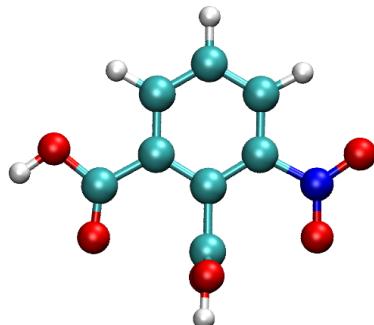
EingenValues - Molecule B

531.402	913.293	1353.16
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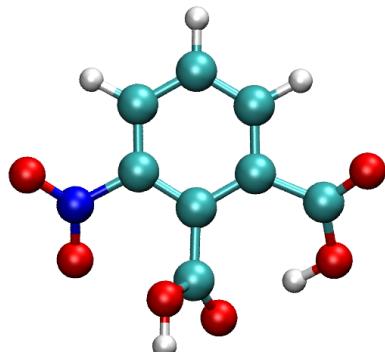
Different



Molecule A 3NFAACa



Molecule B 3NFAACd



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

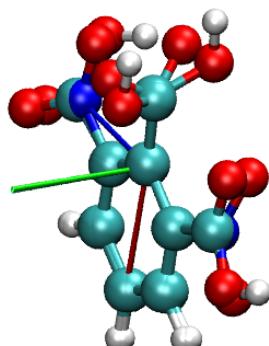
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

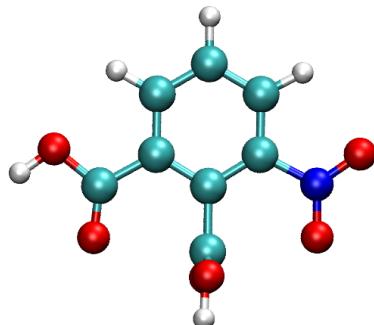
524.175	935.342	1359.19
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Different

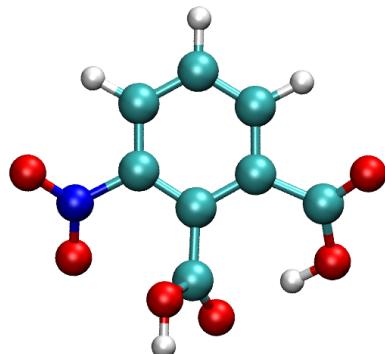


FireTest Número 205

Molecule A 3NFAACa



Molecule B 3NFAACe



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

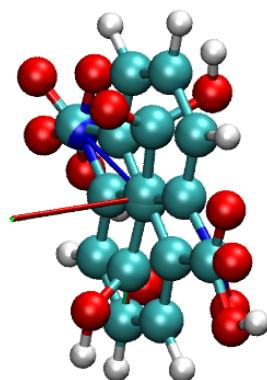
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

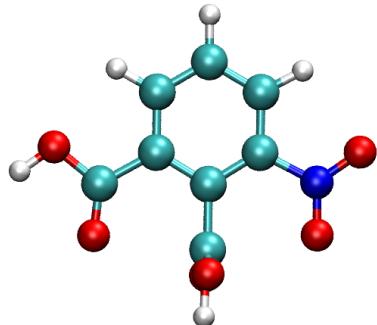
524.162	935.308	1359.22
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Different

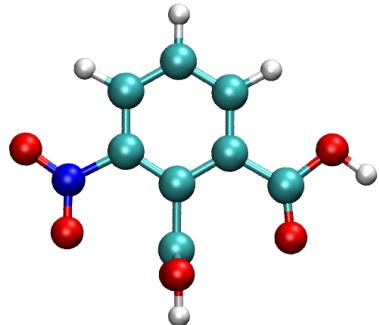


FireTest Número 206

Molecule A 3NFAACa



Molecule B 3NFAACf



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

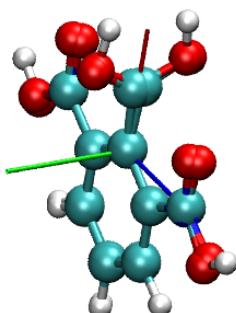
EingenValues - Molecule A

530.124	915.807	1361.14
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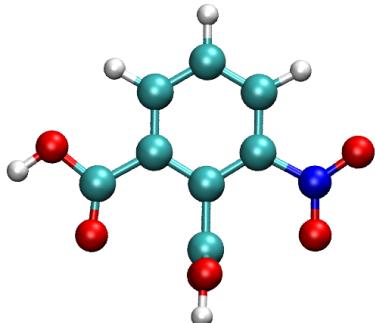
EingenValues - Molecule B

530.045	915.527	1360.79
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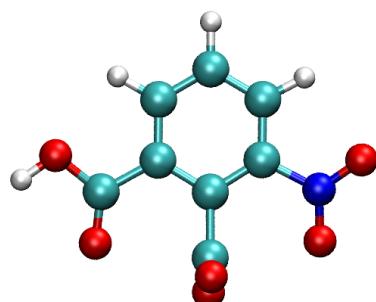
Equal



Molecule A 3NFAACa



Molecule B 3NFAACg



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

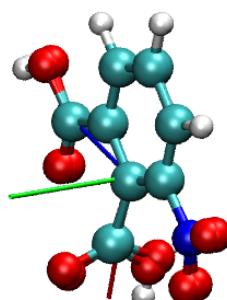
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

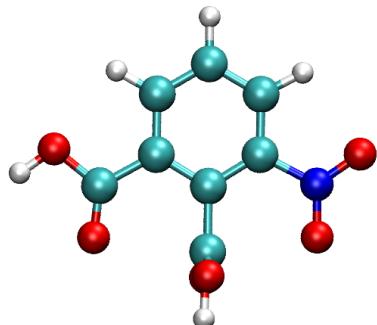
532.89	918.442	1356.93
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Different

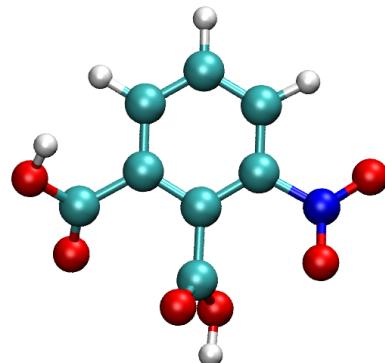


FireTest Número 208

Molecule A 3NFAACa



Molecule B 3NFAACh



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

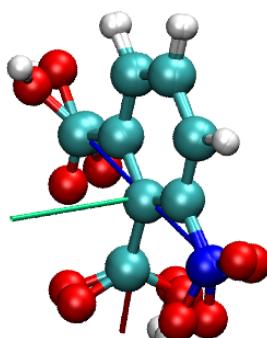
EingenValues - Molecule A

530.124	915.807	1361.14
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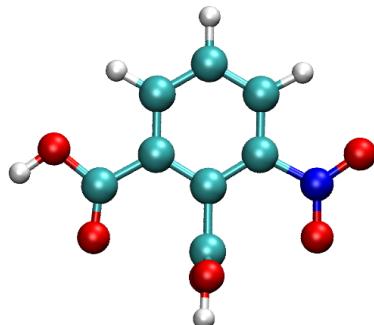
EingenValues - Molecule B

528.663	924.928	1336.12
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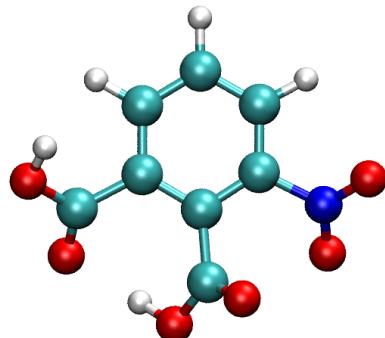
Different



Molecule A 3NFAACa



Molecule B 3NFAACi



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

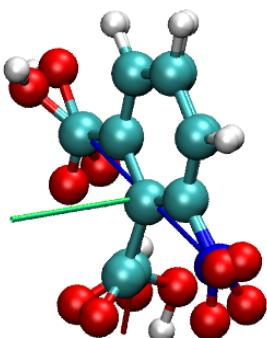
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

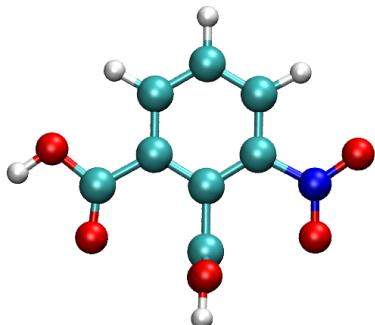
521.475	949.659	1346.18
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Different

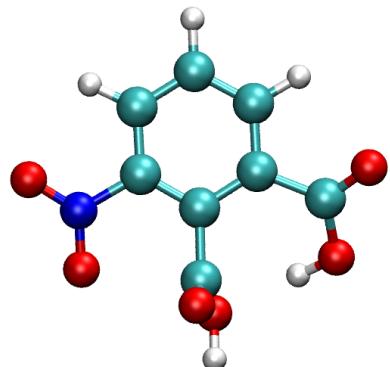


FireTest Número 210

Molecule A 3NFAACa



Molecule B 3NFAACj



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EigenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EigenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

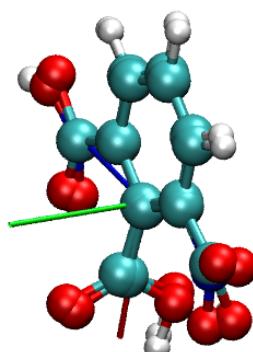
EigenValues - Molecule A

530.124	915.807	1361.14
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EigenValues - Molecule B

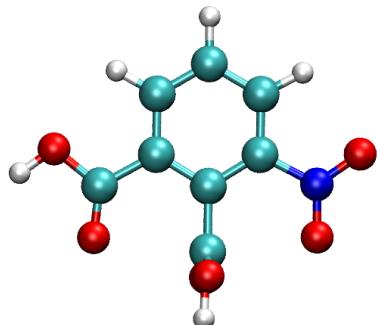
533.726	920.137	1348.3
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Different

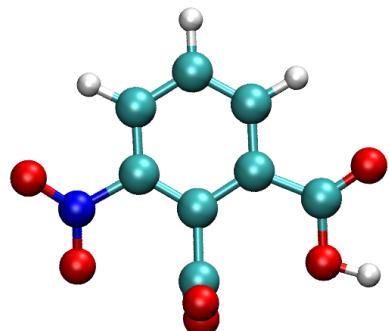


FireTest Número 211

Molecule A 3NFAACa



Molecule B 3NFAACK



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

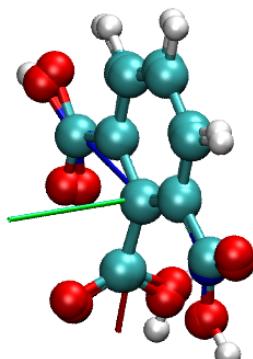
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

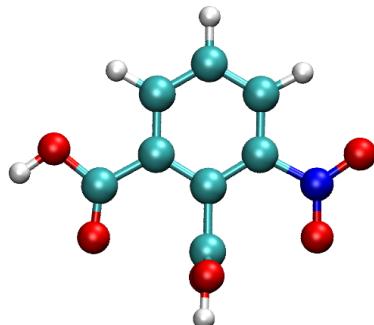
534.81	913.339	1353.78
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Different

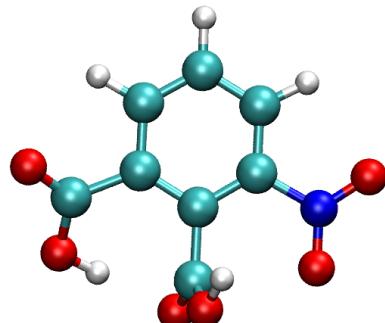


FireTest Número 212

Molecule A 3NFAACa



Molecule B 3NFAACl



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

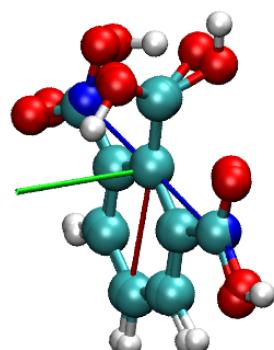
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

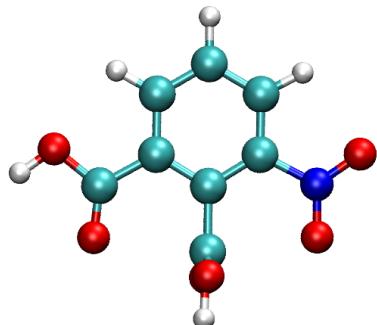
531.691	929.434	1355.4
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Different

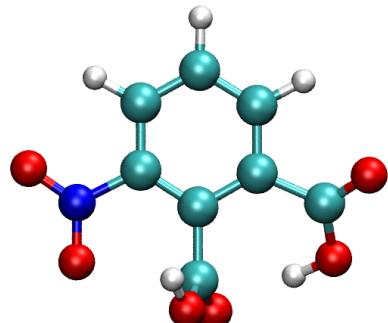


FireTest Número 213

Molecule A 3NFAACa



Molecule B 3NFAACm



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

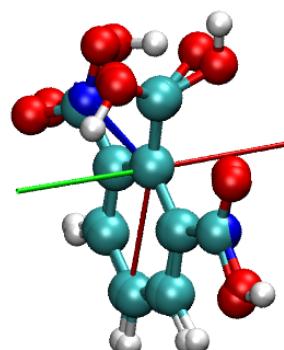
EingenValues - Molecule A

530.124	915.807	1361.14
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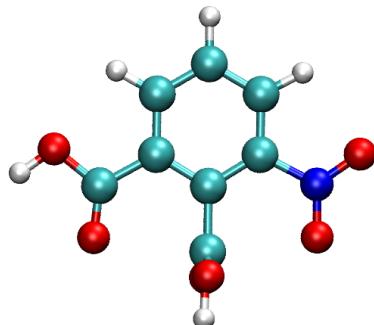
EingenValues - Molecule B

531.698	929.417	1355.4
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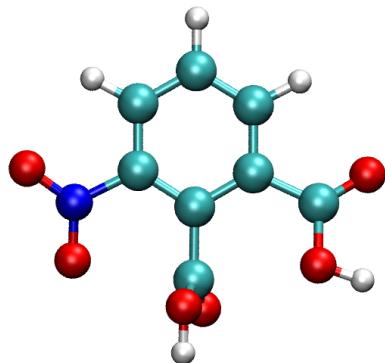
Different



Molecule A 3NFAACa



Molecule B 3NFAACn



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

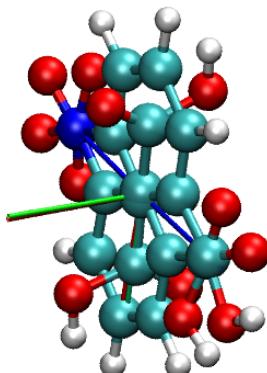
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

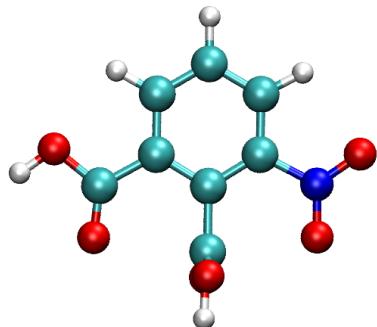
531.43	913.309	1353.35
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Different

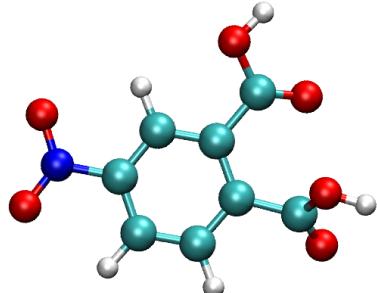


FireTest Número 215

Molecule A 3NFAACa



Molecule B 4NFAACa



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

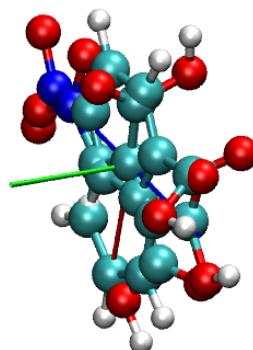
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

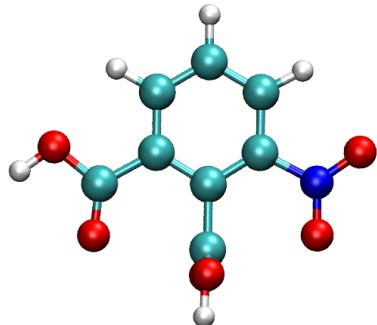
479.363	1242.41	1647.39
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Different

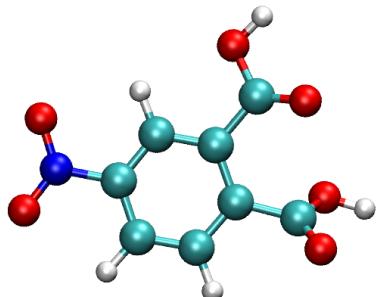


FireTest Número 216

Molecule A 3NFAACa



Molecule B 4NFAACb



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

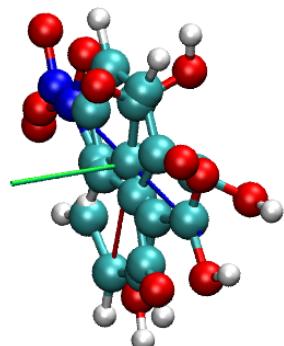
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

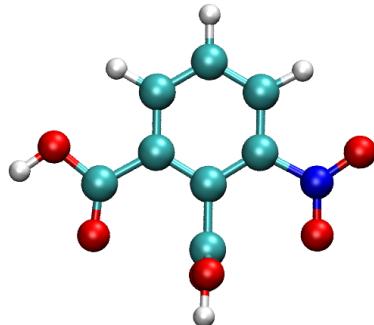
479.308	1242.41	1647.31
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Different

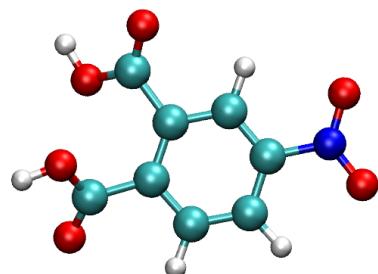


FireTest Número 217

Molecule A 3NFAACa



Molecule B 4NFAACCc



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

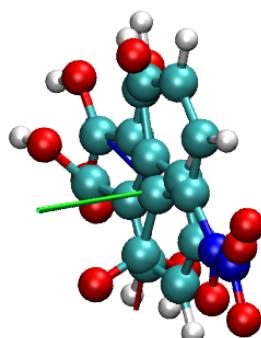
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

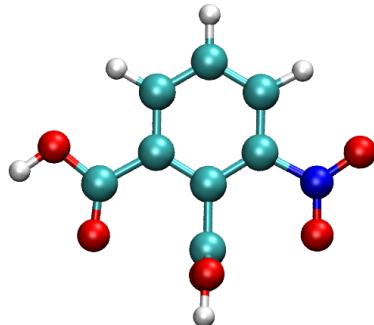
482.027	1240.32	1647.08
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Different

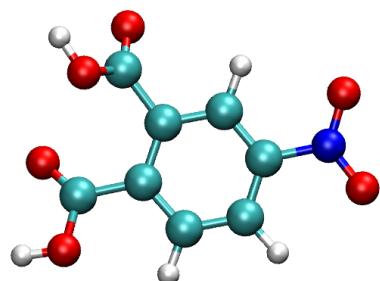


FireTest Número 218

Molecule A 3NFAACa



Molecule B 4NFAACd



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

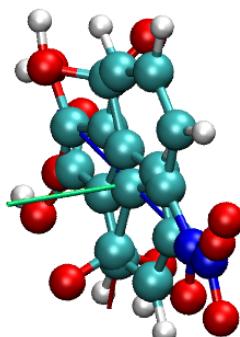
EingenValues - Molecule A

530.124	915.807	1361.14
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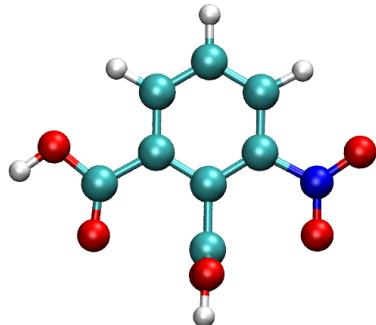
EingenValues - Molecule B

491.663	1231.14	1650.13
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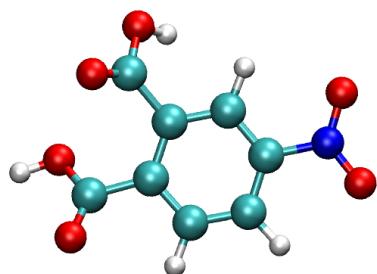
Different



Molecule A 3NFAACa



Molecule B 4NFAACe



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

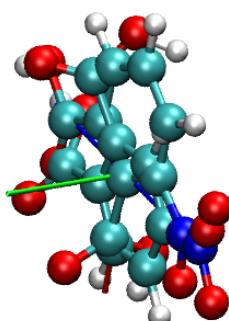
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

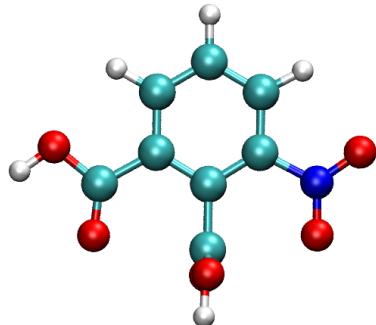
489.011	1233.7	1641.81
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Different

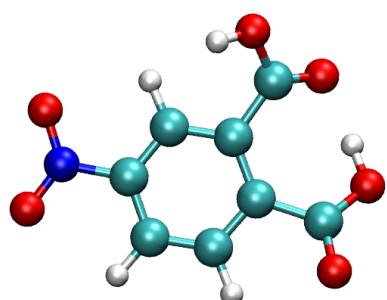


FireTest Número 220

Molecule A 3NFAACa



Molecule B 4NFAACf



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

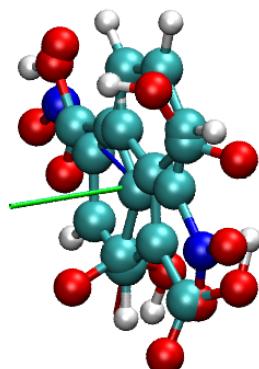
EingenValues - Molecule A

530.124	915.807	1361.14
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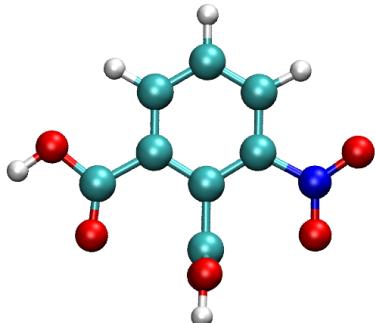
EingenValues - Molecule B

509.668	1219.11	1681.18
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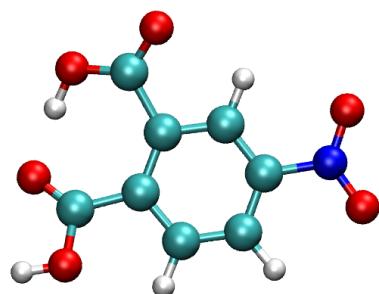
Different



Molecule A 3NFAACa



Molecule B 4NFAACg



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

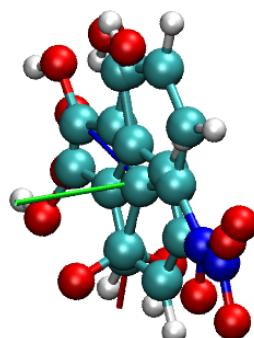
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

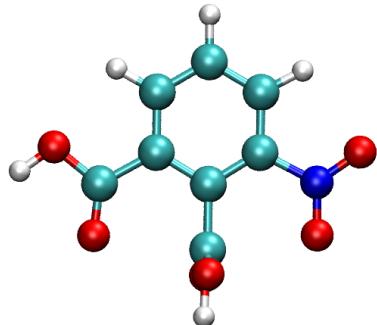
513.751	1208.07	1700.9
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Different

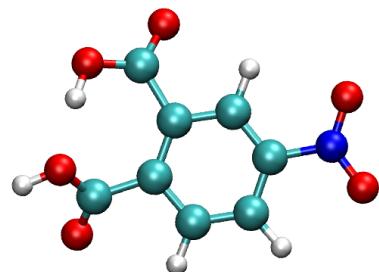


FireTest Número 222

Molecule A 3NFAACa



Molecule B 4NFAACi



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

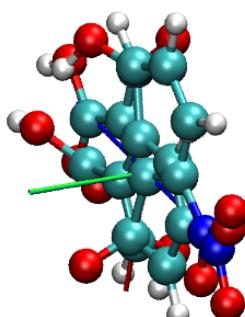
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

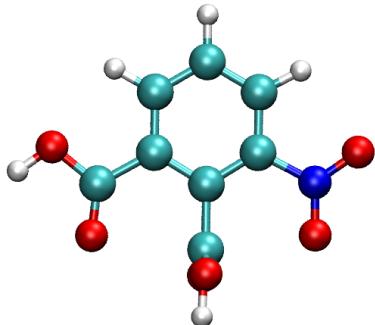
502.409	1232.26	1676.02
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Different

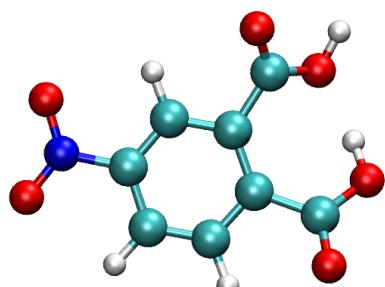


FireTest Número 223

Molecule A 3NFAACa



Molecule B 4NFAACj



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

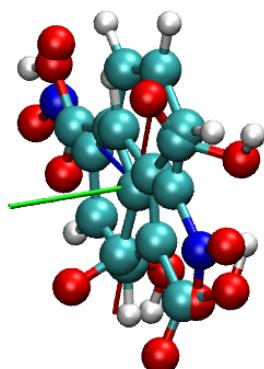
EingenValues - Molecule A

530.124	915.807	1361.14
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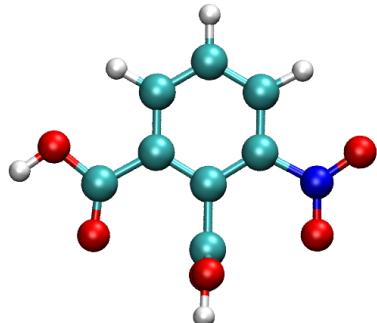
EingenValues - Molecule B

509.897	1225.65	1680.83
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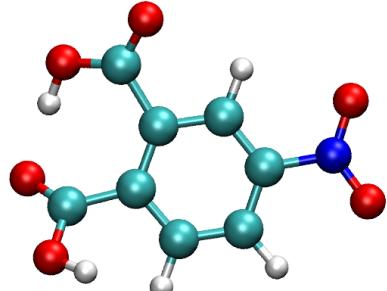
Different



Molecule A 3NFAACa



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

530.125	-0.358211	-0.0456723
-0.358211	915.82	2.40736
-0.0456723	2.40736	1361.13

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-1	-0.000928415	-5.22706e-05
0.000928119	-0.999985	0.00540587
-5.72887e-05	0.00540582	0.999985

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

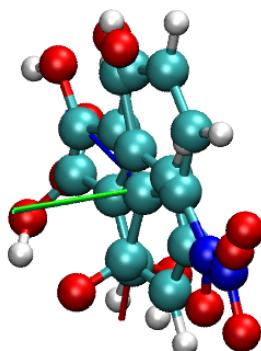
EingenValues - Molecule A

530.124	915.807	1361.14
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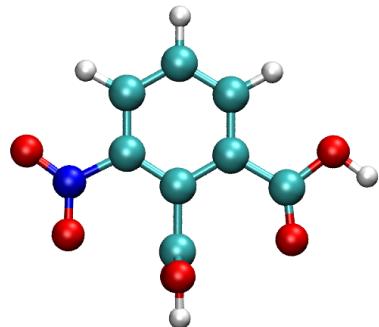
EingenValues - Molecule B

506.607	1222.36	1678.43
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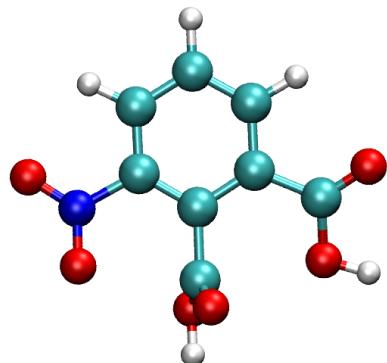
Different



Molecule A 3NFAACb



Molecule B 3NFAACCc



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

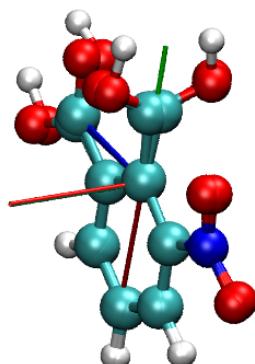
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

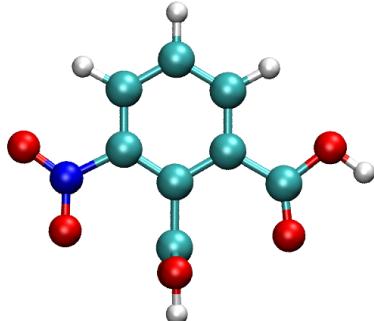
531.402	913.293	1353.16
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Different

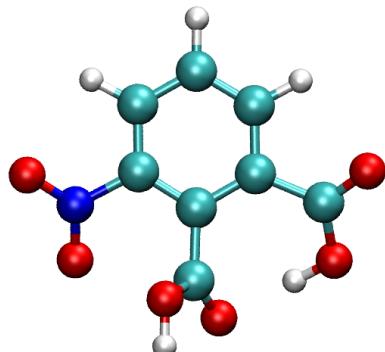


FireTest Número 226

Molecule A 3NFAACb



Molecule B 3NFAACd



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

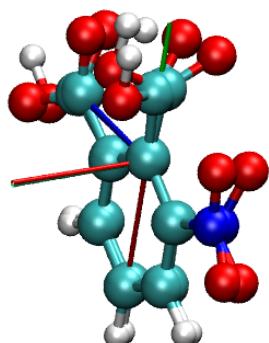
EingenValues - Molecule A

530.103	915.738	1361.08
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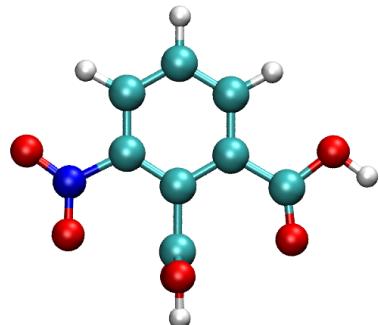
EingenValues - Molecule B

524.175	935.342	1359.19
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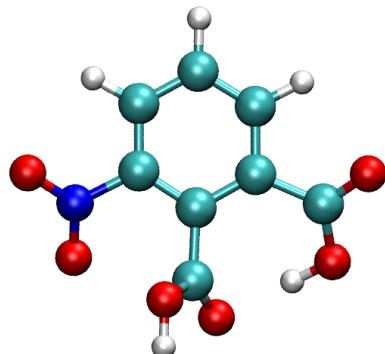
Different



Molecule A 3NFAACb



Molecule B 3NFAACe



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

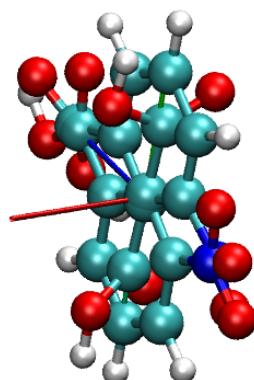
EingenValues - Molecule A

530.103	915.738	1361.08
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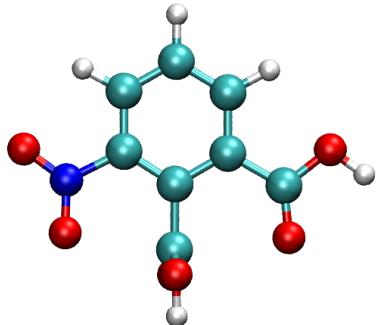
EingenValues - Molecule B

524.162	935.308	1359.22
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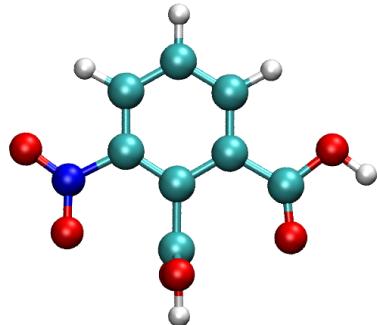
Different



Molecule A 3NFAACb



Molecule B 3NFAACf



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

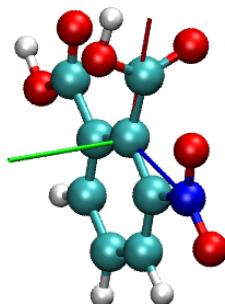
EingenValues - Molecule A

530.103	915.738	1361.08
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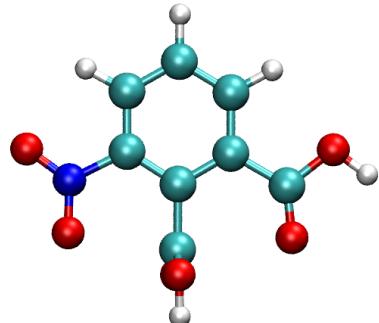
EingenValues - Molecule B

530.045	915.527	1360.79
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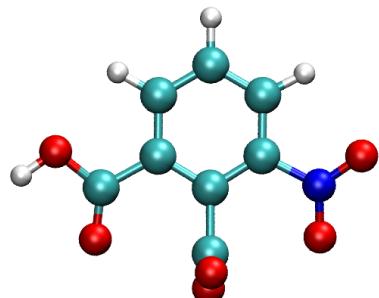
Enantiomers



Molecule A 3NFAACb



Molecule B 3NFAACg



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

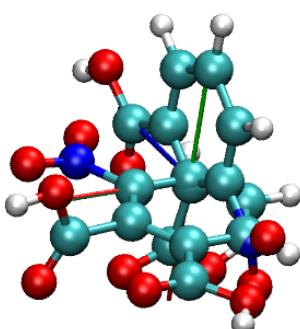
EingenValues - Molecule A

530.103	915.738	1361.08
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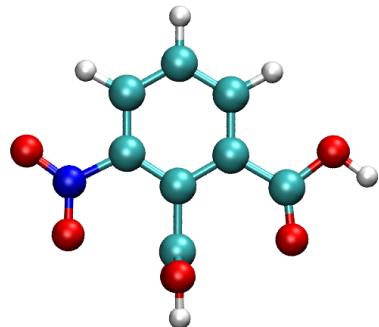
EingenValues - Molecule B

532.89	918.442	1356.93
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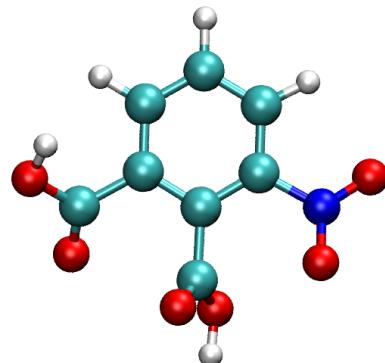
Different



Molecule A 3NFAACb



Molecule B 3NFAACh



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

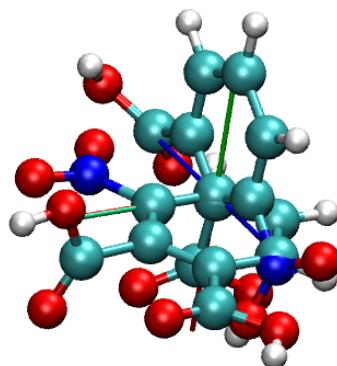
EingenValues - Molecule A

530.103	915.738	1361.08
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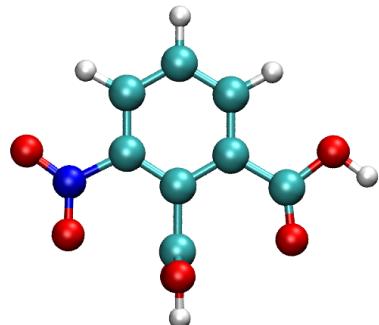
EingenValues - Molecule B

528.663	924.928	1336.12
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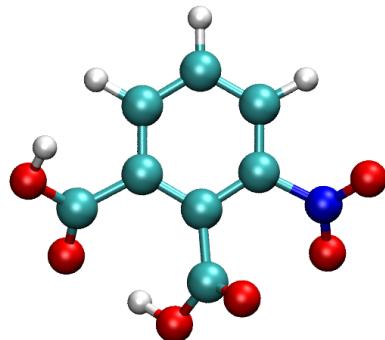
Different



Molecule A 3NFAACb



Molecule B 3NFAACi



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

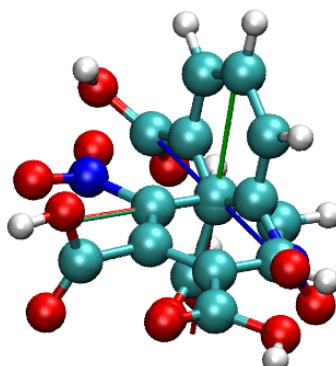
EingenValues - Molecule A

530.103	915.738	1361.08
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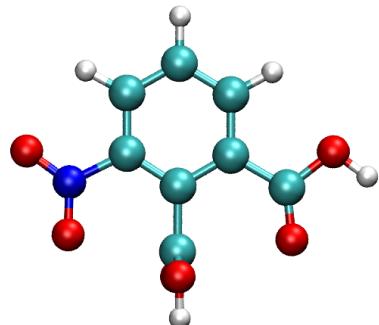
EingenValues - Molecule B

521.475	949.659	1346.18
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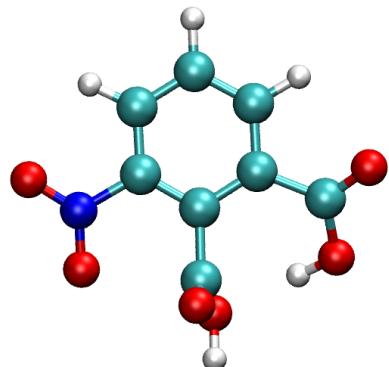
Different



Molecule A 3NFAACb



Molecule B 3NFAACj



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

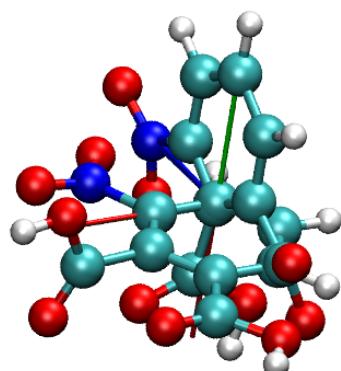
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

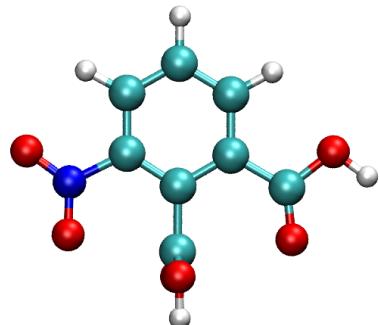
533.726	920.137	1348.3
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Different

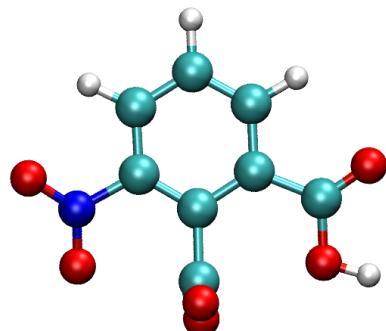


FireTest Número 233

Molecule A 3NFAACb



Molecule B 3NFAACK



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

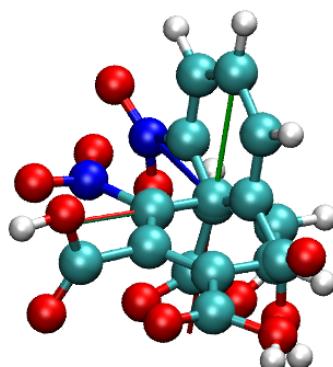
EingenValues - Molecule A

530.103	915.738	1361.08
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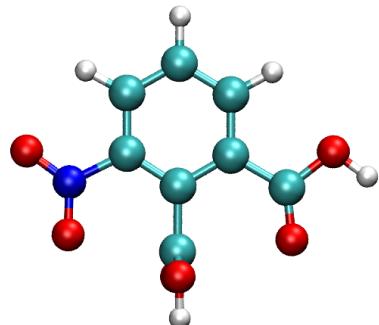
EingenValues - Molecule B

534.81	913.339	1353.78
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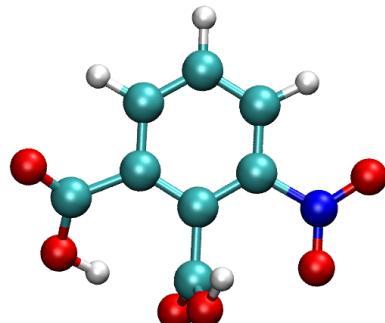
Different



Molecule A 3NFAACb



Molecule B 3NFAACl



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

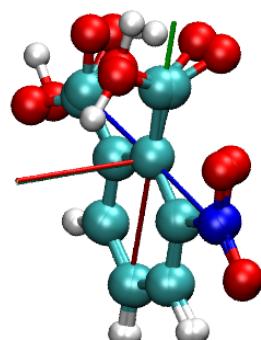
EingenValues - Molecule A

530.103	915.738	1361.08
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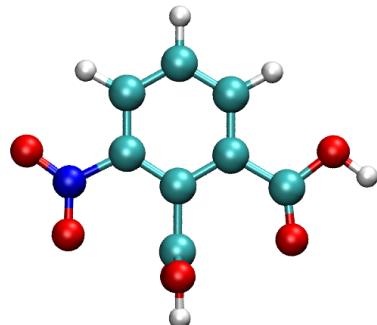
EingenValues - Molecule B

531.691	929.434	1355.4
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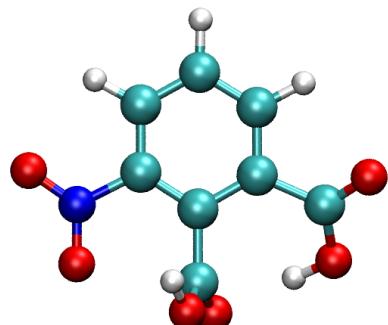
Different



Molecule A 3NFAACb



Molecule B 3NFAACm



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

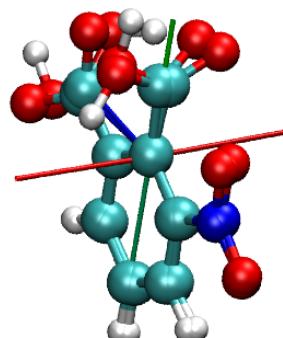
EingenValues - Molecule A

530.103	915.738	1361.08
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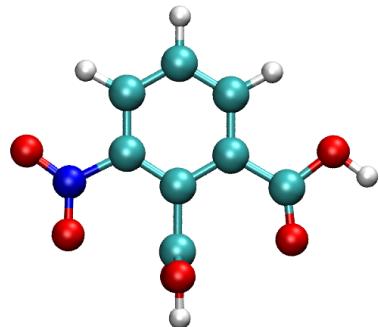
EingenValues - Molecule B

531.698	929.417	1355.4
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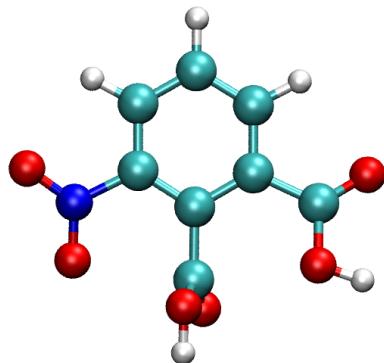
Different



Molecule A 3NFAACb



Molecule B 3NFAACn



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

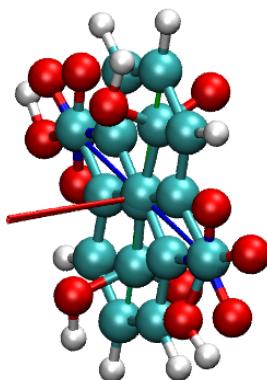
EingenValues - Molecule A

530.103	915.738	1361.08
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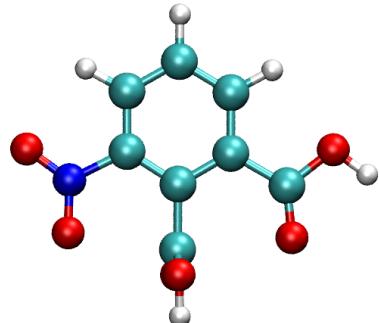
EingenValues - Molecule B

531.43	913.309	1353.35
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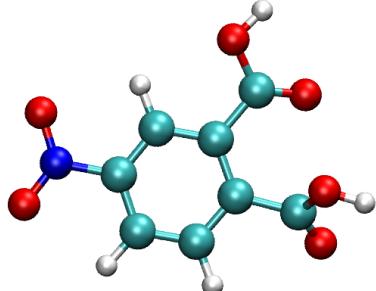
Different



Molecule A 3NFAACb



Molecule B 4NFAACa



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

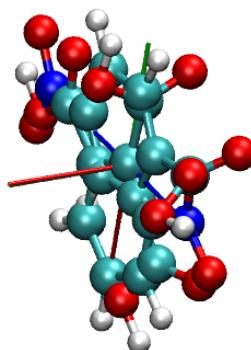
EingenValues - Molecule A

530.103	915.738	1361.08
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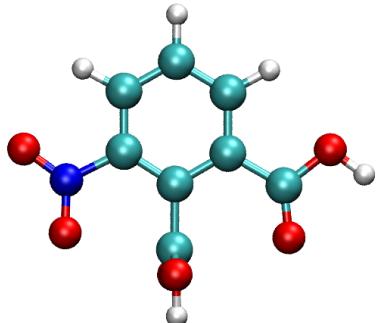
EingenValues - Molecule B

479.363	1242.41	1647.39
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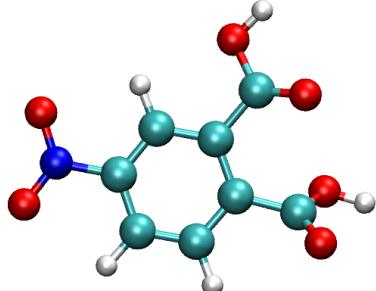
Different



Molecule A 3NFAACb



Molecule B 4NFAACb



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

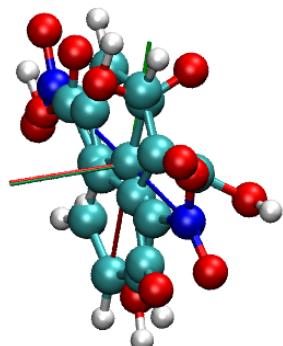
EingenValues - Molecule A

530.103	915.738	1361.08
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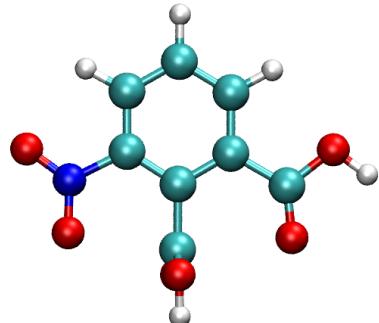
EingenValues - Molecule B

479.308	1242.41	1647.31
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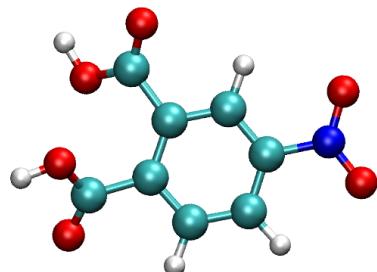
Different



Molecule A 3NFAACb



Molecule B 4NFAACC



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

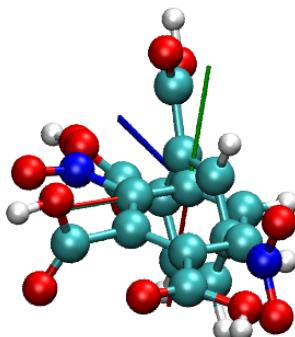
EingenValues - Molecule A

530.103	915.738	1361.08
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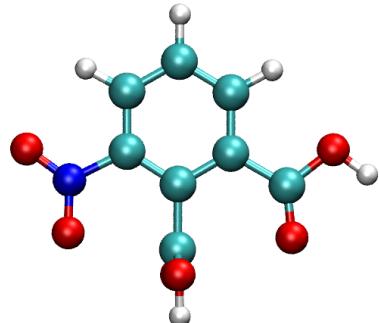
EingenValues - Molecule B

482.027	1240.32	1647.08
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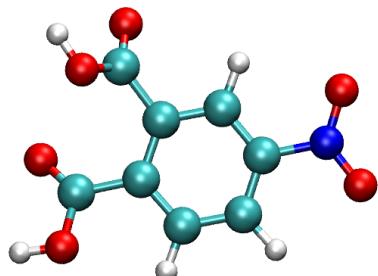
Different



Molecule A 3NFAACb



Molecule B 4NFAACd



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

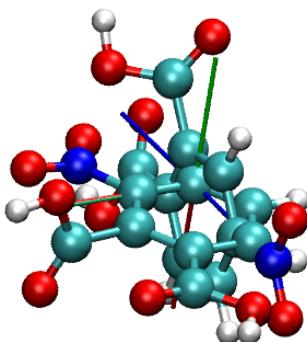
EingenValues - Molecule A

530.103	915.738	1361.08
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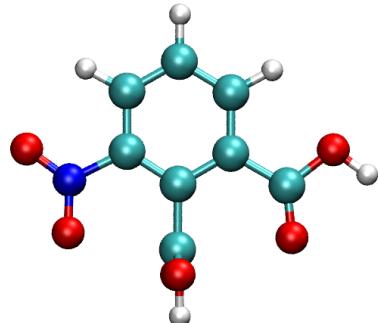
EingenValues - Molecule B

491.663	1231.14	1650.13
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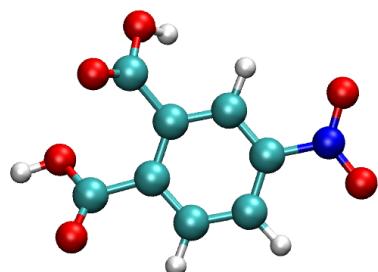
Different



Molecule A 3NFAACb



Molecule B 4NFAACe



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

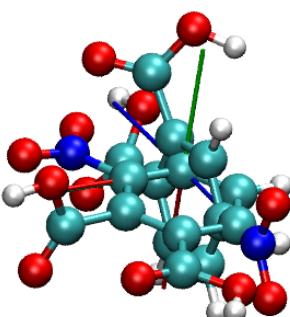
EingenValues - Molecule A

530.103	915.738	1361.08
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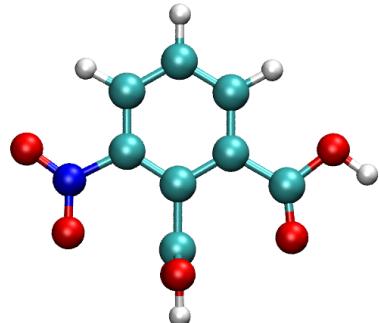
EingenValues - Molecule B

489.011	1233.7	1641.81
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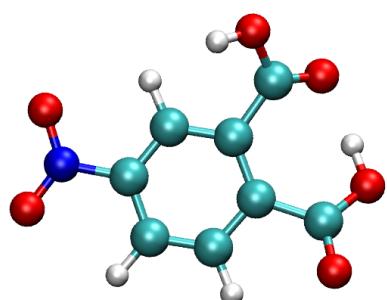
Different



Molecule A 3NFAACb



Molecule B 4NFAACf



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

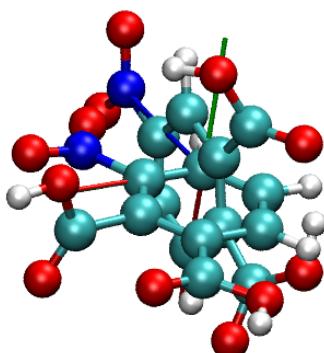
EingenValues - Molecule A

530.103	915.738	1361.08
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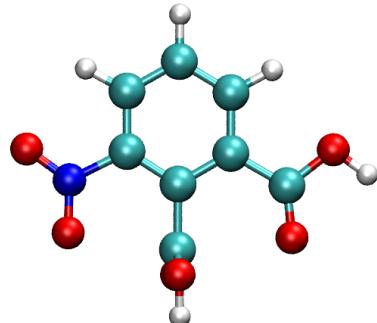
EingenValues - Molecule B

509.668	1219.11	1681.18
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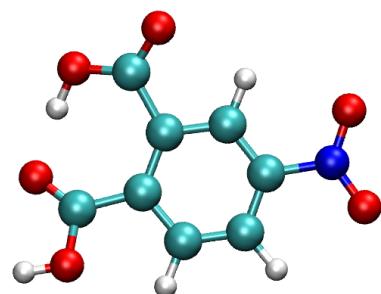
Different



Molecule A 3NFAACb



Molecule B 4NFAACg



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

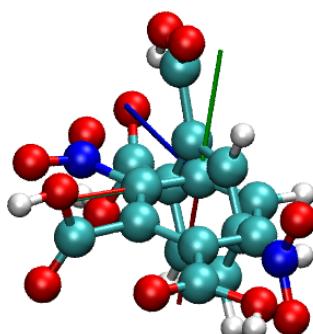
EingenValues - Molecule A

530.103	915.738	1361.08
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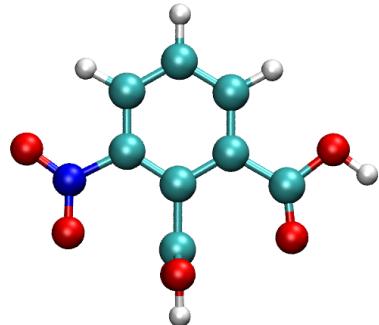
EingenValues - Molecule B

513.751	1208.07	1700.9
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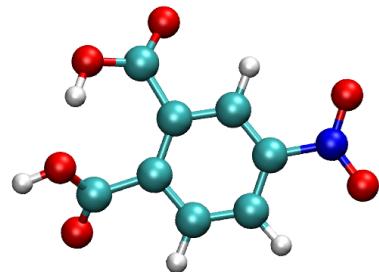
Different



Molecule A 3NFAACb



Molecule B 4NFAACi



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

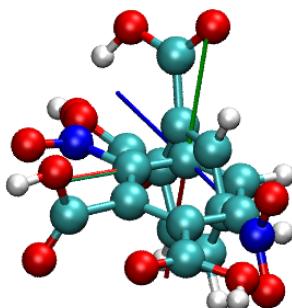
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

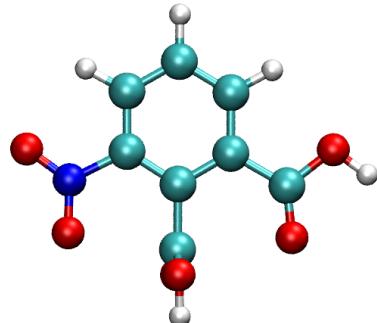
502.409	1232.26	1676.02
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Different

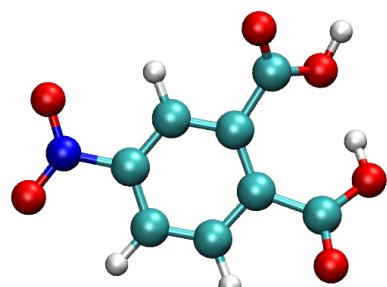


FireTest Número 245

Molecule A 3NFAACb



Molecule B 4NFAACj



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

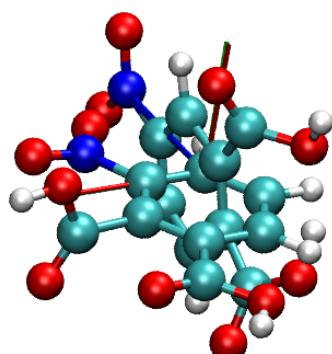
EigenValues - Molecule A

530.103	915.738	1361.08
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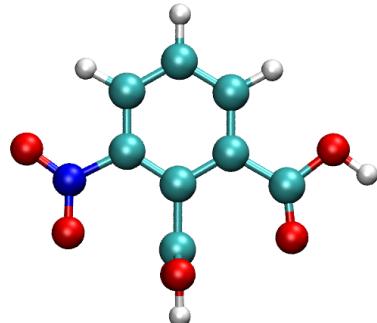
EigenValues - Molecule B

509.897	1225.65	1680.83
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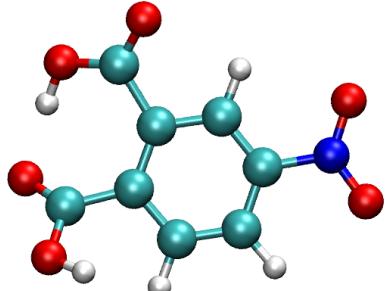
Different



Molecule A 3NFAACb



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

530.265	-1.20883	-7.84653
-1.20883	1361.05	-3.78865
-7.84653	-3.78865	915.61

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999791	-0.00154731	-0.0203648
-0.0203771	0.00845054	0.999757
-0.00137484	0.999963	-0.00848031

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

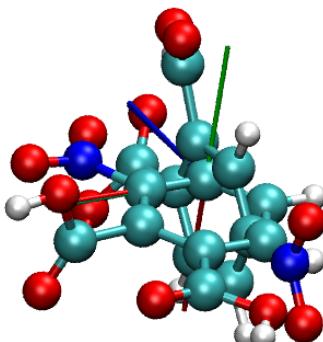
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

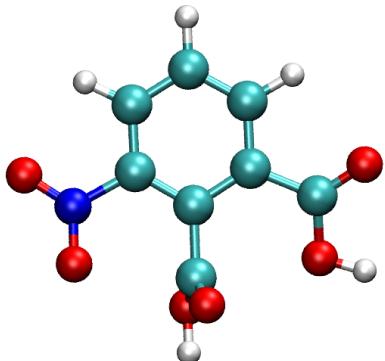
506.607	1222.36	1678.43
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Different

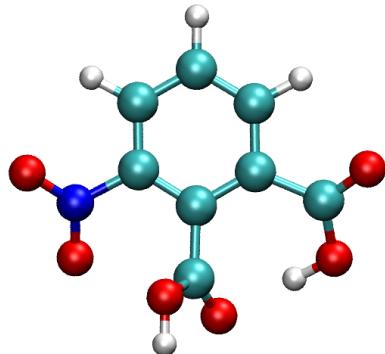


FireTest Número 247

Molecule A 3NFAACc



Molecule B 3NFAACd



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

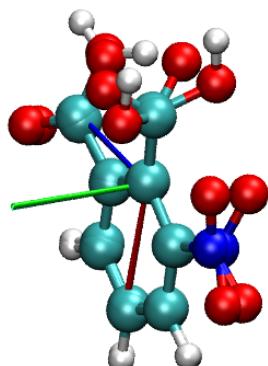
EingenValues - Molecule A

531.402	913.293	1353.16
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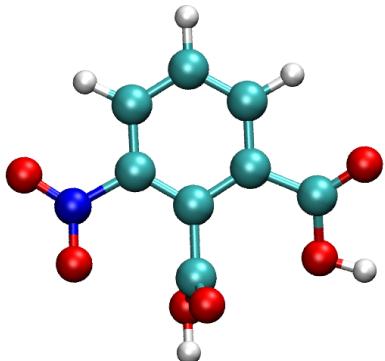
EingenValues - Molecule B

524.175	935.342	1359.19
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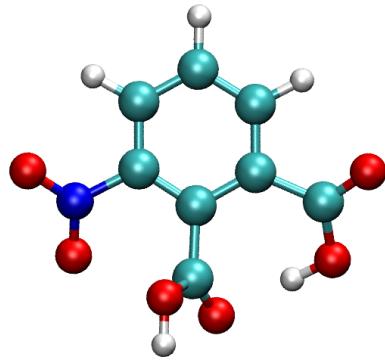
Different



Molecule A 3NFAACc



Molecule B 3NFAACe



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

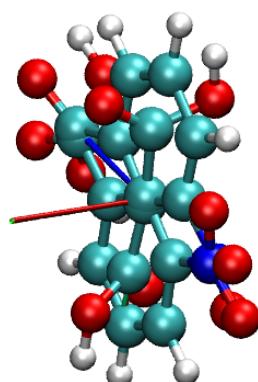
EingenValues - Molecule A

531.402	913.293	1353.16
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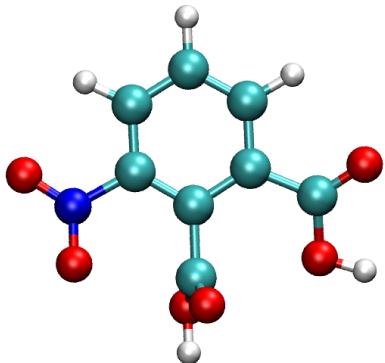
EingenValues - Molecule B

524.162	935.308	1359.22
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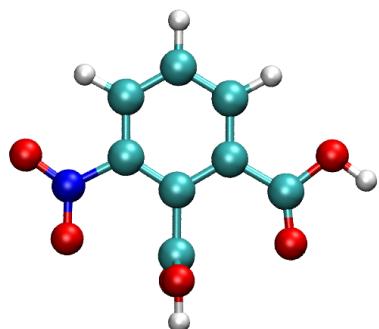
Different



Molecule A 3NFAACc



Molecule B 3NFAACf



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

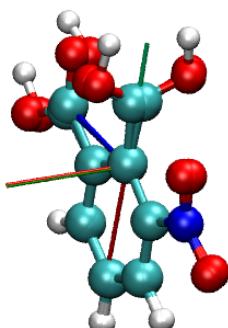
EingenValues - Molecule A

531.402	913.293	1353.16
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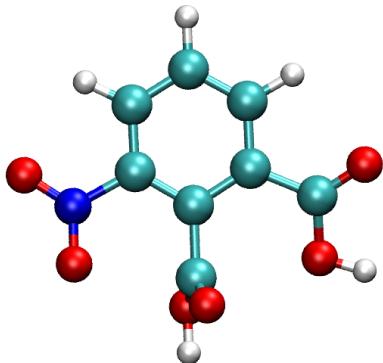
EingenValues - Molecule B

530.045	915.527	1360.79
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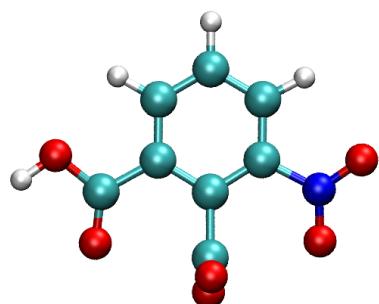
Different



Molecule A 3NFAACc



Molecule B 3NFAACg



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

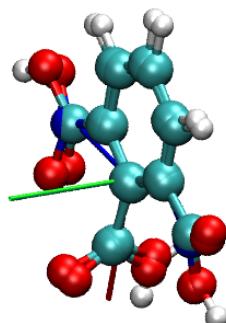
EingenValues - Molecule A

531.402	913.293	1353.16
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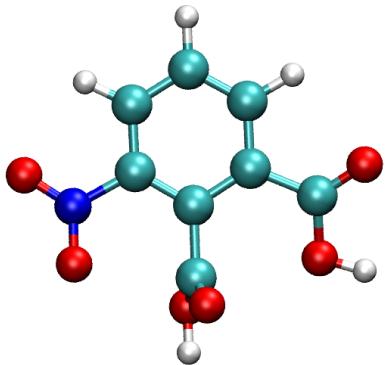
EingenValues - Molecule B

532.89	918.442	1356.93
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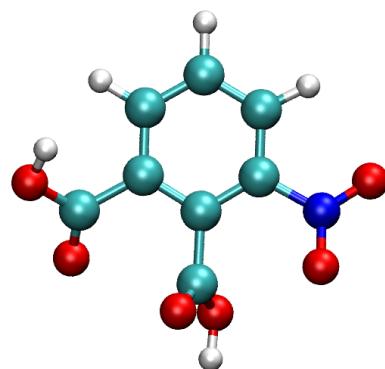
Different



Molecule A 3NFAACc



Molecule B 3NFAACh



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

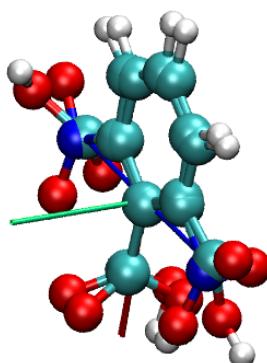
EingenValues - Molecule A

531.402	913.293	1353.16
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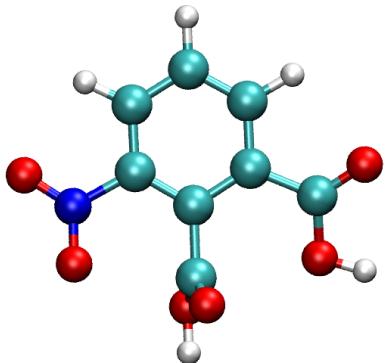
EingenValues - Molecule B

528.663	924.928	1336.12
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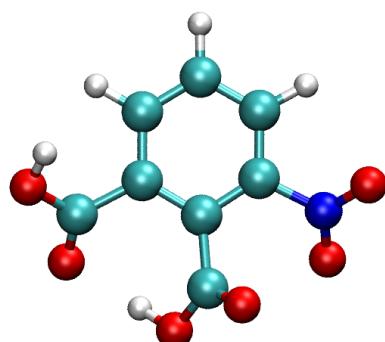
Different



Molecule A 3NFAACc



Molecule B 3NFAACi



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

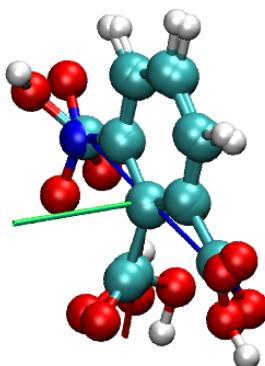
EingenValues - Molecule A

531.402	913.293	1353.16
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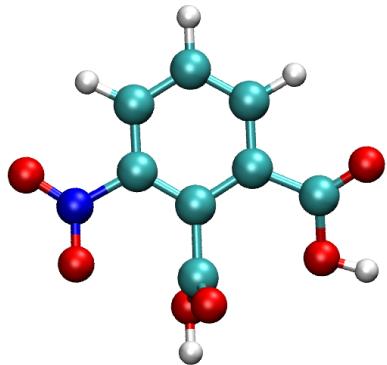
EingenValues - Molecule B

521.475	949.659	1346.18
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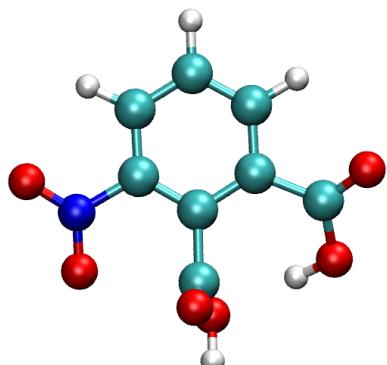
Different



Molecule A 3NFAACc



Molecule B 3NFAACj



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

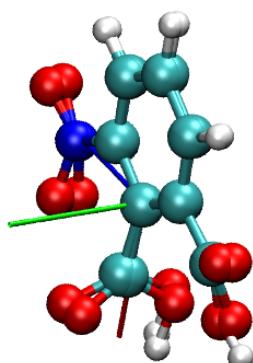
EingenValues - Molecule A

531.402	913.293	1353.16
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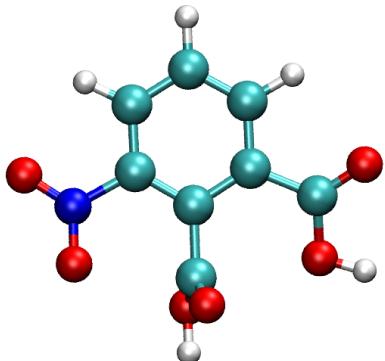
EingenValues - Molecule B

533.726	920.137	1348.3
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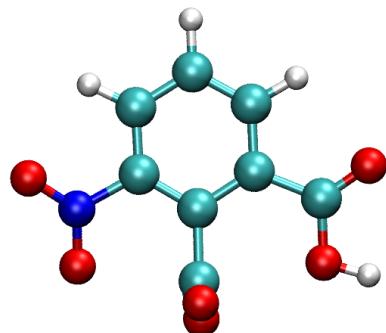
Different



Molecule A 3NFAACc



Molecule B 3NFAACK



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

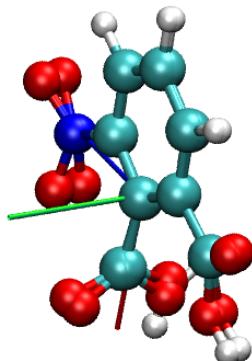
EingenValues - Molecule A

531.402	913.293	1353.16
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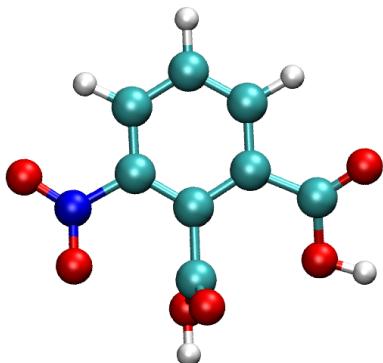
EingenValues - Molecule B

534.81	913.339	1353.78
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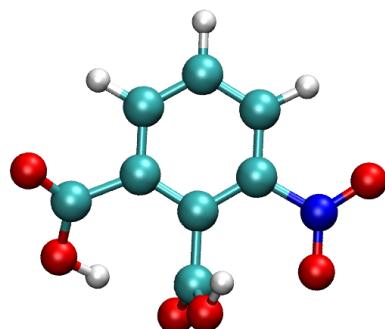
Different



Molecule A 3NFAACc



Molecule B 3NFAACl



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

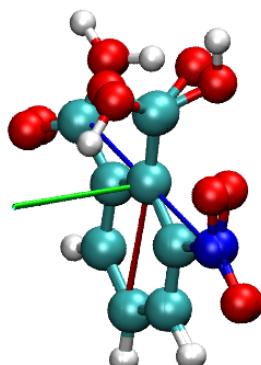
EingenValues - Molecule A

531.402	913.293	1353.16
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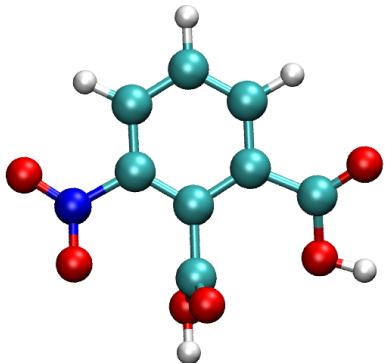
EingenValues - Molecule B

531.691	929.434	1355.4
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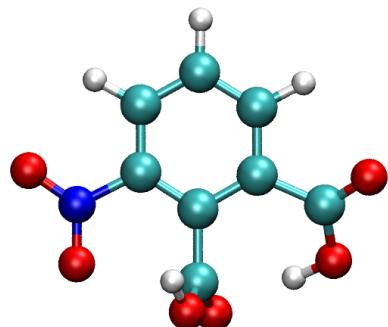
Different



Molecule A 3NFAACc



Molecule B 3NFAACm



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

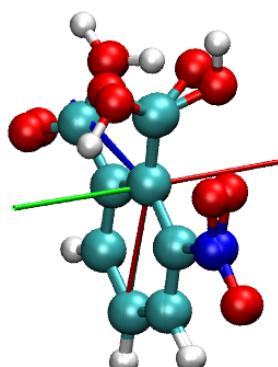
EingenValues - Molecule A

531.402	913.293	1353.16
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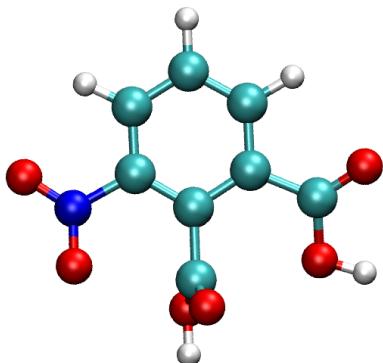
EingenValues - Molecule B

531.698	929.417	1355.4
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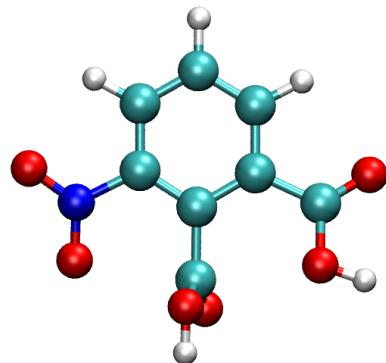
Different



Molecule A 3NFAACc



Molecule B 3NFAACn



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

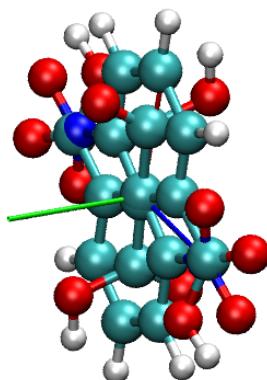
EingenValues - Molecule A

531.402	913.293	1353.16
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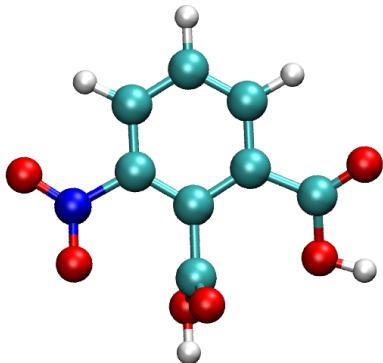
EingenValues - Molecule B

531.43	913.309	1353.35
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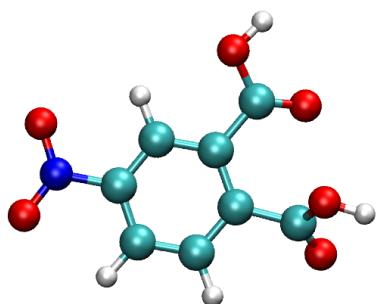
Enantiomers



Molecule A 3NFAACc



Molecule B 4NFAACa



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

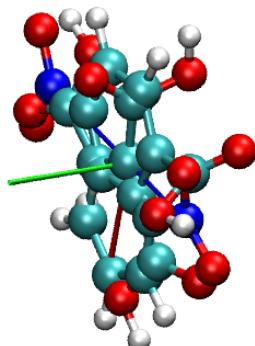
EingenValues - Molecule A

531.402	913.293	1353.16
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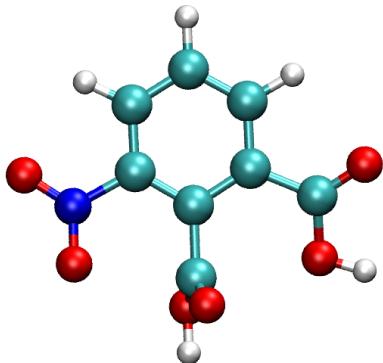
EingenValues - Molecule B

479.363	1242.41	1647.39
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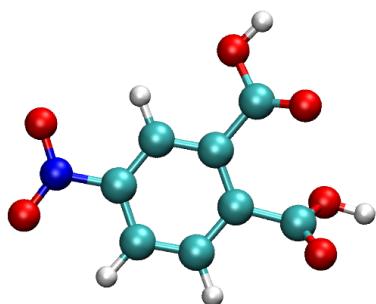
Different



Molecule A 3NFAACc



Molecule B 4NFAACb



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

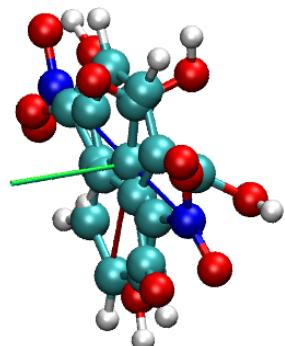
EingenValues - Molecule A

531.402	913.293	1353.16
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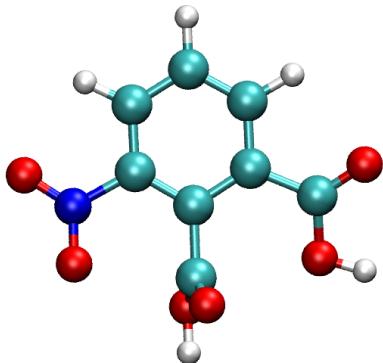
EingenValues - Molecule B

479.308	1242.41	1647.31
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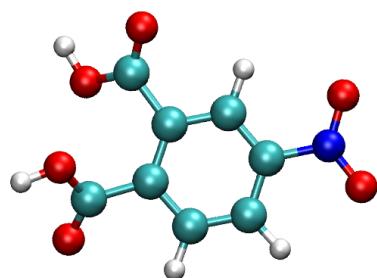
Different



Molecule A 3NFAACc



Molecule B 4NFAACc



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

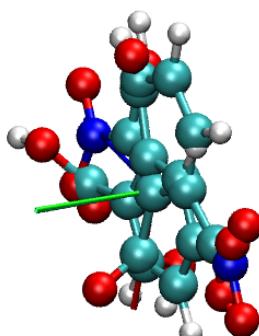
EingenValues - Molecule A

531.402	913.293	1353.16
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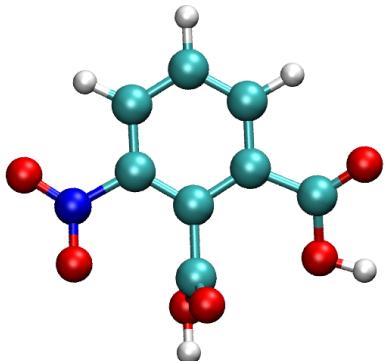
EingenValues - Molecule B

482.027	1240.32	1647.08
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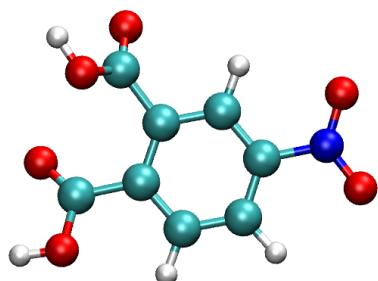
Different



Molecule A 3NFAACc



Molecule B 4NFAACd



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

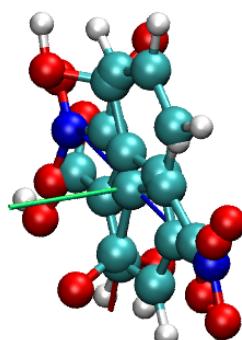
EingenValues - Molecule A

531.402	913.293	1353.16
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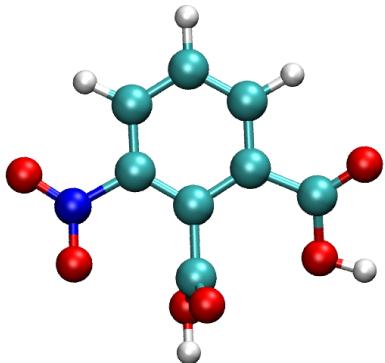
EingenValues - Molecule B

491.663	1231.14	1650.13
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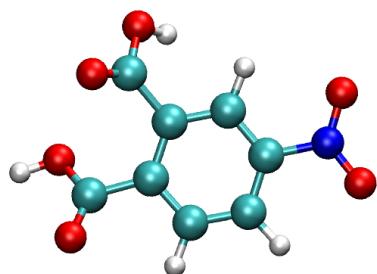
Different



Molecule A 3NFAACc



Molecule B 4NFAACe



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

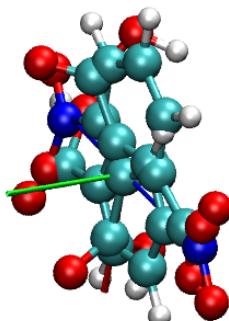
EingenValues - Molecule A

531.402	913.293	1353.16
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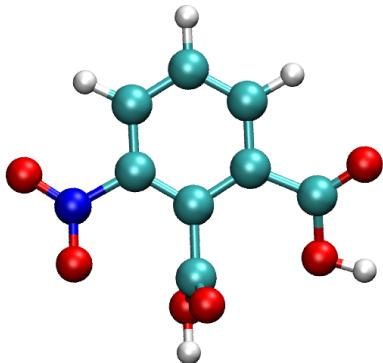
EingenValues - Molecule B

489.011	1233.7	1641.81
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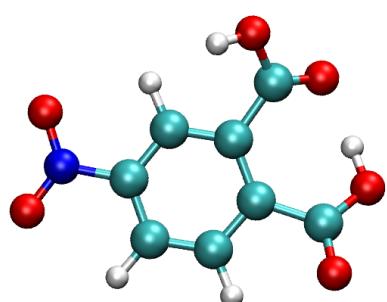
Different



Molecule A 3NFAACc



Molecule B 4NFAACf



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

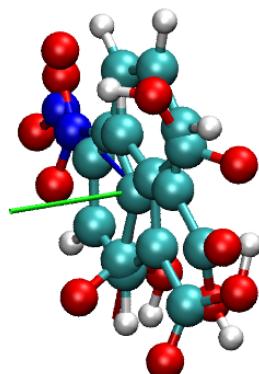
EingenValues - Molecule A

531.402	913.293	1353.16
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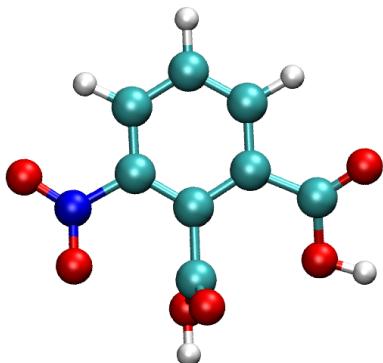
EingenValues - Molecule B

509.668	1219.11	1681.18
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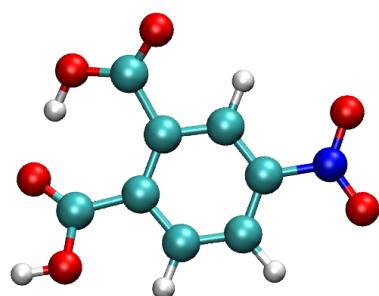
Different



Molecule A 3NFAACc



Molecule B 4NFAACg



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

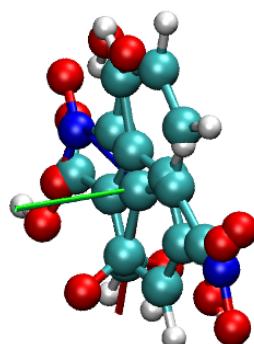
EingenValues - Molecule A

531.402	913.293	1353.16
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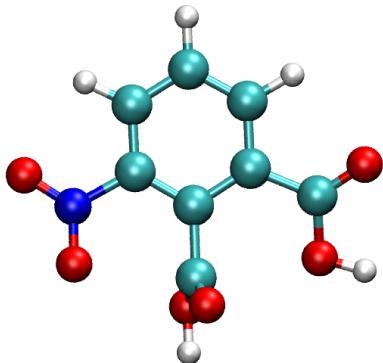
EingenValues - Molecule B

513.751	1208.07	1700.9
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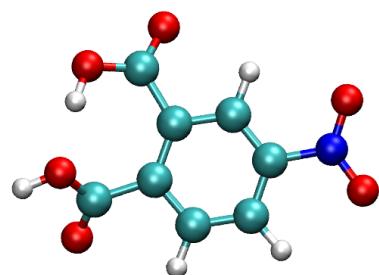
Different



Molecule A 3NFAACc



Molecule B 4NFAACi



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

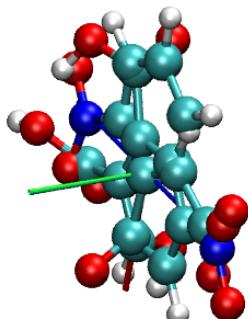
EingenValues - Molecule A

531.402	913.293	1353.16
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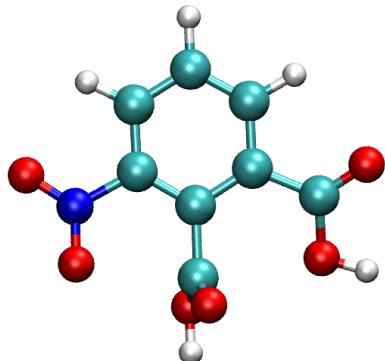
EingenValues - Molecule B

502.409	1232.26	1676.02
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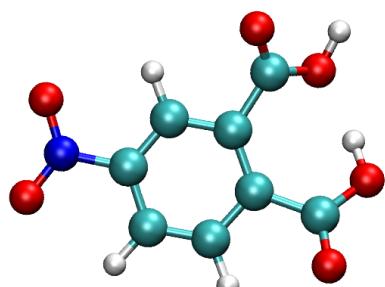
Different



Molecule A 3NFAACc



Molecule B 4NFAACj



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

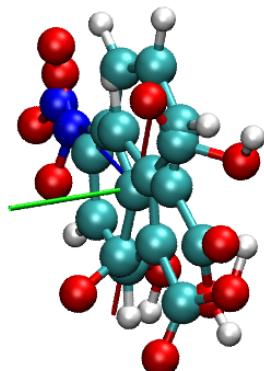
EingenValues - Molecule A

531.402	913.293	1353.16
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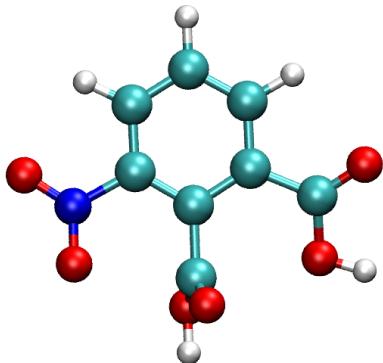
EingenValues - Molecule B

509.897	1225.65	1680.83
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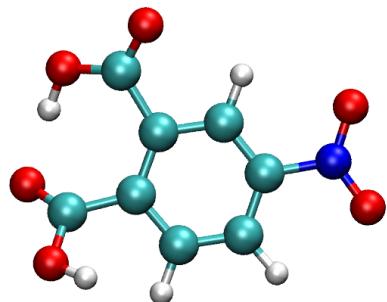
Different



Molecule A 3NFAACc



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

531.482	-5.48557	-0.978638
-5.48557	913.233	2.89201
-0.978638	2.89201	1353.14

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999896	-0.0143563	-0.00114029
0.0143485	-0.999875	0.00660611
-0.00123498	0.00658906	0.999978

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

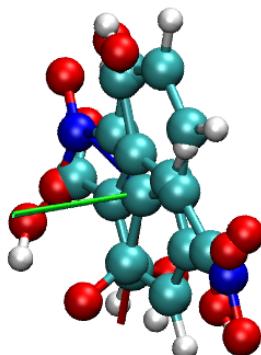
EingenValues - Molecule A

531.402	913.293	1353.16
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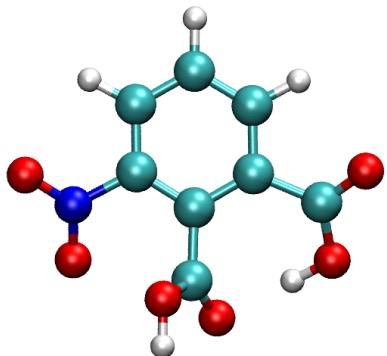
EingenValues - Molecule B

506.607	1222.36	1678.43
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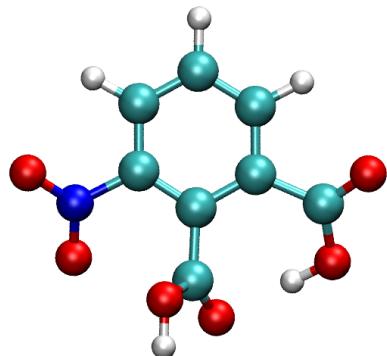
Different



Molecule A 3NFAACd



Molecule B 3NFAACe



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

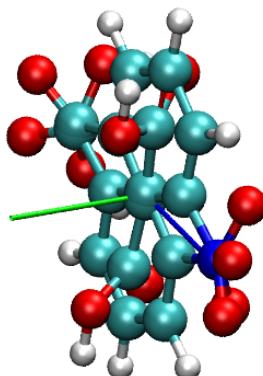
EingenValues - Molecule A

524.175	935.342	1359.19
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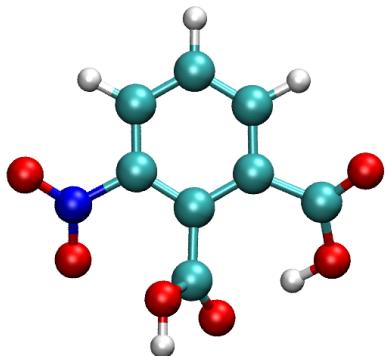
EingenValues - Molecule B

524.162	935.308	1359.22
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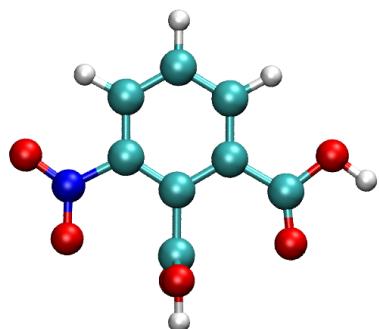
Equal



Molecule A 3NFAACd



Molecule B 3NFAACf



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

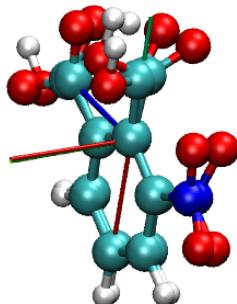
EingenValues - Molecule A

524.175	935.342	1359.19
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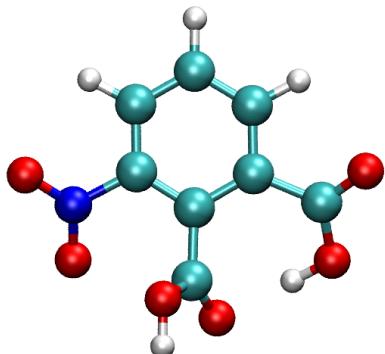
EingenValues - Molecule B

530.045	915.527	1360.79
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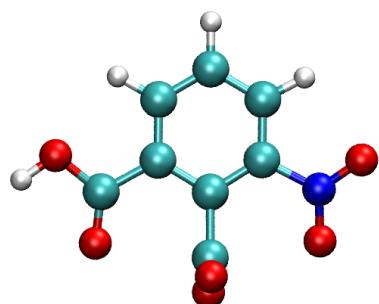
Different



Molecule A 3NFAACd



Molecule B 3NFAACg



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

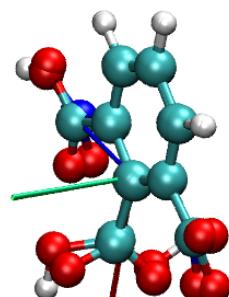
EingenValues - Molecule A

524.175	935.342	1359.19
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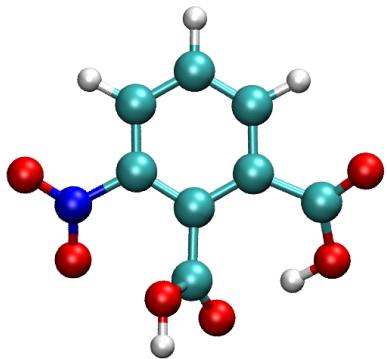
EingenValues - Molecule B

532.89	918.442	1356.93
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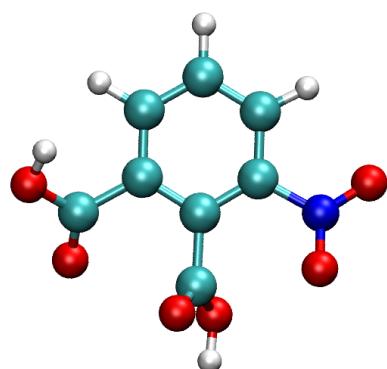
Different



Molecule A 3NFAACd



Molecule B 3NFAACh



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

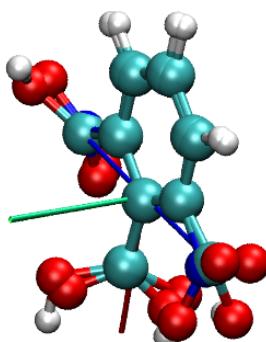
EingenValues - Molecule A

524.175	935.342	1359.19
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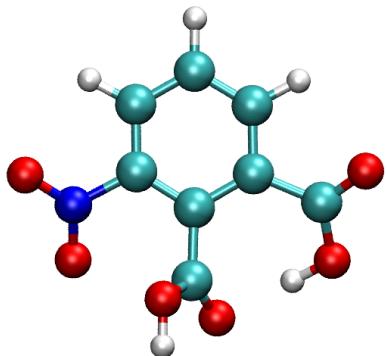
EingenValues - Molecule B

528.663	924.928	1336.12
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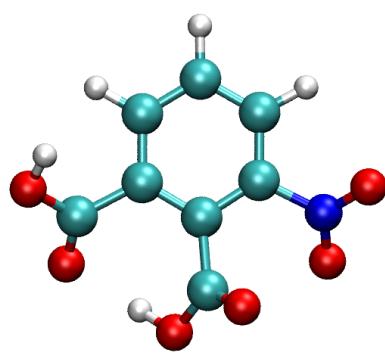
Different



Molecule A 3NFAACd



Molecule B 3NFAACi



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

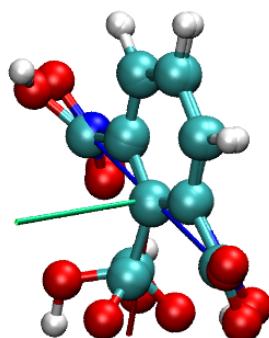
EingenValues - Molecule A

524.175	935.342	1359.19
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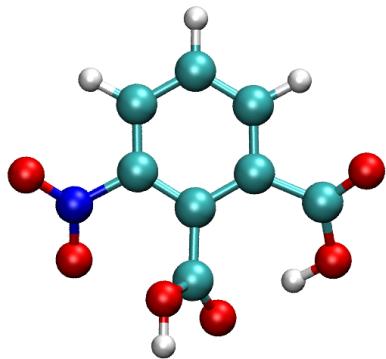
EingenValues - Molecule B

521.475	949.659	1346.18
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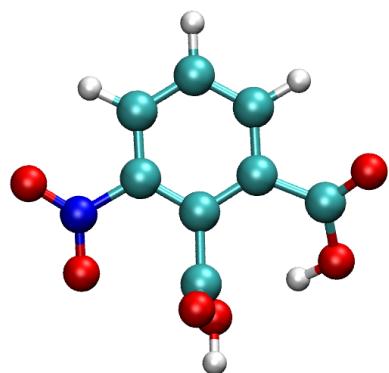
Different



Molecule A 3NFAACd



Molecule B 3NFAACj



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

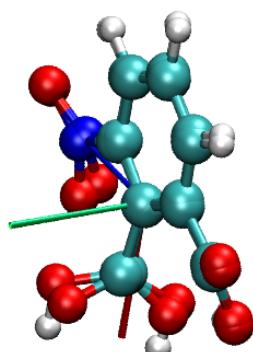
EingenValues - Molecule A

524.175	935.342	1359.19
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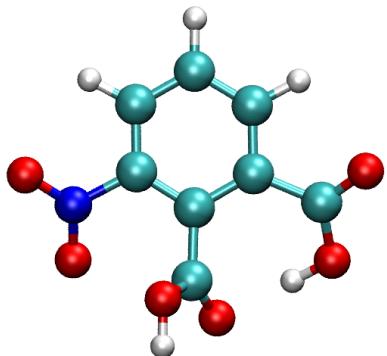
EingenValues - Molecule B

533.726	920.137	1348.3
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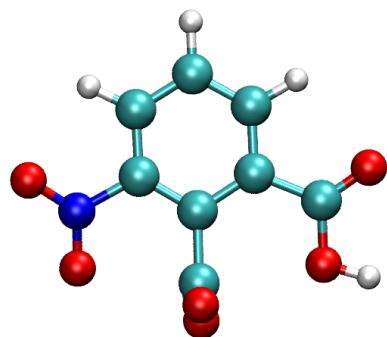
Different



Molecule A 3NFAACd



Molecule B 3NFAACK



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

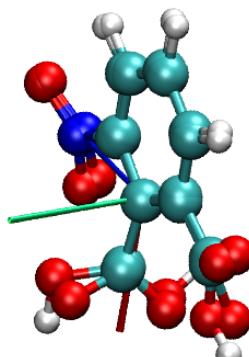
EingenValues - Molecule A

524.175	935.342	1359.19
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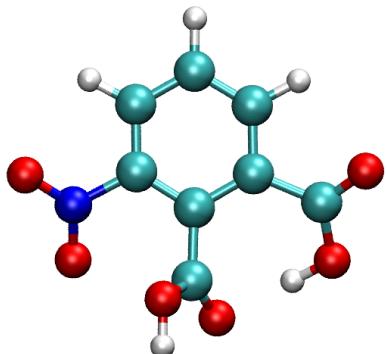
EingenValues - Molecule B

534.81	913.339	1353.78
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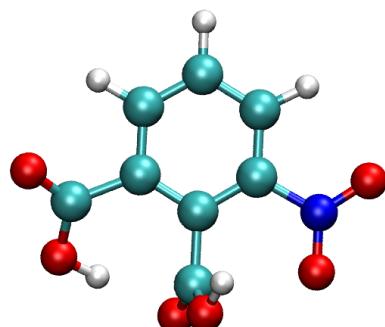
Different



Molecule A 3NFAACd



Molecule B 3NFAACl



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

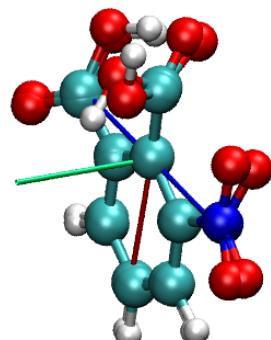
EingenValues - Molecule A

524.175	935.342	1359.19
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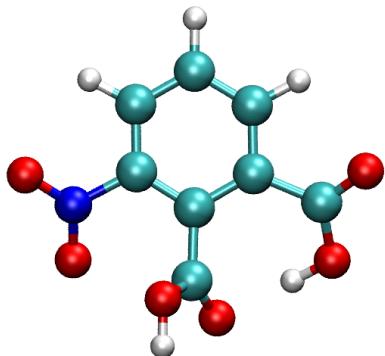
EingenValues - Molecule B

531.691	929.434	1355.4
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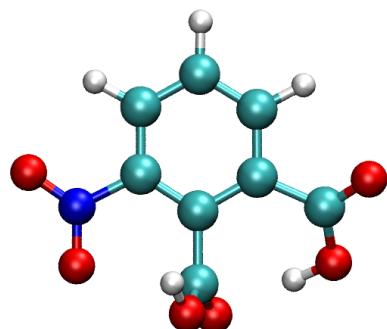
Different



Molecule A 3NFAACd



Molecule B 3NFAACm



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

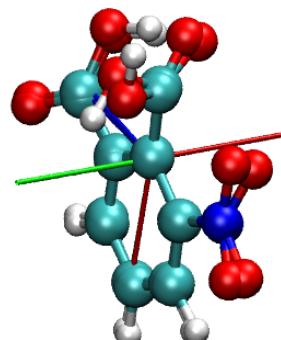
EingenValues - Molecule A

524.175	935.342	1359.19
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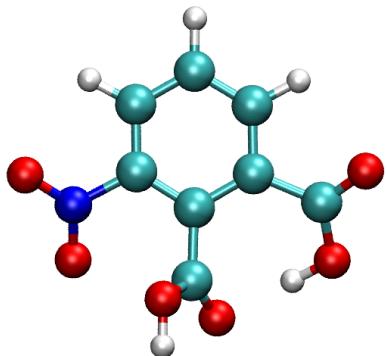
EingenValues - Molecule B

531.698	929.417	1355.4
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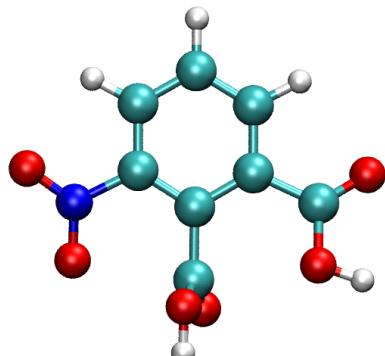
Different



Molecule A 3NFAACd



Molecule B 3NFAACn



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

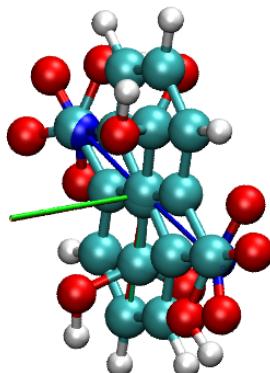
EingenValues - Molecule A

524.175	935.342	1359.19
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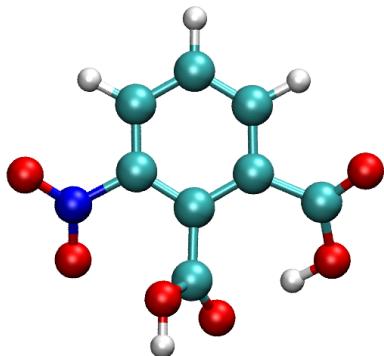
EingenValues - Molecule B

531.43	913.309	1353.35
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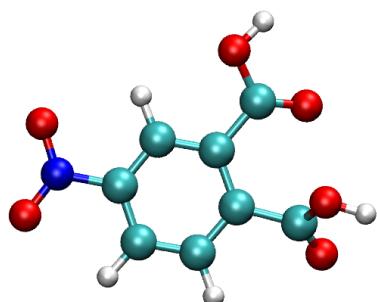
Different



Molecule A 3NFAACd



Molecule B 4NFAACa



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

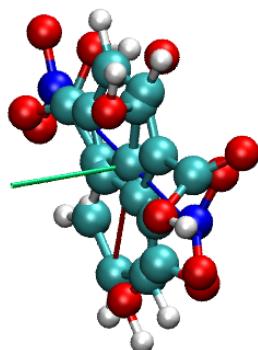
EingenValues - Molecule A

524.175	935.342	1359.19
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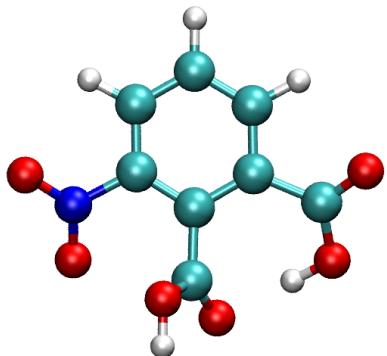
EingenValues - Molecule B

479.363	1242.41	1647.39
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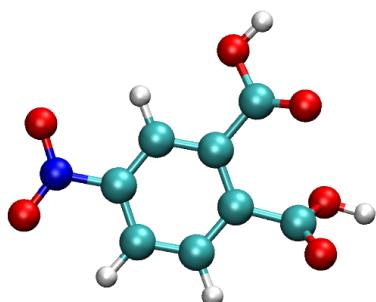
Different



Molecule A 3NFAACd



Molecule B 4NFAACb



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

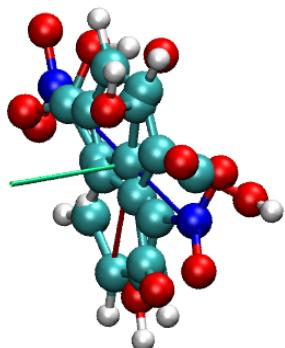
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

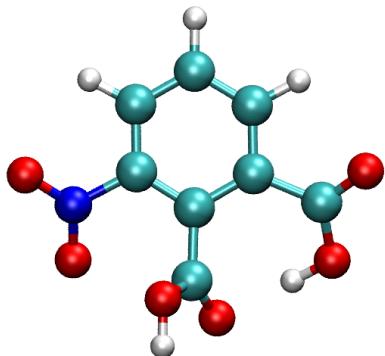
479.308	1242.41	1647.31
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Different

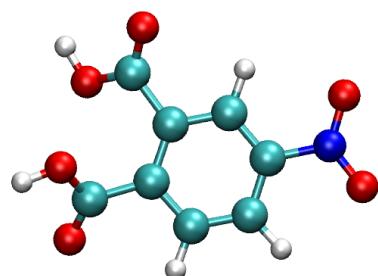


FireTest Número 280

Molecule A 3NFAACd



Molecule B 4NFAACC



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

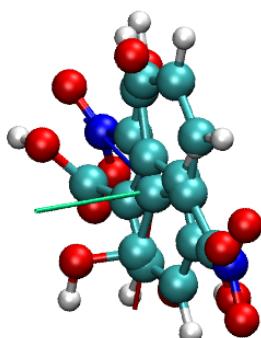
EingenValues - Molecule A

524.175	935.342	1359.19
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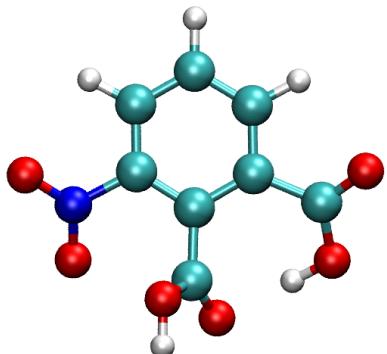
EingenValues - Molecule B

482.027	1240.32	1647.08
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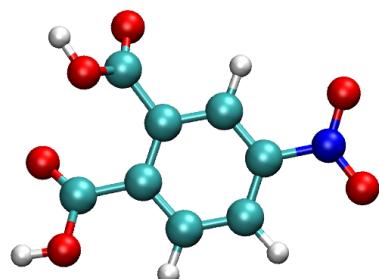
Different



Molecule A 3NFAACd



Molecule B 4NFAACd



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

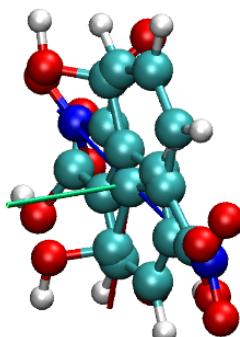
EingenValues - Molecule A

524.175	935.342	1359.19
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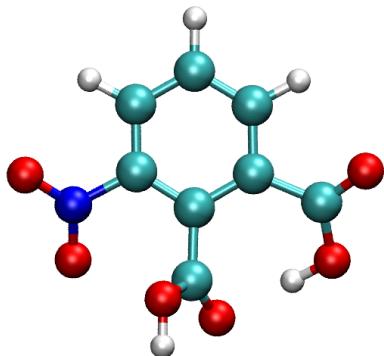
EingenValues - Molecule B

491.663	1231.14	1650.13
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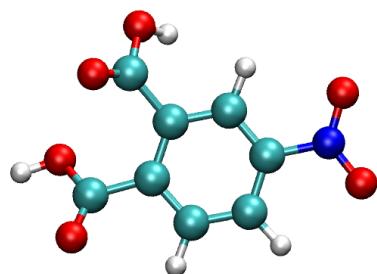
Different



Molecule A 3NFAACd



Molecule B 4NFAACe



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

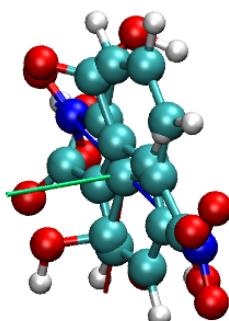
EingenValues - Molecule A

524.175	935.342	1359.19
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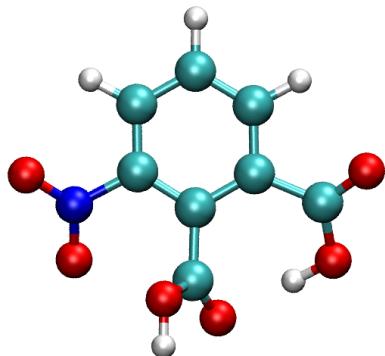
EingenValues - Molecule B

489.011	1233.7	1641.81
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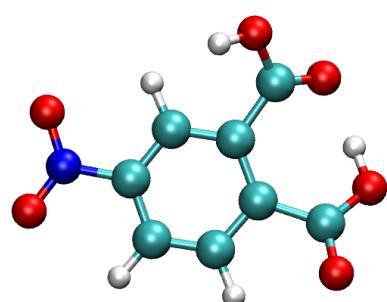
Different



Molecule A 3NFAACd



Molecule B 4NFAACf



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

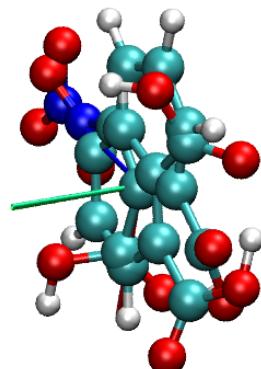
EingenValues - Molecule A

524.175	935.342	1359.19
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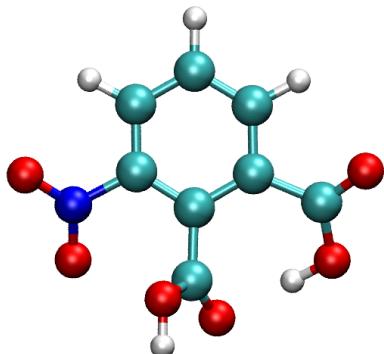
EingenValues - Molecule B

509.668	1219.11	1681.18
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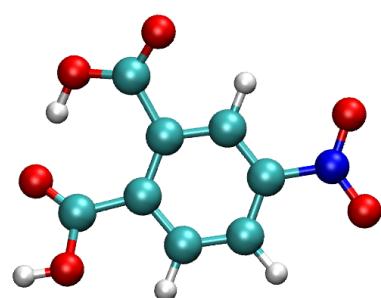
Different



Molecule A 3NFAACd



Molecule B 4NFAACg



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

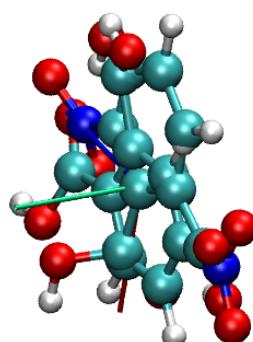
EingenValues - Molecule A

524.175	935.342	1359.19
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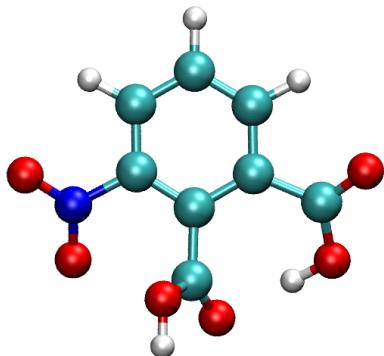
EingenValues - Molecule B

513.751	1208.07	1700.9
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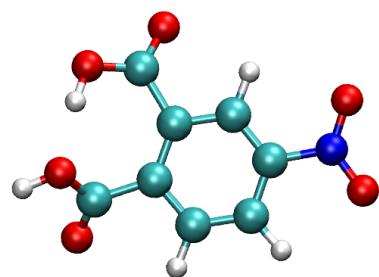
Different



Molecule A 3NFAACd



Molecule B 4NFAACi



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

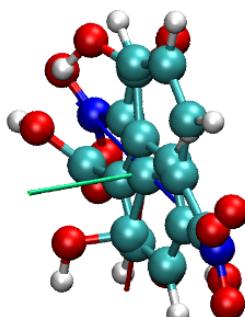
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

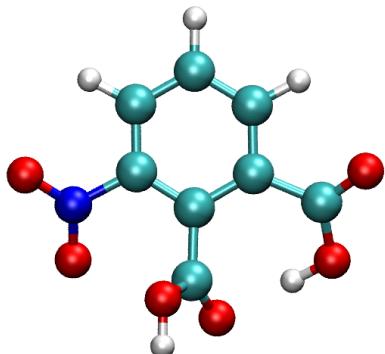
502.409	1232.26	1676.02
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Different

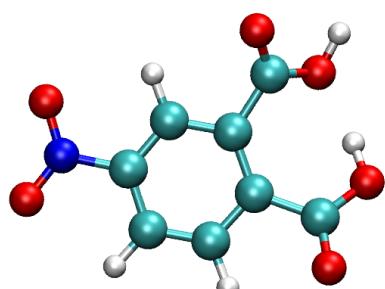


FireTest Número 286

Molecule A 3NFAACd



Molecule B 4NFAACj



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

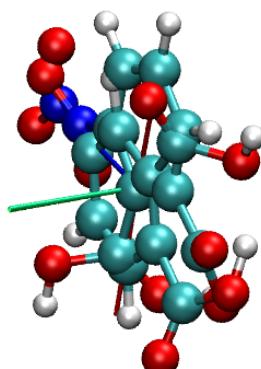
EigenValues - Molecule A

524.175	935.342	1359.19
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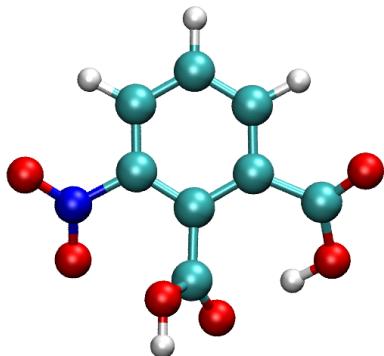
EigenValues - Molecule B

509.897	1225.65	1680.83
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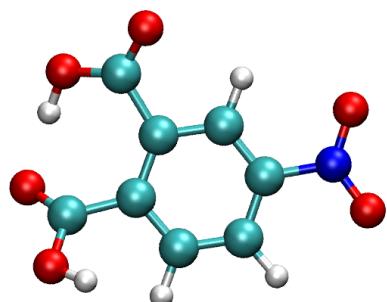
Different



Molecule A 3NFAACd



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

524.186	-1.32648	-2.36411
-1.32648	935.358	-2.91274
-2.36411	-2.91274	1359.16

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999991	-0.00324612	-0.00284261
0.00326554	-0.999971	-0.0068542
-0.00282028	-0.00686342	0.999972

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

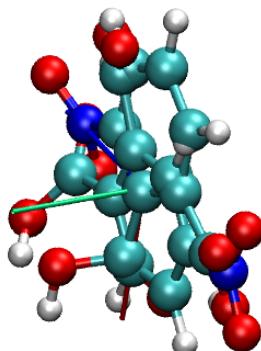
EingenValues - Molecule A

524.175	935.342	1359.19
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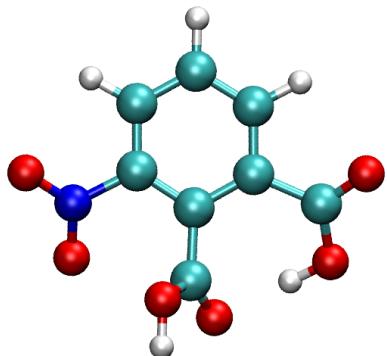
EingenValues - Molecule B

506.607	1222.36	1678.43
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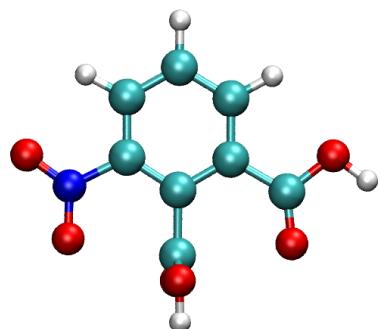
Different



Molecule A 3NFAACe



Molecule B 3NFAACf



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

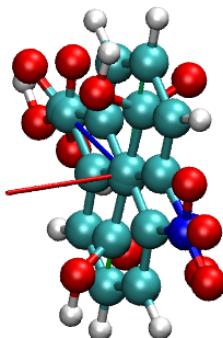
EingenValues - Molecule A

524.162	935.308	1359.22
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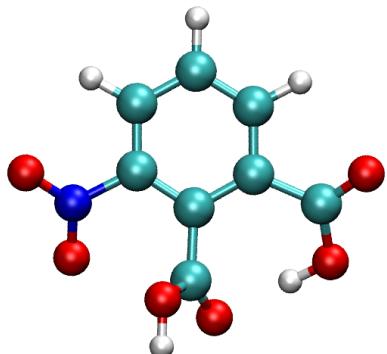
EingenValues - Molecule B

530.045	915.527	1360.79
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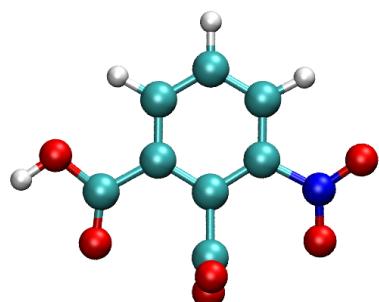
Different



Molecule A 3NFAACe



Molecule B 3NFAACg



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

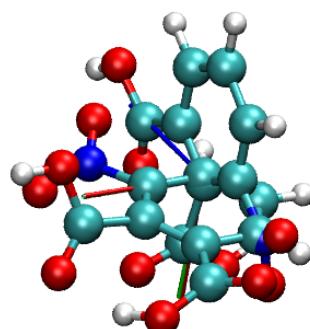
EingenValues - Molecule A

524.162	935.308	1359.22
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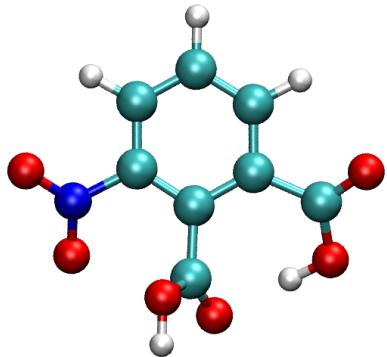
EingenValues - Molecule B

532.89	918.442	1356.93
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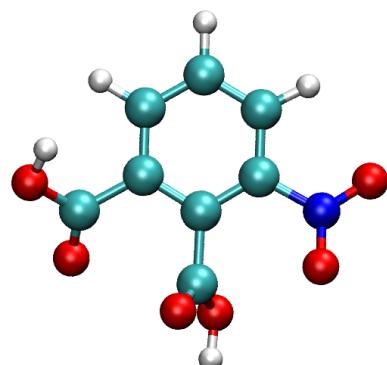
Different



Molecule A 3NFAACe



Molecule B 3NFAACh



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

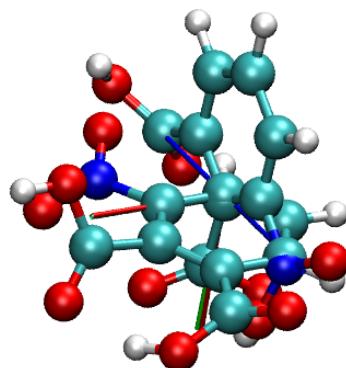
EingenValues - Molecule A

524.162	935.308	1359.22
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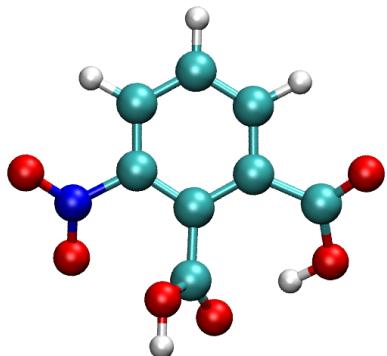
EingenValues - Molecule B

528.663	924.928	1336.12
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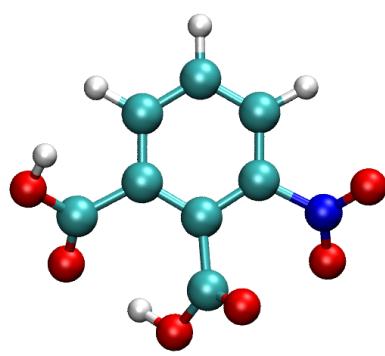
Different



Molecule A 3NFAACe



Molecule B 3NFAACi



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

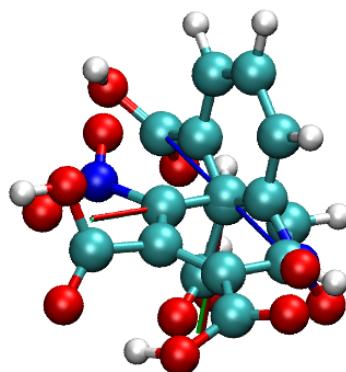
EingenValues - Molecule A

524.162	935.308	1359.22
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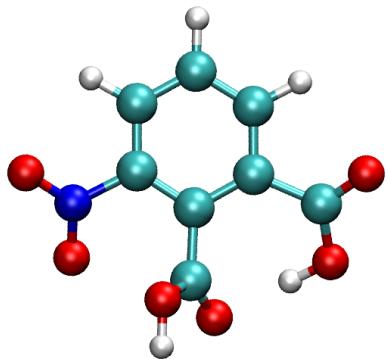
EingenValues - Molecule B

521.475	949.659	1346.18
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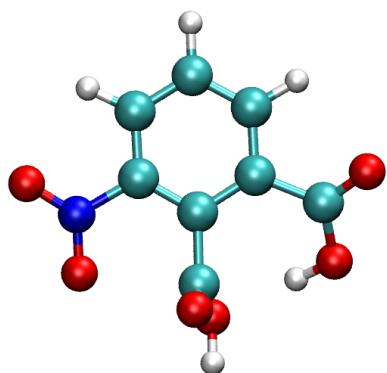
Different



Molecule A 3NFAACe



Molecule B 3NFAACj



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

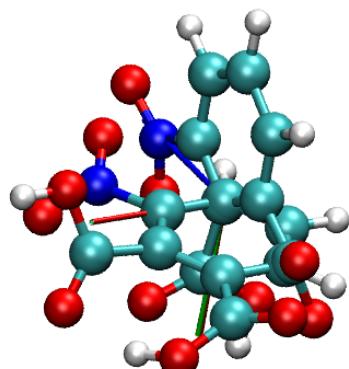
EingenValues - Molecule A

524.162	935.308	1359.22
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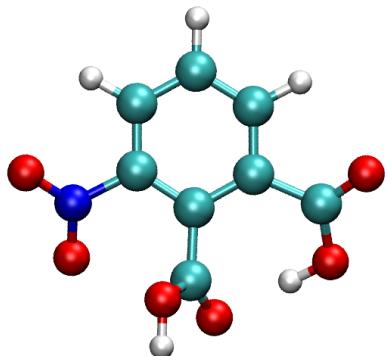
EingenValues - Molecule B

533.726	920.137	1348.3
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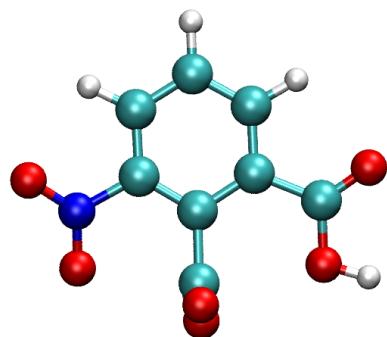
Different



Molecule A 3NFAACe



Molecule B 3NFAACK



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

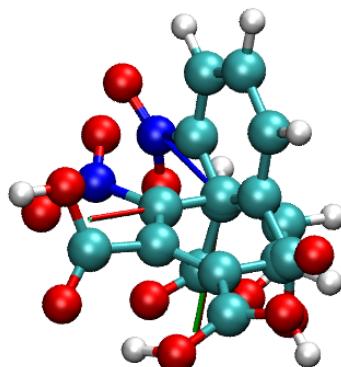
EingenValues - Molecule A

524.162	935.308	1359.22
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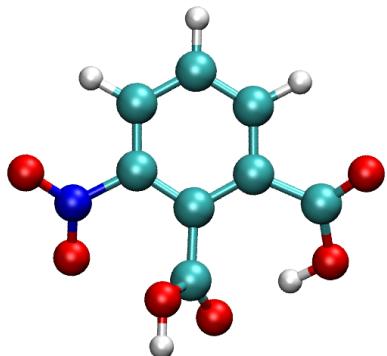
EingenValues - Molecule B

534.81	913.339	1353.78
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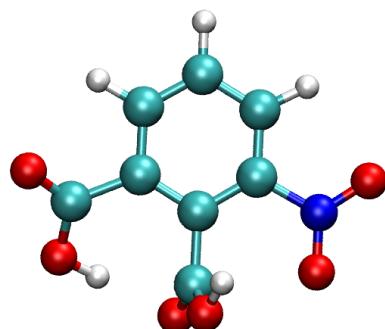
Different



Molecule A 3NFAACe



Molecule B 3NFAACl



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

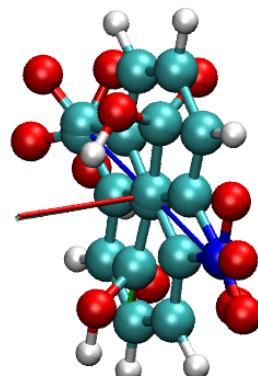
EingenValues - Molecule A

524.162	935.308	1359.22
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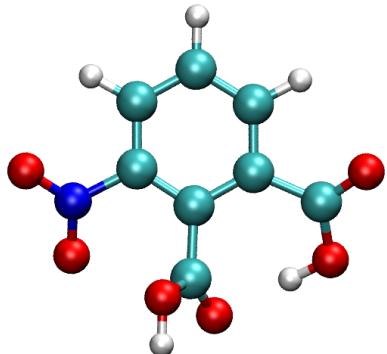
EingenValues - Molecule B

531.691	929.434	1355.4
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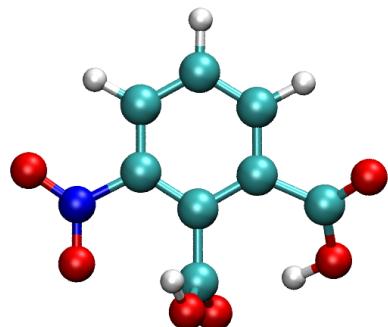
Different



Molecule A 3NFAACe



Molecule B 3NFAACm



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

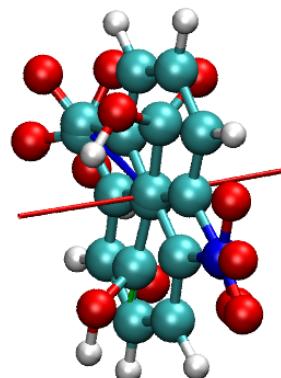
EingenValues - Molecule A

524.162	935.308	1359.22
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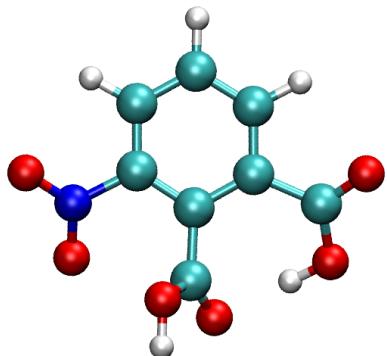
EingenValues - Molecule B

531.698	929.417	1355.4
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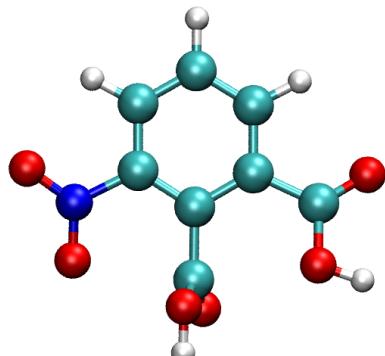
Different



Molecule A 3NFAACe



Molecule B 3NFAACn



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

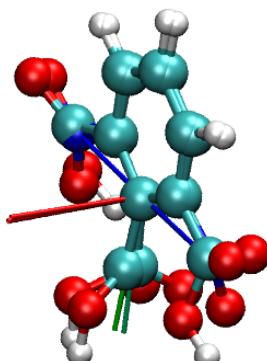
EingenValues - Molecule A

524.162	935.308	1359.22
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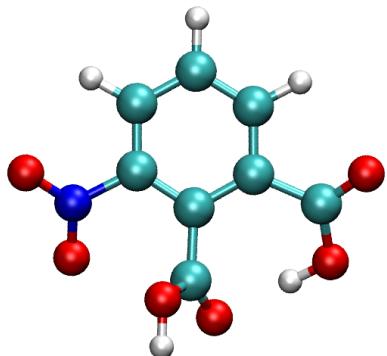
EingenValues - Molecule B

531.43	913.309	1353.35
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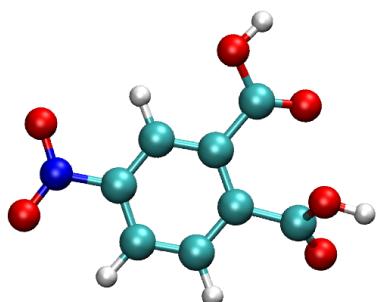
Different



Molecule A 3NFAACe



Molecule B 4NFAACa



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

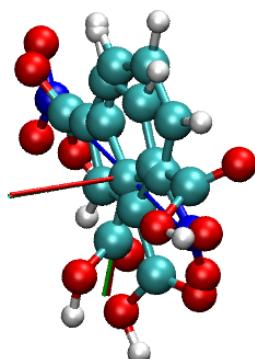
EingenValues - Molecule A

524.162	935.308	1359.22
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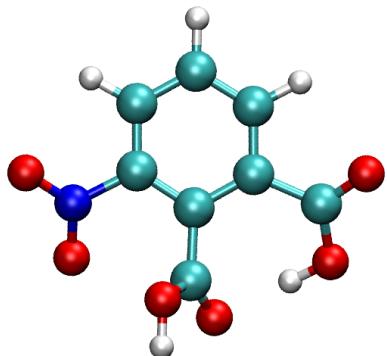
EingenValues - Molecule B

479.363	1242.41	1647.39
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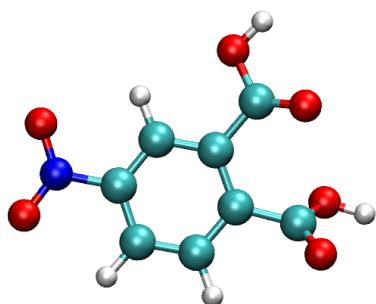
Different



Molecule A 3NFAACe



Molecule B 4NFAACb



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

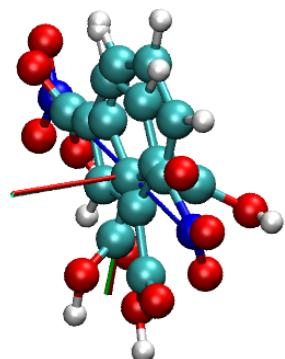
EingenValues - Molecule A

524.162	935.308	1359.22
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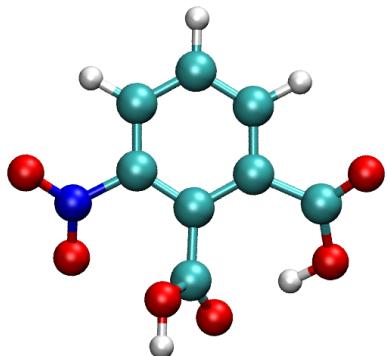
EingenValues - Molecule B

479.308	1242.41	1647.31
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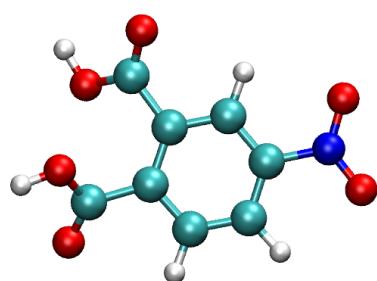
Different



Molecule A 3NFAACe



Molecule B 4NFAACCc



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

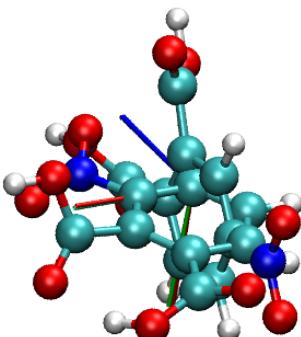
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

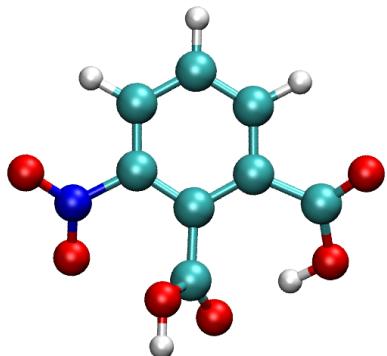
482.027	1240.32	1647.08
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Different

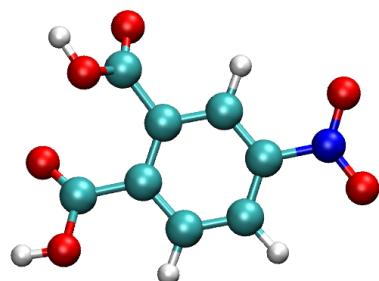


FireTest Número 300

Molecule A 3NFAACe



Molecule B 4NFAACd



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

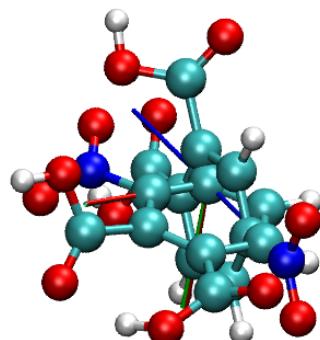
EingenValues - Molecule A

524.162	935.308	1359.22
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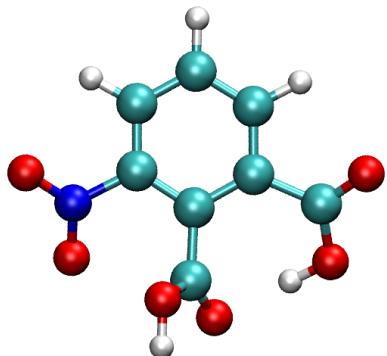
EingenValues - Molecule B

491.663	1231.14	1650.13
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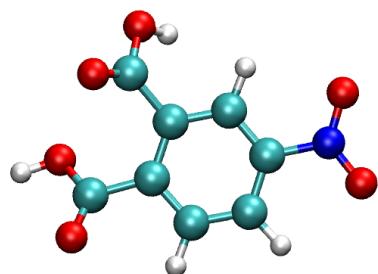
Different



Molecule A 3NFAACe



Molecule B 4NFAACe



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

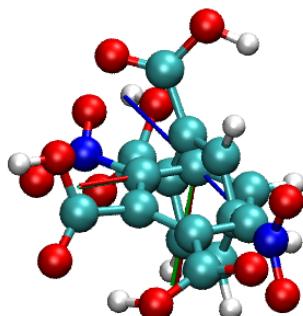
EingenValues - Molecule A

524.162	935.308	1359.22
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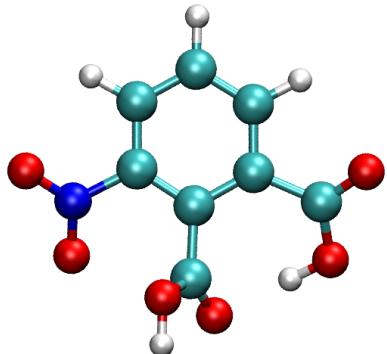
EingenValues - Molecule B

489.011	1233.7	1641.81
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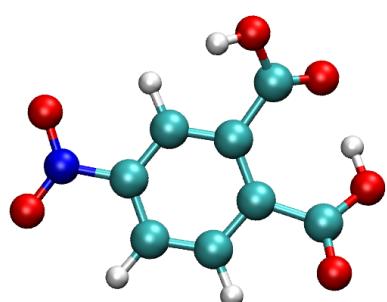
Different



Molecule A 3NFAACe



Molecule B 4NFAACf



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

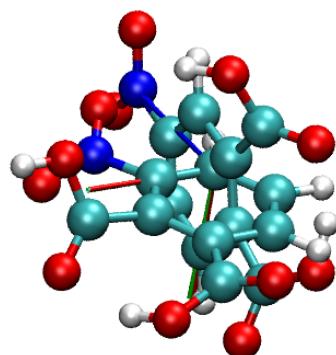
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

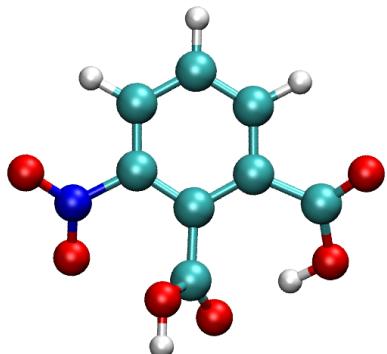
509.668	1219.11	1681.18
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Different

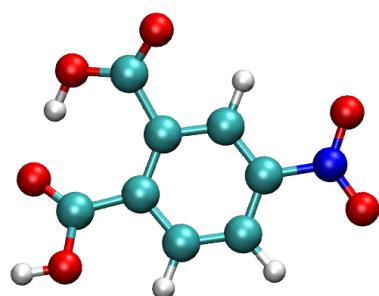


# FireTest Número 303

Molecule A 3NFAACe



Molecule B 4NFAACg



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EigenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EigenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

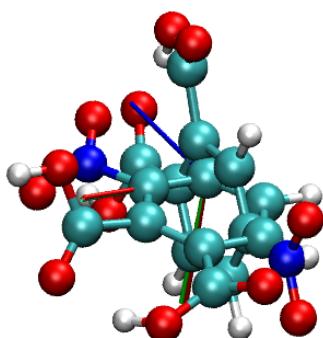
EigenValues - Molecule A

524.162	935.308	1359.22
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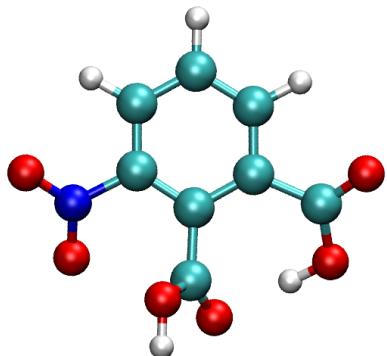
EigenValues - Molecule B

513.751	1208.07	1700.9
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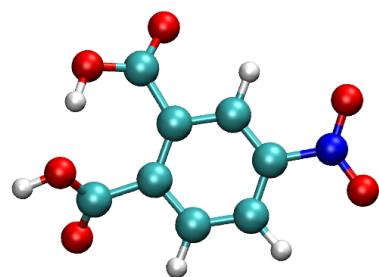
Different



Molecule A 3NFAACe



Molecule B 4NFAACi



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

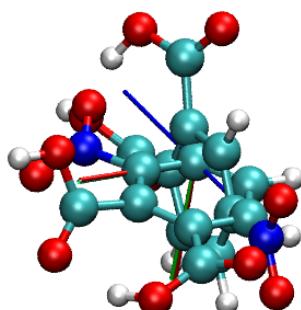
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

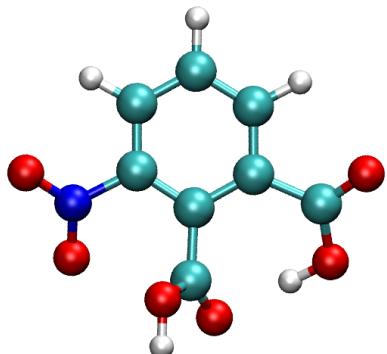
502.409	1232.26	1676.02
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Different

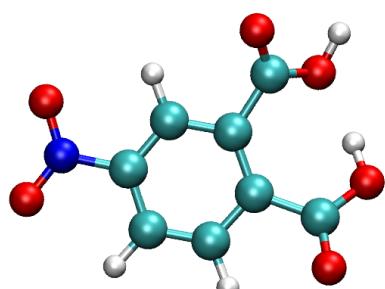


# FireTest Número 305

Molecule A 3NFAACe



Molecule B 4NFAACj



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

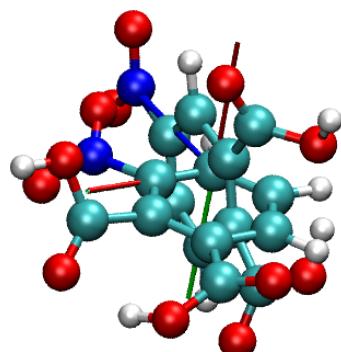
EigenValues - Molecule A

524.162	935.308	1359.22
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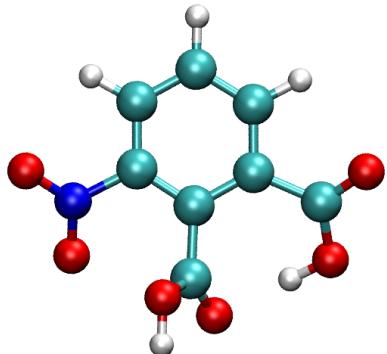
EigenValues - Molecule B

509.897	1225.65	1680.83
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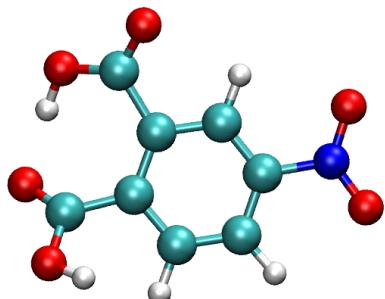
Different



Molecule A 3NFAACe



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

524.508	15.8785	-4.02001
15.8785	1358.65	10.8723
-4.02001	10.8723	935.54

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999764	0.0191573	-0.0102761
0.0107588	0.025269	-0.999623
0.0188904	0.999497	0.0254692

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

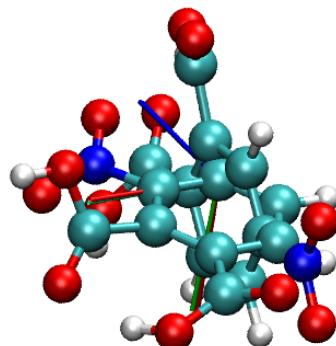
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

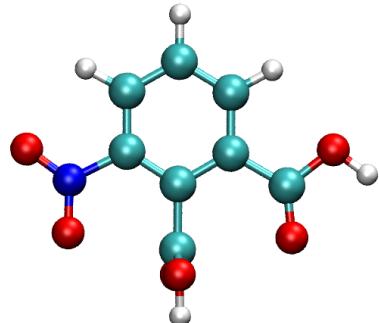
506.607	1222.36	1678.43
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Different

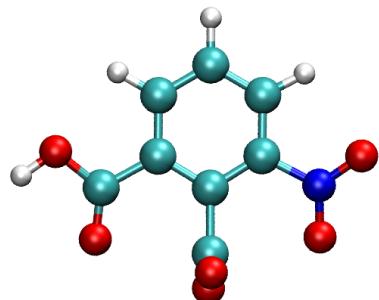


FireTest Número 307

Molecule A 3NFAACf



Molecule B 3NFAACg



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

EigenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EigenVectors - Molecule B

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

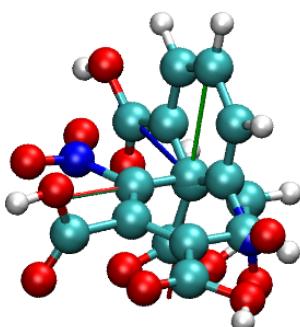
EigenValues - Molecule A

530.045	915.527	1360.79
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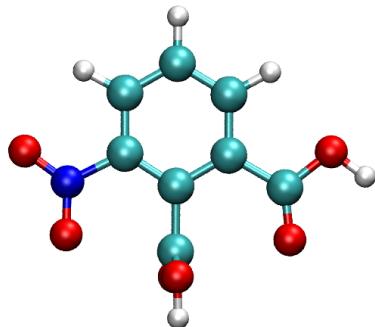
EigenValues - Molecule B

532.89	918.442	1356.93
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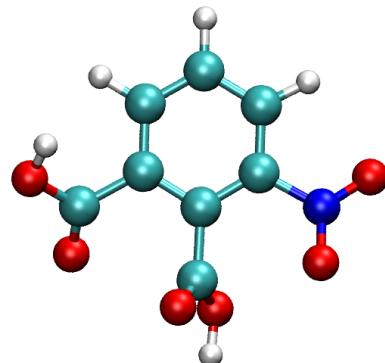
Different



Molecule A 3NFAACf



Molecule B 3NFAACh



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

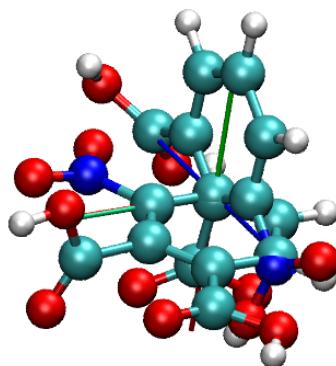
EingenValues - Molecule A

530.045	915.527	1360.79
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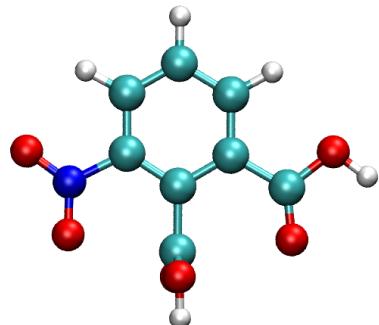
EingenValues - Molecule B

528.663	924.928	1336.12
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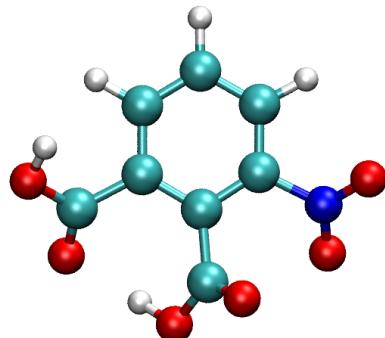
Different



Molecule A 3NFAACf



Molecule B 3NFAACi



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

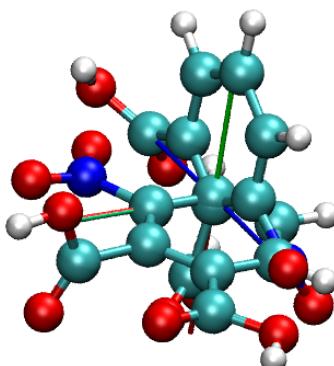
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

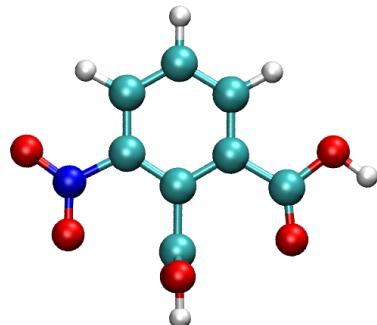
521.475	949.659	1346.18
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Different

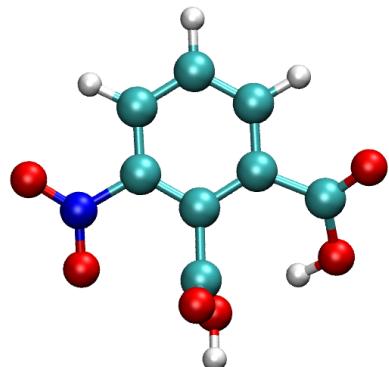


FireTest Número 310

Molecule A 3NFAACf



Molecule B 3NFAACj



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EigenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EigenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

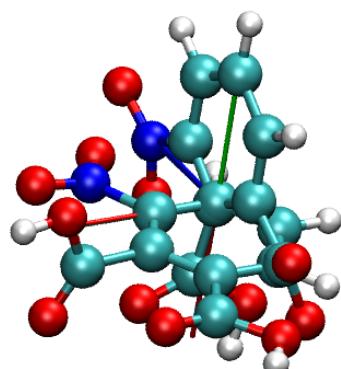
EigenValues - Molecule A

530.045	915.527	1360.79
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EigenValues - Molecule B

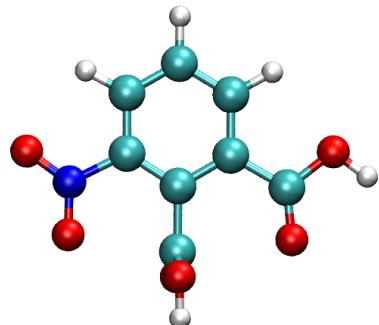
533.726	920.137	1348.3
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Different

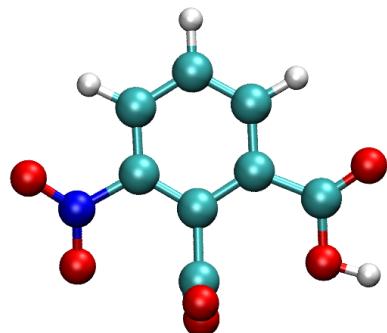


FireTest Número 311

Molecule A 3NFAACf



Molecule B 3NFAACK



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

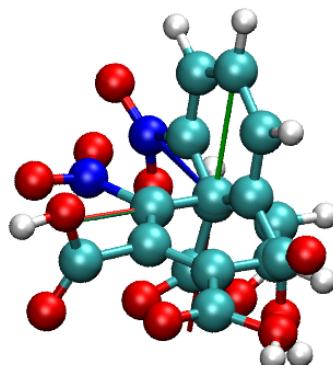
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

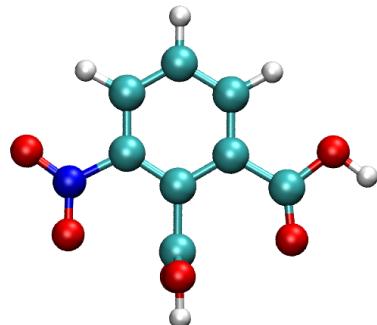
534.81	913.339	1353.78
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Different

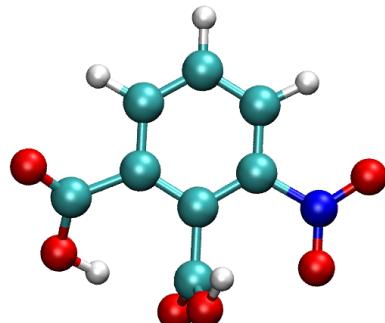


FireTest Número 312

Molecule A 3NFAACf



Molecule B 3NFAACl



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

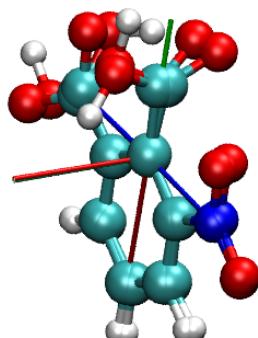
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

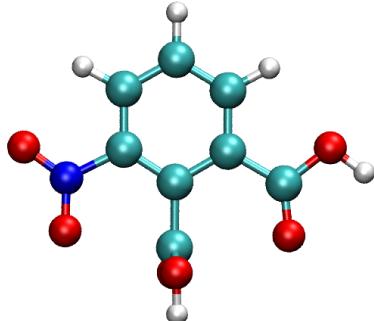
531.691	929.434	1355.4
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Different

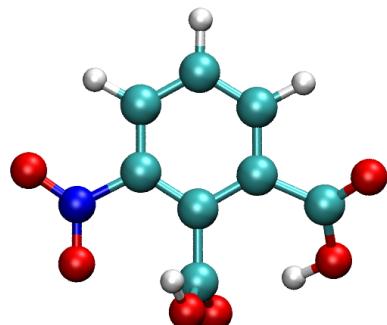


FireTest Número 313

Molecule A 3NFAACf



Molecule B 3NFAACm



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

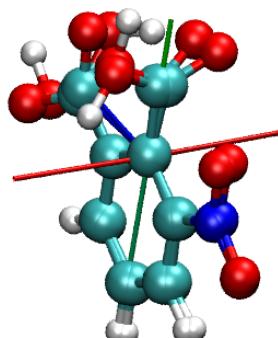
EingenValues - Molecule A

530.045	915.527	1360.79
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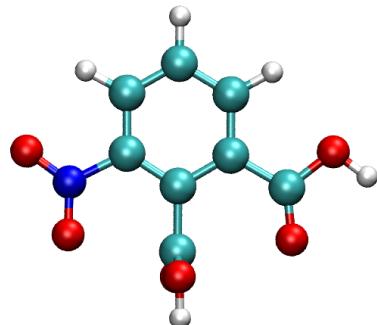
EingenValues - Molecule B

531.698	929.417	1355.4
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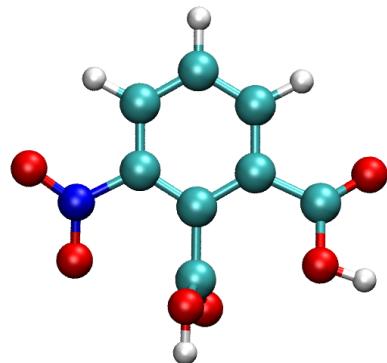
Different



Molecule A 3NFAACf



Molecule B 3NFAACn



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

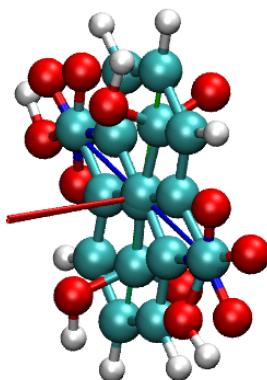
EingenValues - Molecule A

530.045	915.527	1360.79
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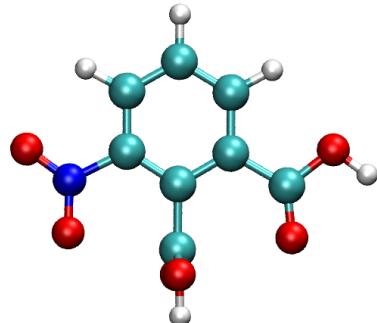
EingenValues - Molecule B

531.43	913.309	1353.35
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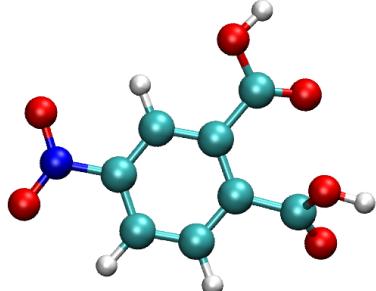
Different



Molecule A 3NFAACf



Molecule B 4NFAACa



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

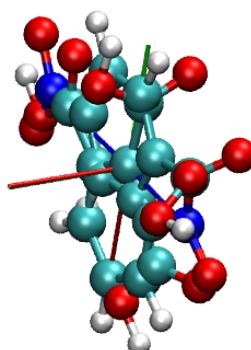
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

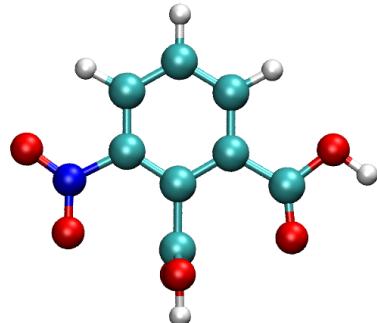
479.363	1242.41	1647.39
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Different

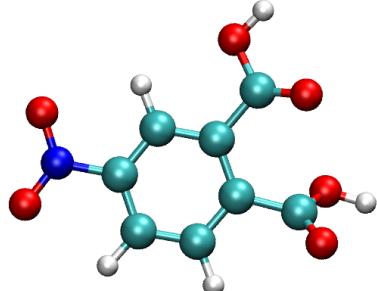


FireTest Número 316

Molecule A 3NFAACf



Molecule B 4NFAACb



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

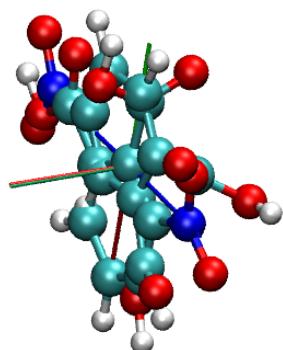
EingenValues - Molecule A

530.045	915.527	1360.79
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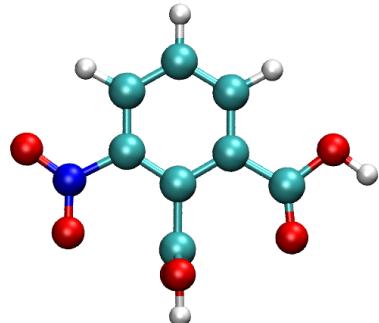
EingenValues - Molecule B

479.308	1242.41	1647.31
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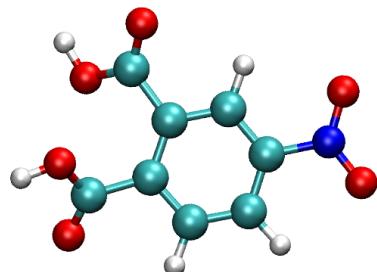
Different



Molecule A 3NFAACf



Molecule B 4NFAACC



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

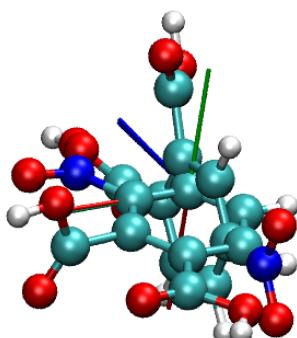
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

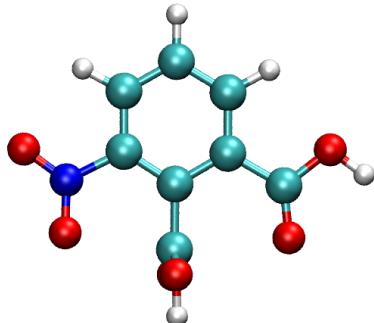
482.027	1240.32	1647.08
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Different

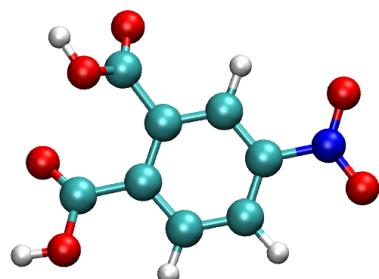


FireTest Número 318

Molecule A 3NFAACf



Molecule B 4NFAACd



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

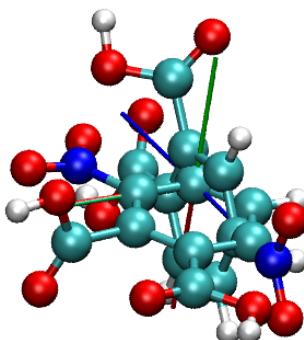
EingenValues - Molecule A

530.045	915.527	1360.79
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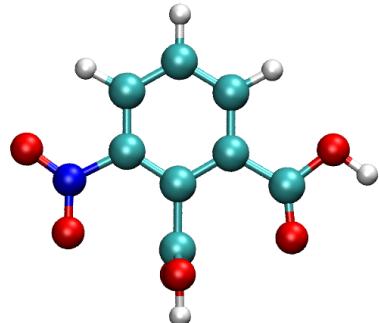
EingenValues - Molecule B

491.663	1231.14	1650.13
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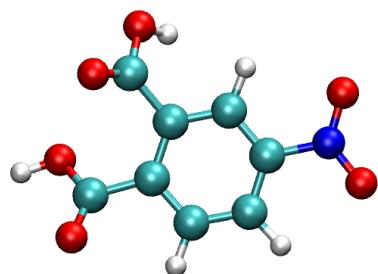
Different



Molecule A 3NFAACf



Molecule B 4NFAACe



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

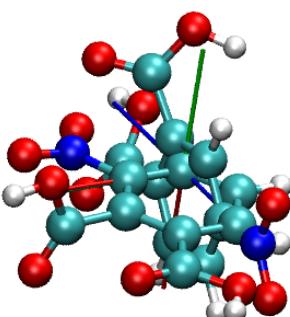
EingenValues - Molecule A

530.045	915.527	1360.79
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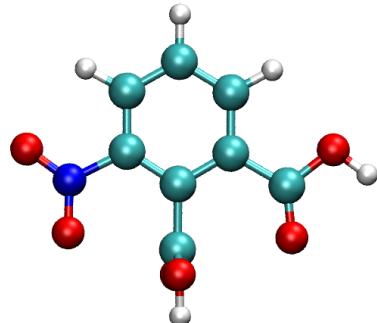
EingenValues - Molecule B

489.011	1233.7	1641.81
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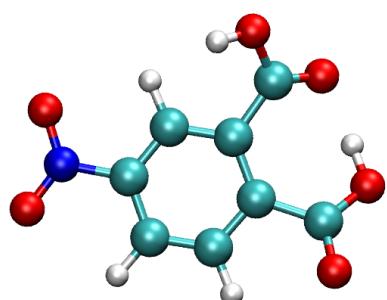
Different



Molecule A 3NFAACf



Molecule B 4NFAACf



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

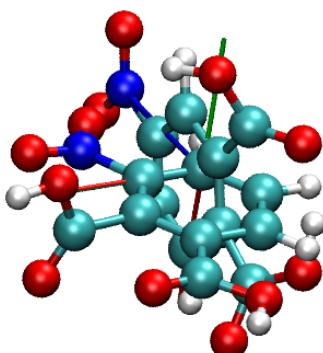
EingenValues - Molecule A

530.045	915.527	1360.79
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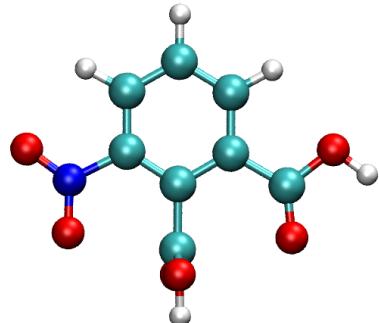
EingenValues - Molecule B

509.668	1219.11	1681.18
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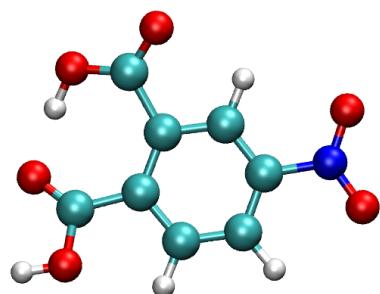
Different



Molecule A 3NFAACf



Molecule B 4NFAACg



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

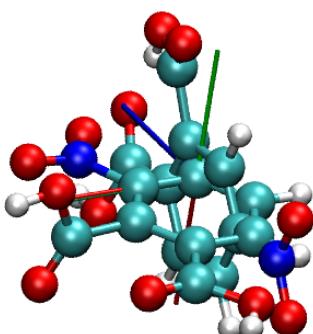
EingenValues - Molecule A

530.045	915.527	1360.79
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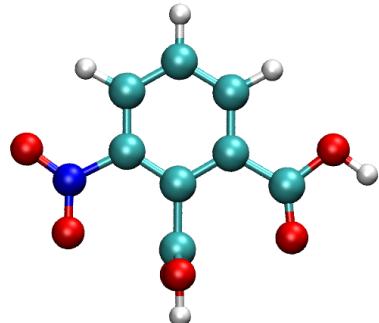
EingenValues - Molecule B

513.751	1208.07	1700.9
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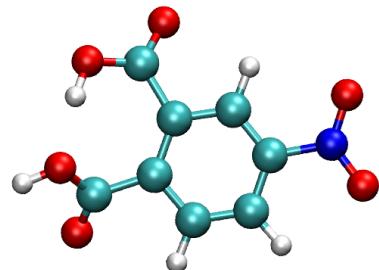
Different



Molecule A 3NFAACf



Molecule B 4NFAACi



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

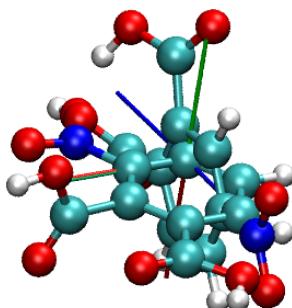
EingenValues - Molecule A

530.045	915.527	1360.79
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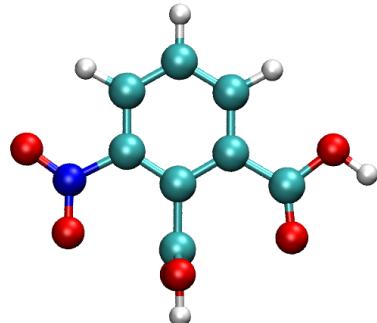
EingenValues - Molecule B

502.409	1232.26	1676.02
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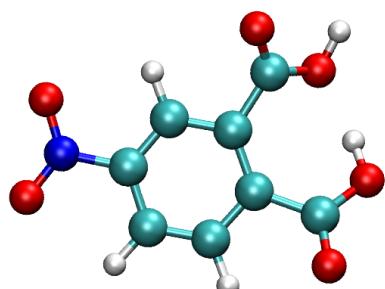
Different



Molecule A 3NFAACf



Molecule B 4NFAACj



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

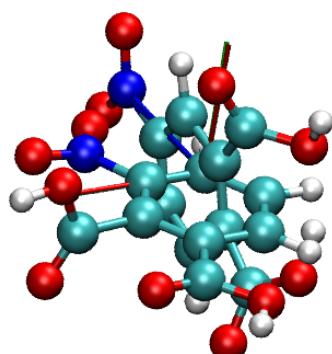
EingenValues - Molecule A

530.045	915.527	1360.79
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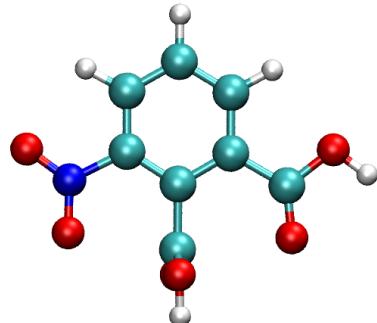
EingenValues - Molecule B

509.897	1225.65	1680.83
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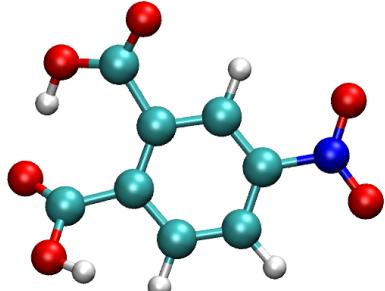
Different



Molecule A 3NFAACf



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

530.208	-1.63273	-7.84857
-1.63273	1360.76	-3.6411
-7.84857	-3.6411	915.396

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.99979	-0.00205437	-0.0203824
-0.0203985	0.00810116	0.999759
-0.00188875	0.999965	-0.00814137

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

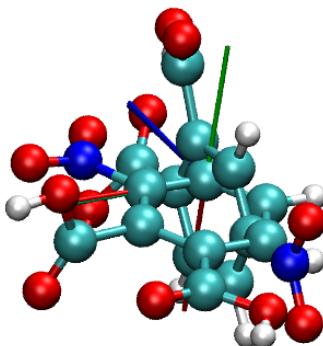
EingenValues - Molecule A

530.045	915.527	1360.79
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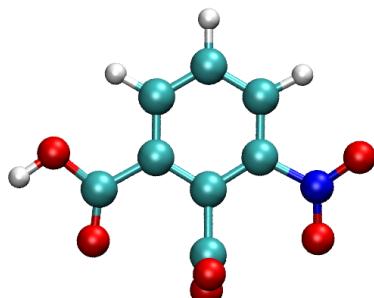
EingenValues - Molecule B

506.607	1222.36	1678.43
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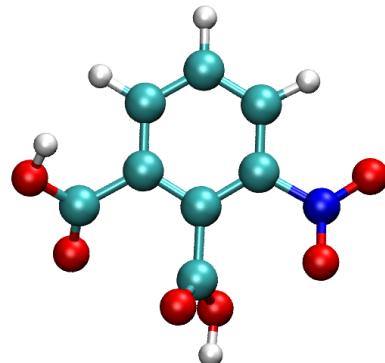
Different



Molecule A 3NFAACg



Molecule B 3NFAACh



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

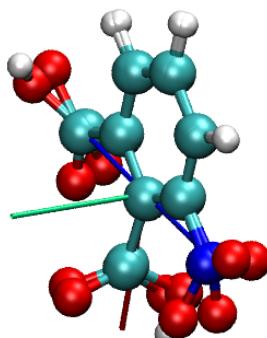
EingenValues - Molecule A

532.89	918.442	1356.93
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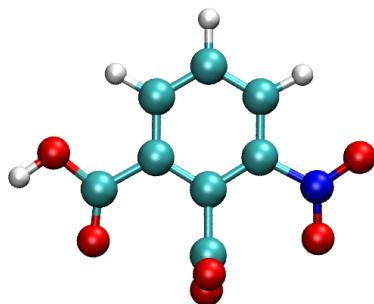
EingenValues - Molecule B

528.663	924.928	1336.12
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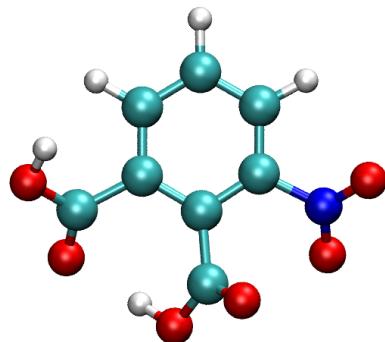
Different



Molecule A 3NFAACg



Molecule B 3NFAACi



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

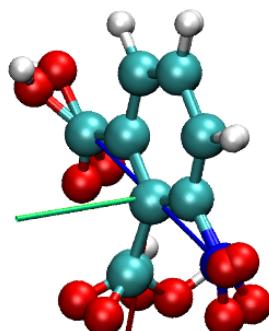
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

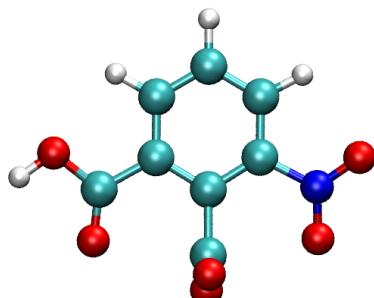
521.475	949.659	1346.18
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Different

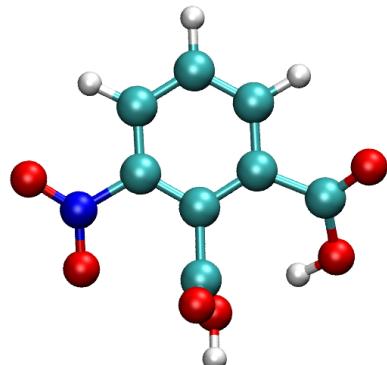


FireTest Número 327

Molecule A 3NFAACg



Molecule B 3NFAACj



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

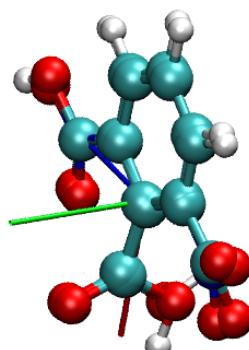
EingenValues - Molecule A

532.89	918.442	1356.93
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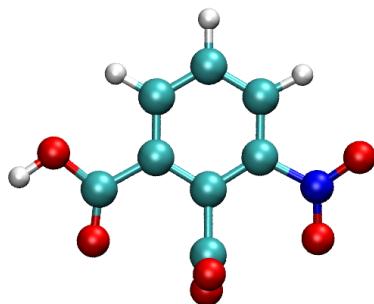
EingenValues - Molecule B

533.726	920.137	1348.3
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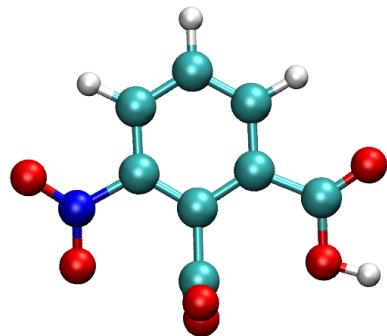
Different



Molecule A 3NFAACg



Molecule B 3NFAACK



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

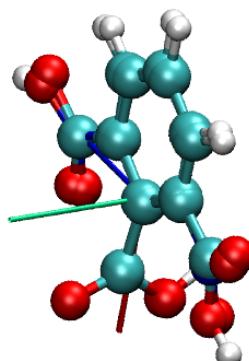
EingenValues - Molecule A

532.89	918.442	1356.93
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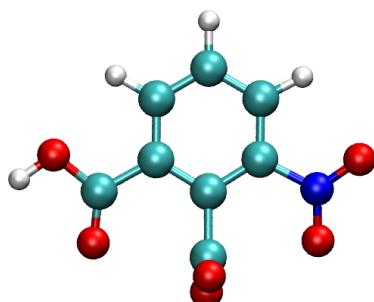
EingenValues - Molecule B

534.81	913.339	1353.78
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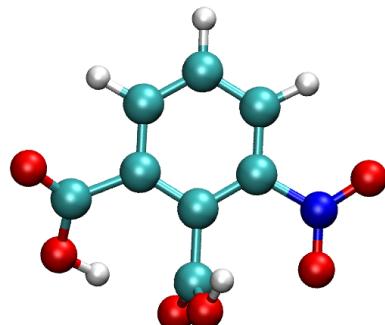
Different



Molecule A 3NFAACg



Molecule B 3NFAACl



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

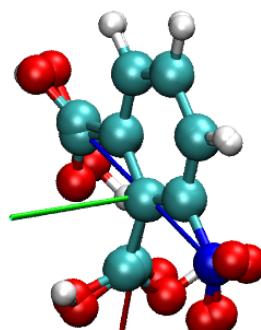
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

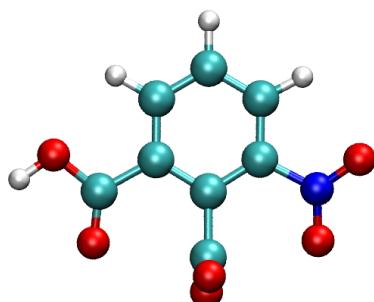
531.691	929.434	1355.4
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Different

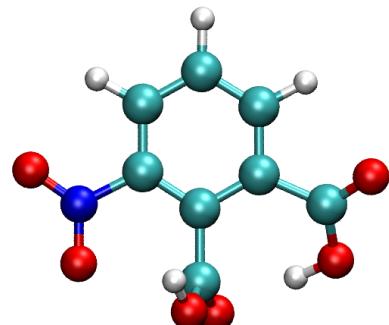


FireTest Número 330

Molecule A 3NFAACg



Molecule B 3NFAACm



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

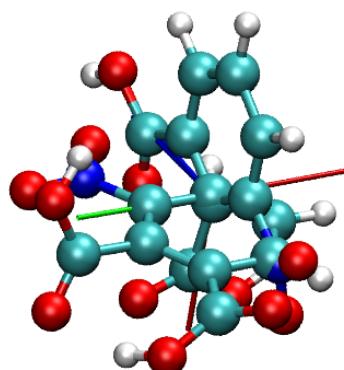
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

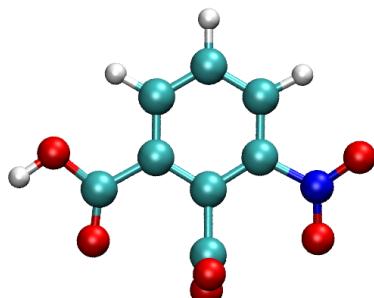
531.698	929.417	1355.4
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Different

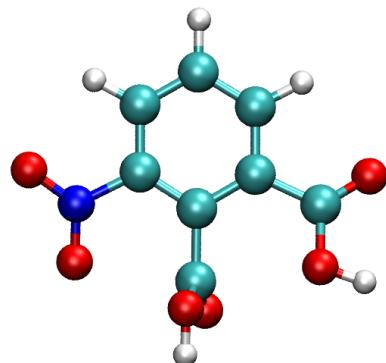


FireTest Número 331

Molecule A 3NFAACg



Molecule B 3NFAACn



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

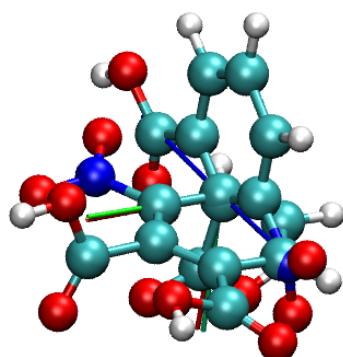
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

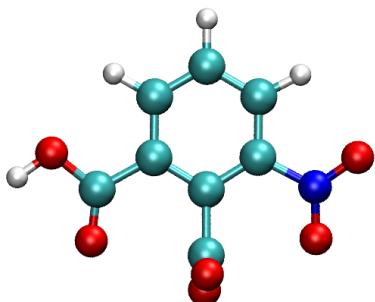
531.43	913.309	1353.35
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Different

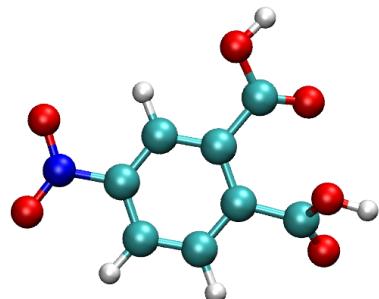


# FireTest Número 332

Molecule A 3NFAACg



Molecule B 4NFAACa



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

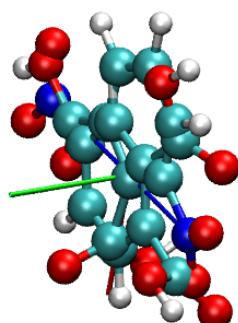
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

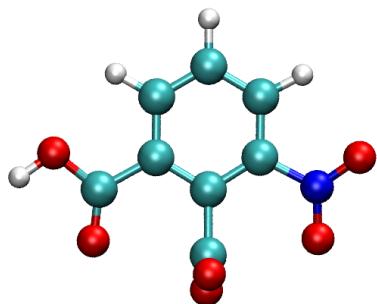
479.363	1242.41	1647.39
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Different

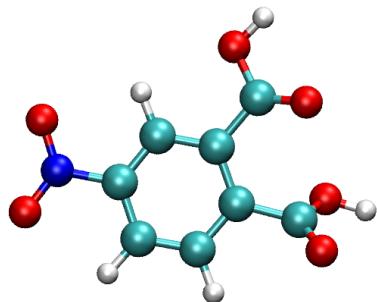


# FireTest Número 333

Molecule A 3NFAACg



Molecule B 4NFAACb



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

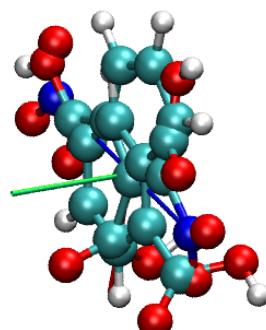
EingenValues - Molecule A

532.89	918.442	1356.93
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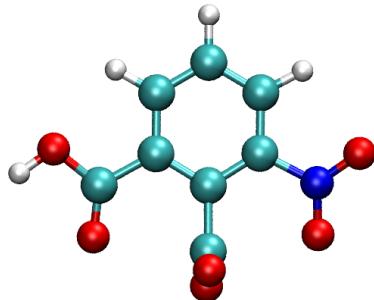
EingenValues - Molecule B

479.308	1242.41	1647.31
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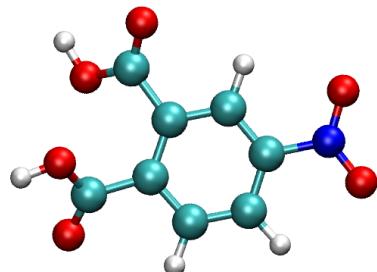
Different



Molecule A 3NFAACg



Molecule B 4NFAACC



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

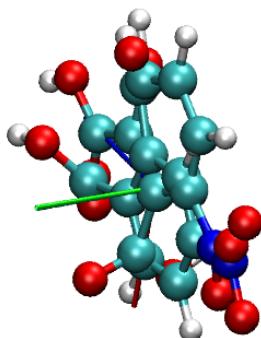
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

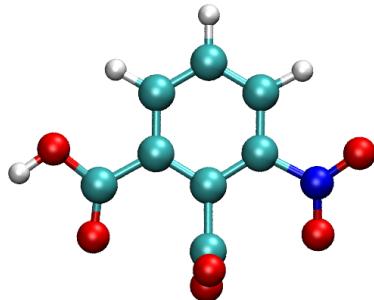
482.027	1240.32	1647.08
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Different

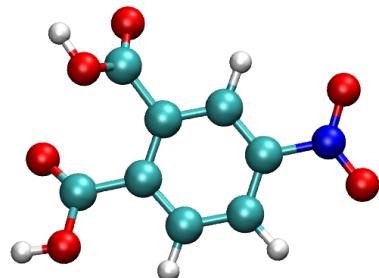


FireTest Número 335

Molecule A 3NFAACg



Molecule B 4NFAACd



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

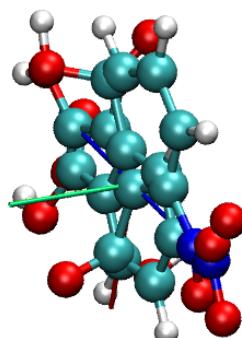
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

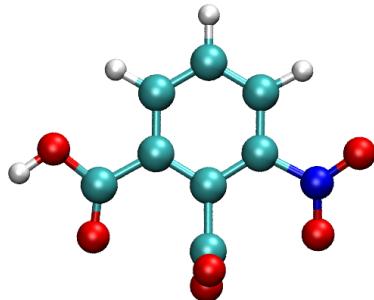
491.663	1231.14	1650.13
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Different

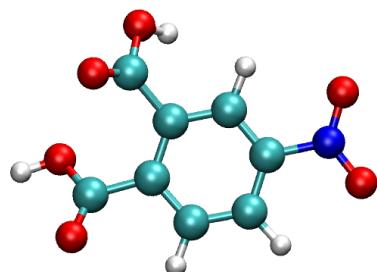


FireTest Número 336

Molecule A 3NFAACg



Molecule B 4NFAACe



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

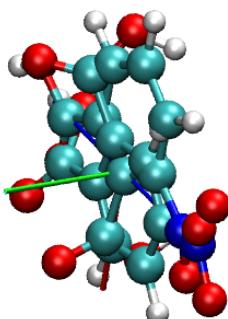
EingenValues - Molecule A

532.89	918.442	1356.93
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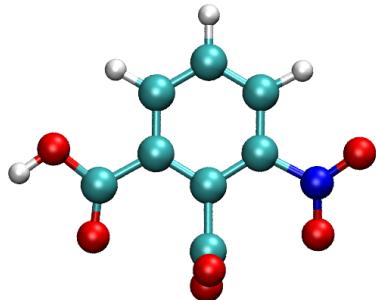
EingenValues - Molecule B

489.011	1233.7	1641.81
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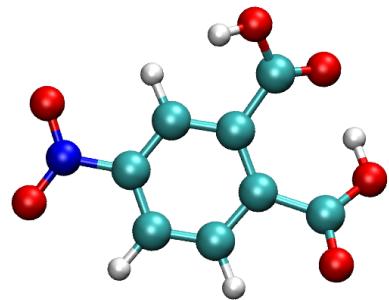
Different



Molecule A 3NFAACg



Molecule B 4NFAACf



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

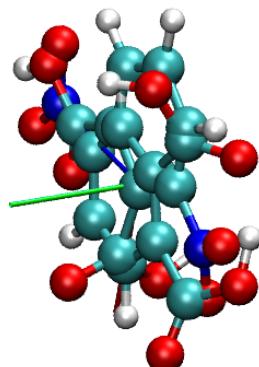
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

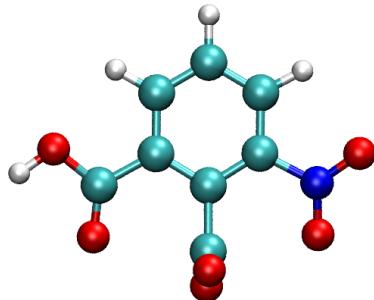
509.668	1219.11	1681.18
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Different

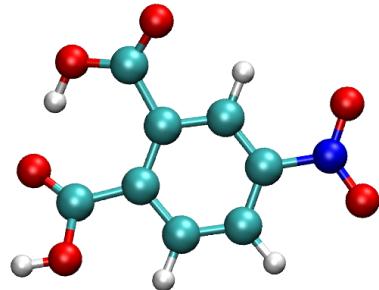


FireTest Número 338

Molecule A 3NFAACg



Molecule B 4NFAACg



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

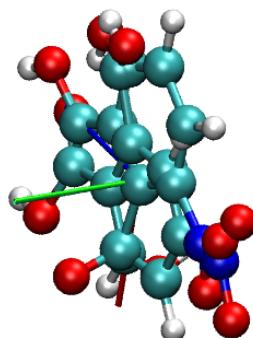
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

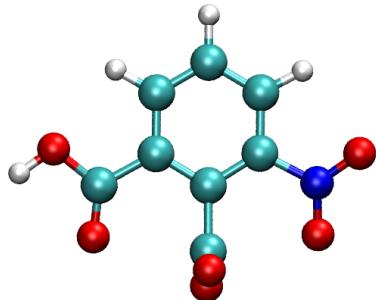
513.751	1208.07	1700.9
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Different

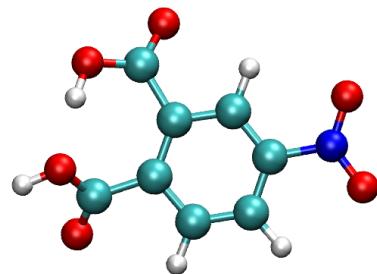


FireTest Número 339

Molecule A 3NFAACg



Molecule B 4NFAACi



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

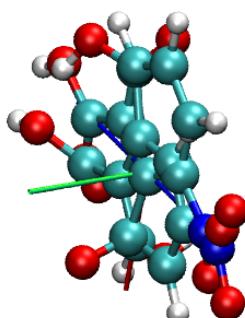
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

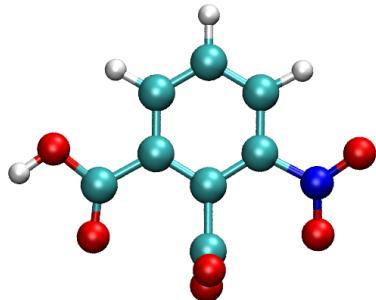
502.409	1232.26	1676.02
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Different

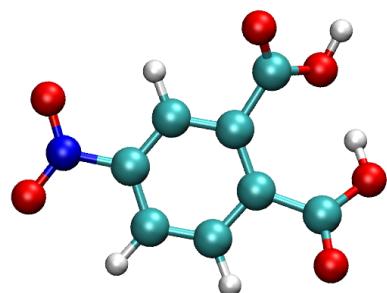


FireTest Número 340

Molecule A 3NFAACg



Molecule B 4NFAACj



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

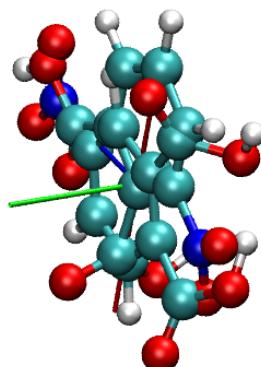
EingenValues - Molecule A

532.89	918.442	1356.93
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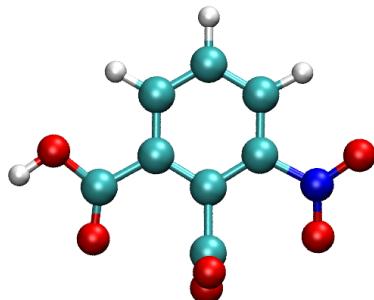
EingenValues - Molecule B

509.897	1225.65	1680.83
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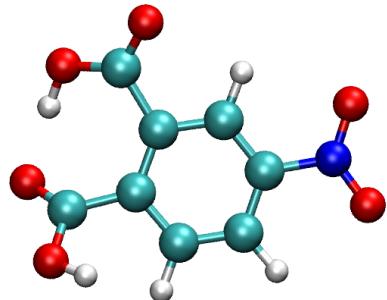
Different



Molecule A 3NFAACg



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

532.891	-0.526938	-0.504713
-0.526938	918.454	2.35809
-0.504713	2.35809	1356.91

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999999	-0.00136295	-0.000608598
0.00135965	-0.999985	0.00537946
-0.000615921	0.00537863	0.999985

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

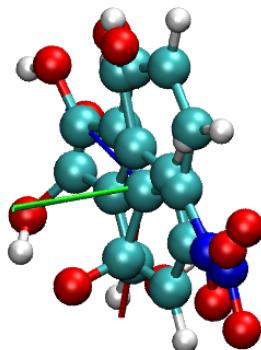
EingenValues - Molecule A

532.89	918.442	1356.93
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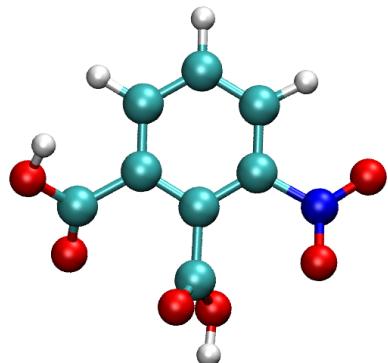
EingenValues - Molecule B

506.607	1222.36	1678.43
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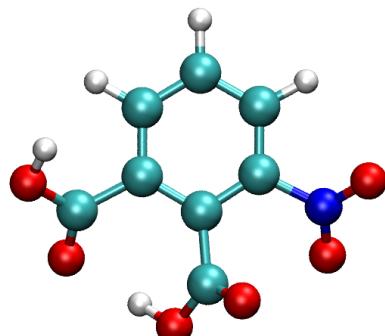
Different



Molecule A 3NFAACh



Molecule B 3NFAACi



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

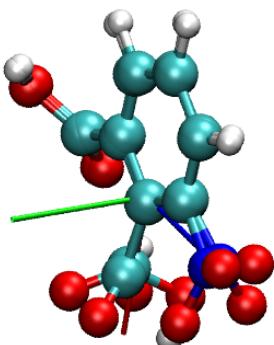
EingenValues - Molecule A

528.663	924.928	1336.12
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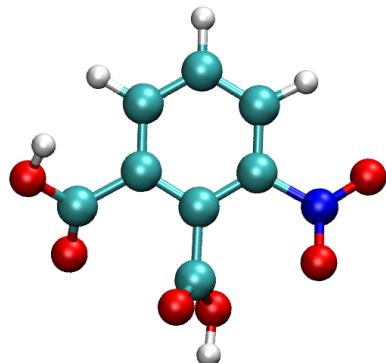
EingenValues - Molecule B

521.475	949.659	1346.18
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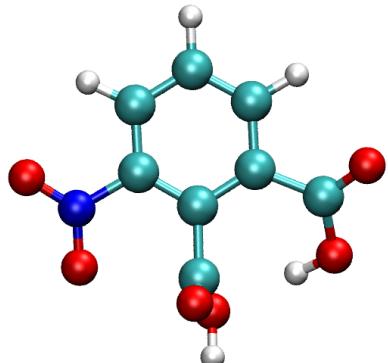
Different



Molecule A 3NFAACh



Molecule B 3NFAACj



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

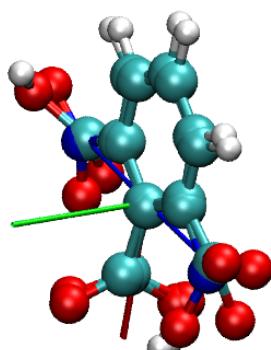
EingenValues - Molecule A

528.663	924.928	1336.12
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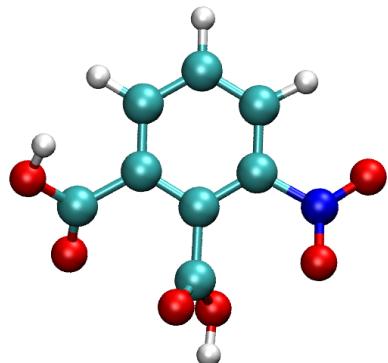
EingenValues - Molecule B

533.726	920.137	1348.3
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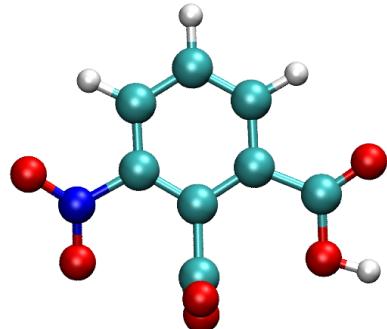
Different



Molecule A 3NFAACh



Molecule B 3NFAACK



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

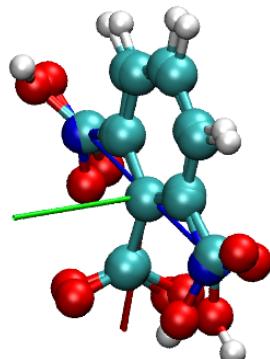
EingenValues - Molecule A

528.663	924.928	1336.12
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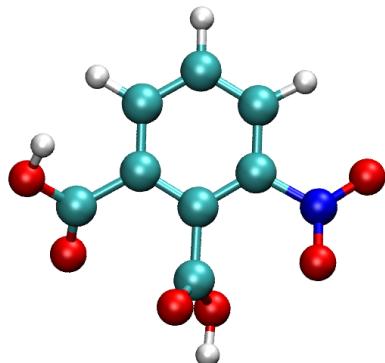
EingenValues - Molecule B

534.81	913.339	1353.78
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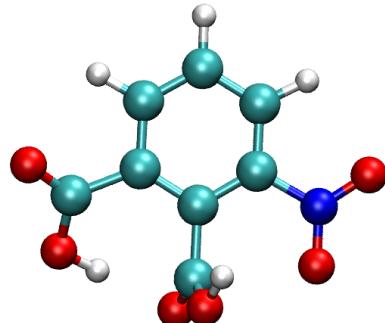
Different



Molecule A 3NFAACh



Molecule B 3NFAACl



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

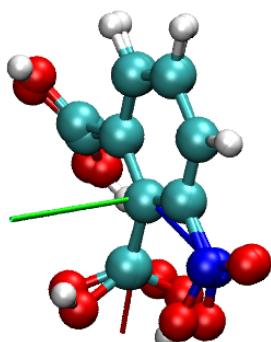
EingenValues - Molecule A

528.663	924.928	1336.12
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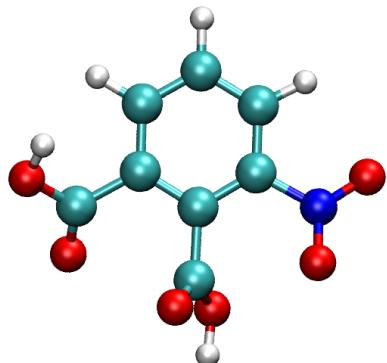
EingenValues - Molecule B

531.691	929.434	1355.4
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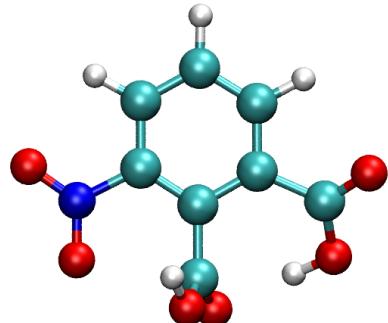
Different



Molecule A 3NFAACh



Molecule B 3NFAACm



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

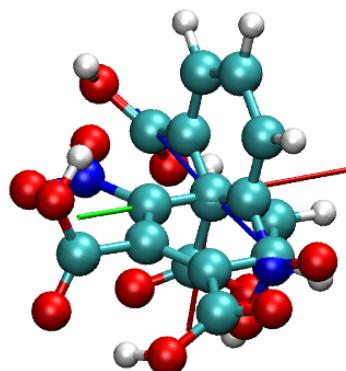
EingenValues - Molecule A

528.663	924.928	1336.12
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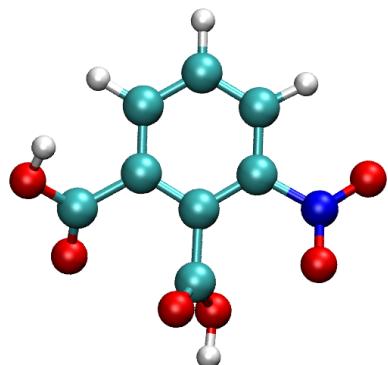
EingenValues - Molecule B

531.698	929.417	1355.4
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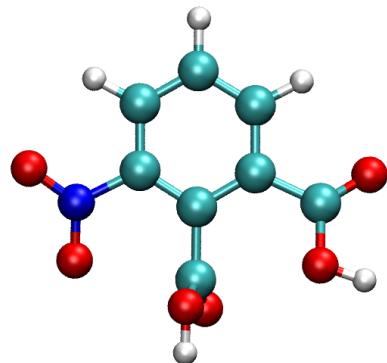
Different



Molecule A 3NFAACh



Molecule B 3NFAACn



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

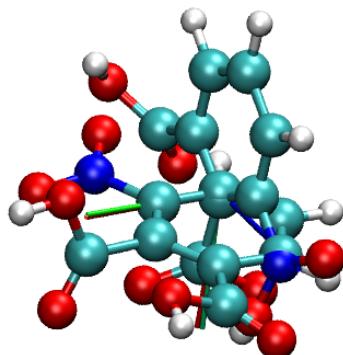
EingenValues - Molecule A

528.663	924.928	1336.12
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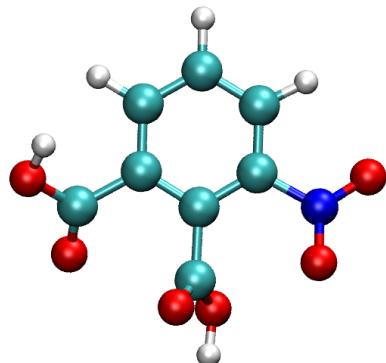
EingenValues - Molecule B

531.43	913.309	1353.35
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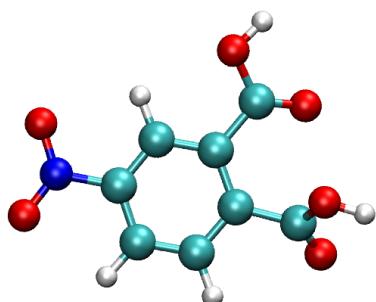
Different



Molecule A 3NFAACh



Molecule B 4NFAACa



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

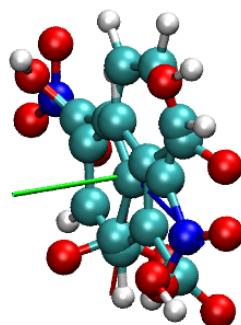
EingenValues - Molecule A

528.663	924.928	1336.12
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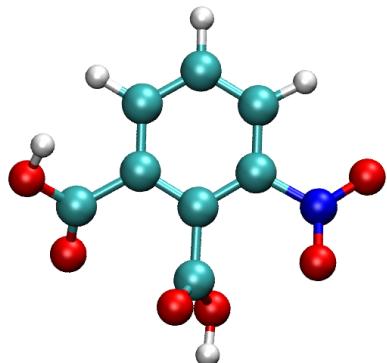
EingenValues - Molecule B

479.363	1242.41	1647.39
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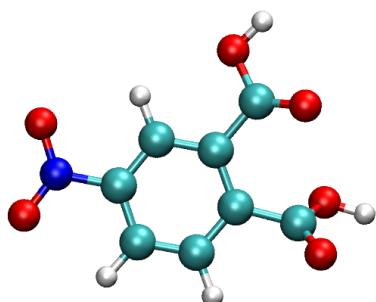
Different



Molecule A 3NFAACh



Molecule B 4NFAACb



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

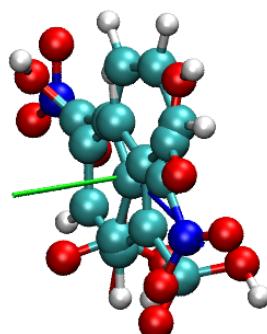
EingenValues - Molecule A

528.663	924.928	1336.12
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EingenValues - Molecule B

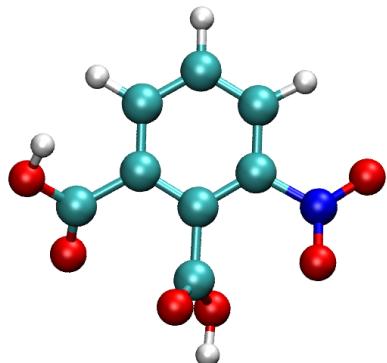
479.308	1242.41	1647.31
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Different

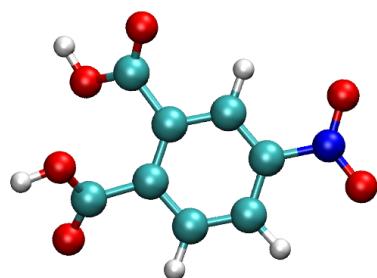


FireTest Número 350

Molecule A 3NFAACh



Molecule B 4NFAACC



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

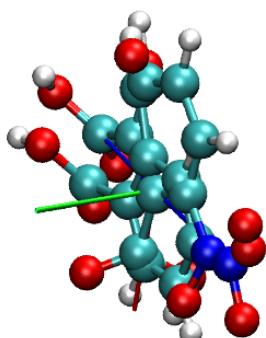
EingenValues - Molecule A

528.663	924.928	1336.12
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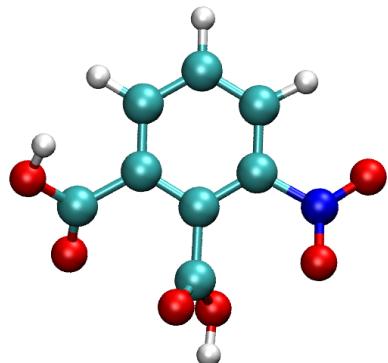
EingenValues - Molecule B

482.027	1240.32	1647.08
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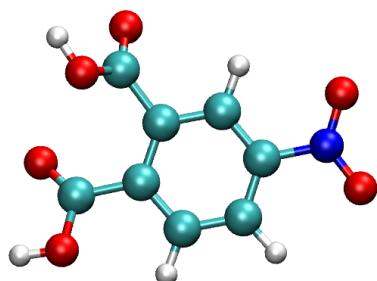
Different



Molecule A 3NFAACh



Molecule B 4NFAACd



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

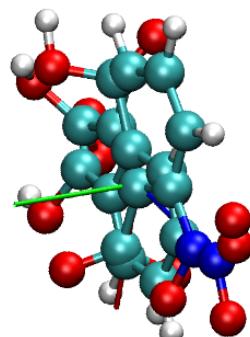
EingenValues - Molecule A

528.663	924.928	1336.12
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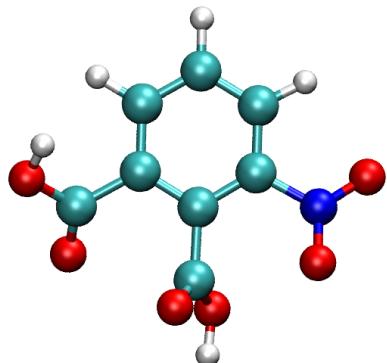
EingenValues - Molecule B

491.663	1231.14	1650.13
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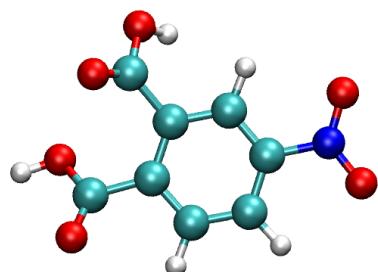
Different



Molecule A 3NFAACh



Molecule B 4NFAACe



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

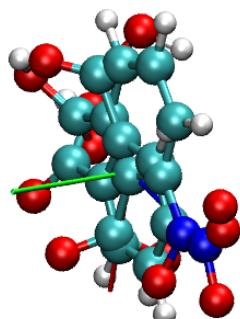
EingenValues - Molecule A

528.663	924.928	1336.12
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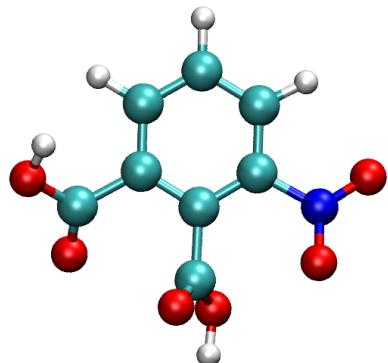
EingenValues - Molecule B

489.011	1233.7	1641.81
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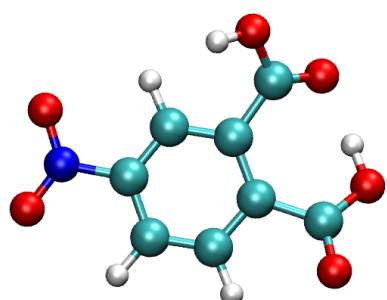
Different



Molecule A 3NFAACh



Molecule B 4NFAACf



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

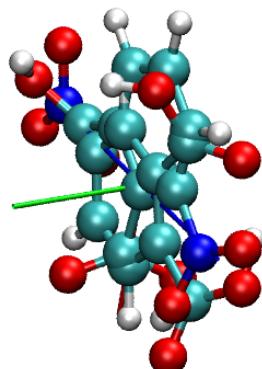
EingenValues - Molecule A

528.663	924.928	1336.12
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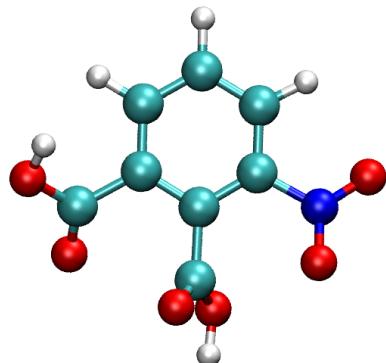
EingenValues - Molecule B

509.668	1219.11	1681.18
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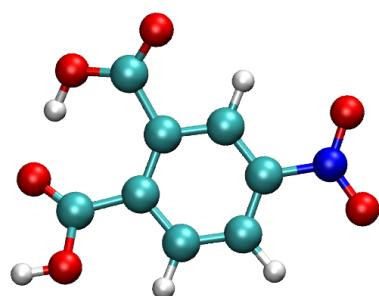
Different



Molecule A 3NFAACh



Molecule B 4NFAACg



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

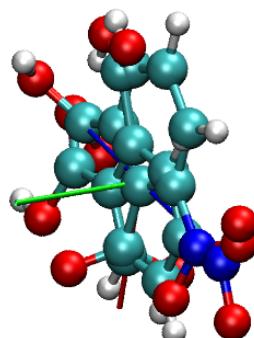
EingenValues - Molecule A

528.663	924.928	1336.12
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EingenValues - Molecule B

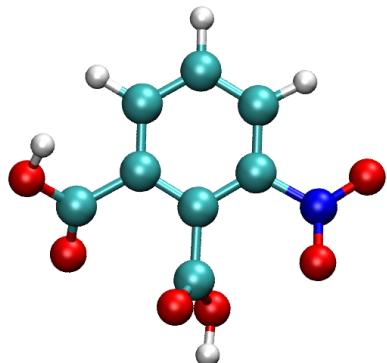
513.751	1208.07	1700.9
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Different

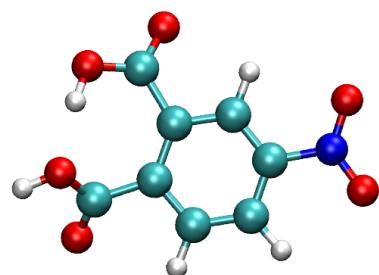


FireTest Número 355

Molecule A 3NFAACh



Molecule B 4NFAACi



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

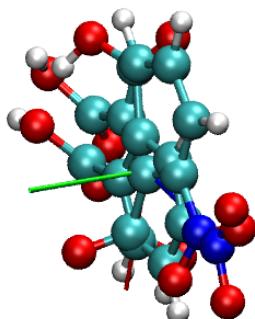
EingenValues - Molecule A

528.663	924.928	1336.12
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EingenValues - Molecule B

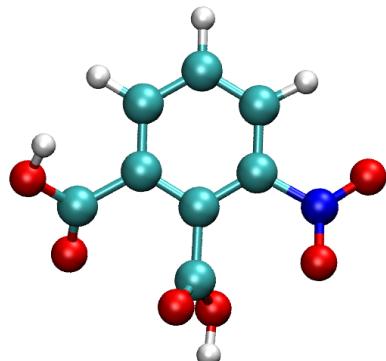
502.409	1232.26	1676.02
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Different

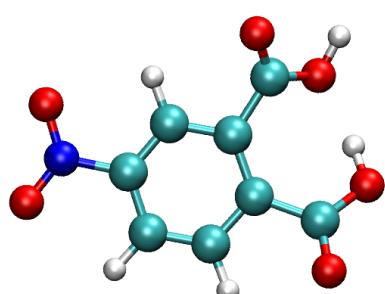


FireTest Número 356

Molecule A 3NFAACh



Molecule B 4NFAACj



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

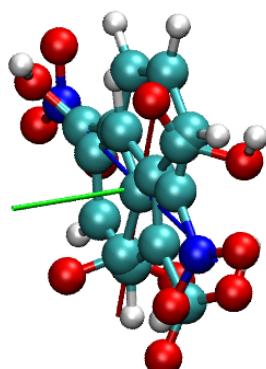
EigenValues - Molecule A

528.663	924.928	1336.12
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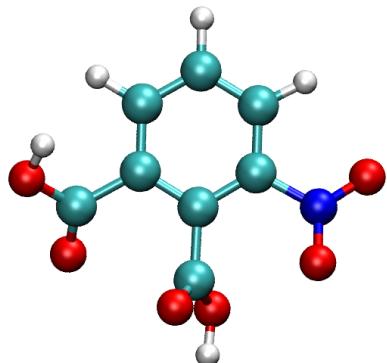
EigenValues - Molecule B

509.897	1225.65	1680.83
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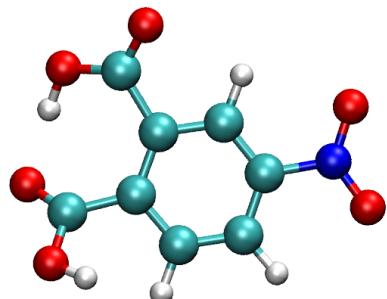
Different



Molecule A 3NFAACh



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

528.718	-3.89066	-3.66882
-3.89066	924.911	2.93817
-3.66882	2.93817	1336.08

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

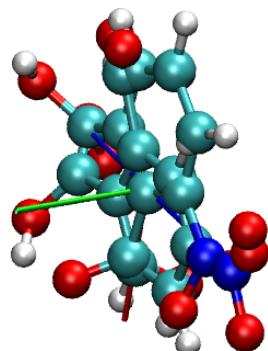
EingenValues - Molecule A

528.663	924.928	1336.12
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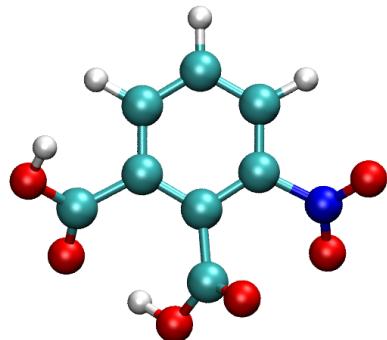
EingenValues - Molecule B

506.607	1222.36	1678.43
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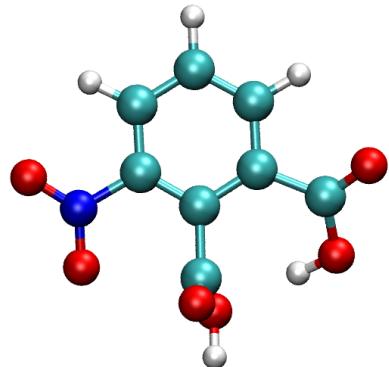
Different



Molecule A 3NFAACi



Molecule B 3NFAACj



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

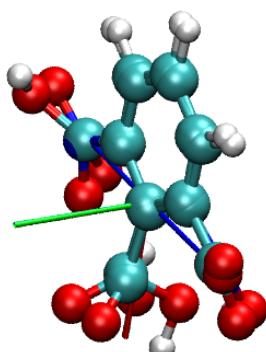
EingenValues - Molecule A

521.475	949.659	1346.18
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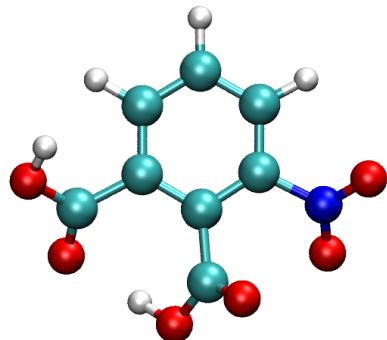
EingenValues - Molecule B

533.726	920.137	1348.3
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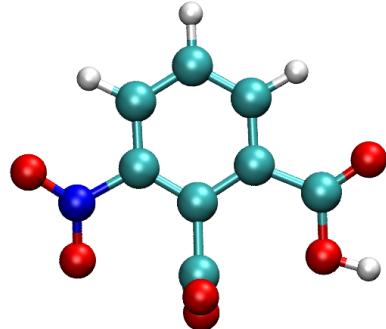
Different



Molecule A 3NFAACi



Molecule B 3NFAACK



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

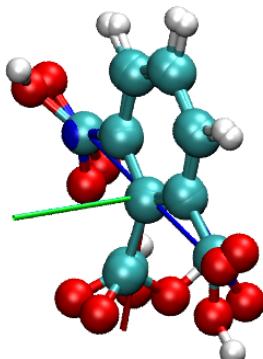
EingenValues - Molecule A

521.475	949.659	1346.18
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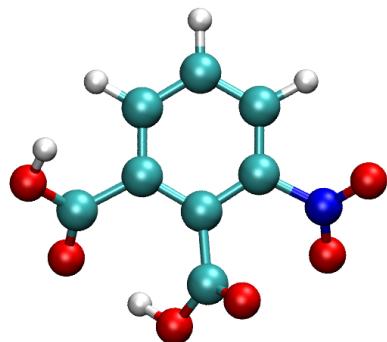
EingenValues - Molecule B

534.81	913.339	1353.78
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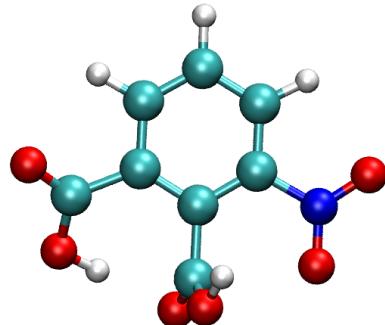
Different



Molecule A 3NFAACi



Molecule B 3NFAACl



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

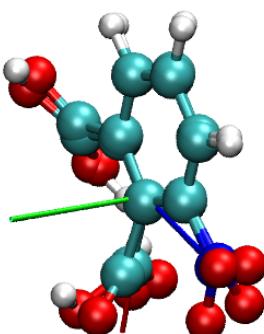
EingenValues - Molecule A

521.475	949.659	1346.18
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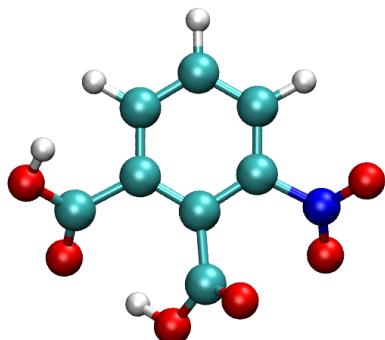
EingenValues - Molecule B

531.691	929.434	1355.4
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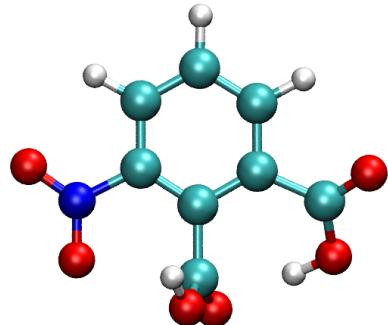
Different



Molecule A 3NFAACi



Molecule B 3NFAACm



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

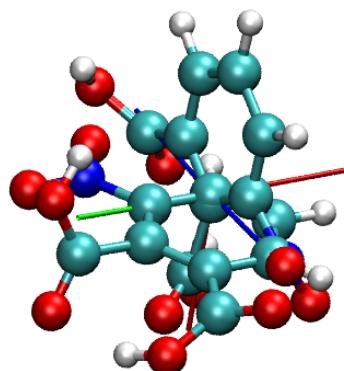
EingenValues - Molecule A

521.475	949.659	1346.18
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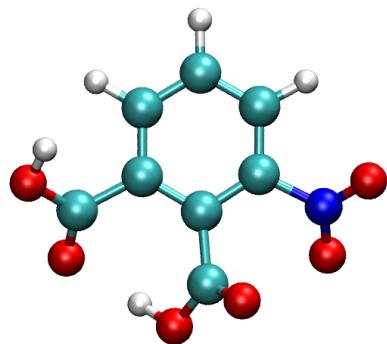
EingenValues - Molecule B

531.698	929.417	1355.4
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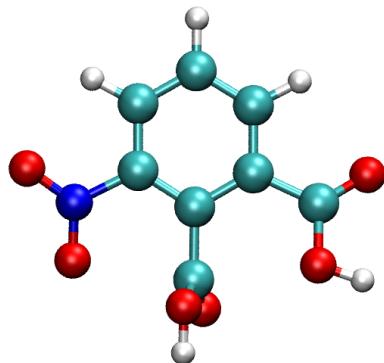
Different



Molecule A 3NFAACi



Molecule B 3NFAACn



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

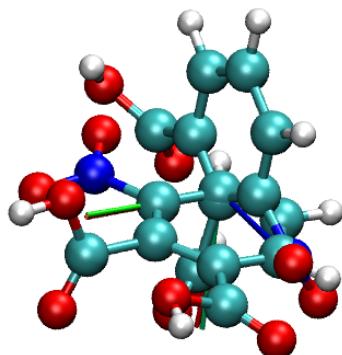
EingenValues - Molecule A

521.475	949.659	1346.18
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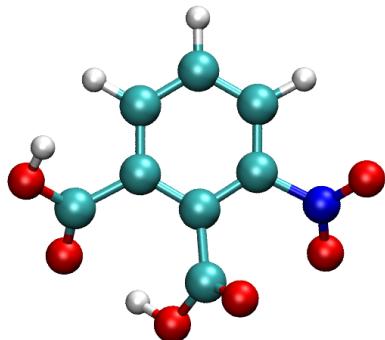
EingenValues - Molecule B

531.43	913.309	1353.35
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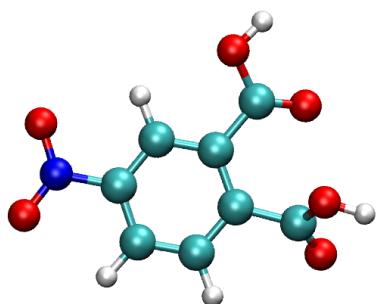
Different



Molecule A 3NFAACi



Molecule B 4NFAACa



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

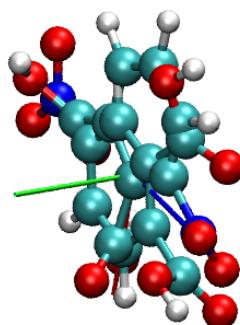
EingenValues - Molecule A

521.475	949.659	1346.18
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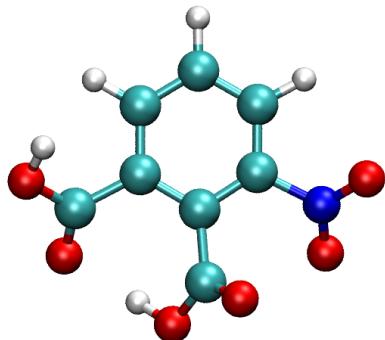
EingenValues - Molecule B

479.363	1242.41	1647.39
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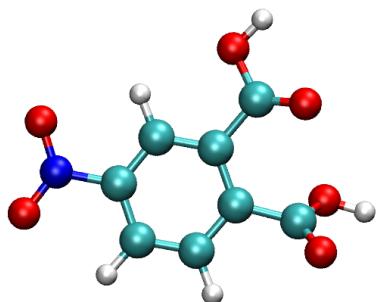
Different



Molecule A 3NFAACi



Molecule B 4NFAACb



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

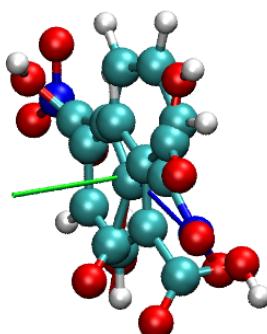
EingenValues - Molecule A

521.475	949.659	1346.18
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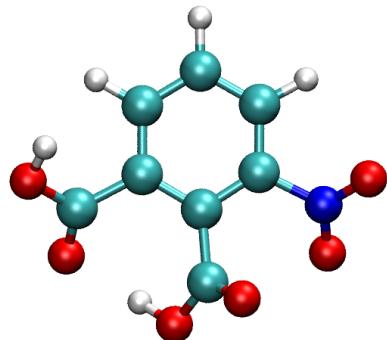
EingenValues - Molecule B

479.308	1242.41	1647.31
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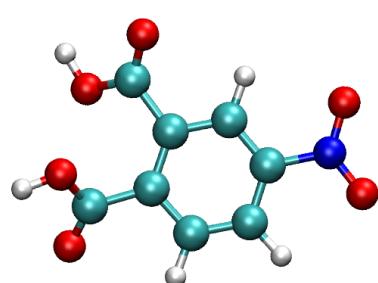
Different



Molecule A 3NFAACi



Molecule B 4NFAACCc



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

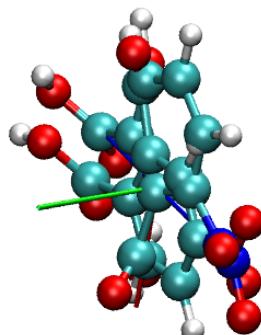
EingenValues - Molecule A

521.475	949.659	1346.18
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EingenValues - Molecule B

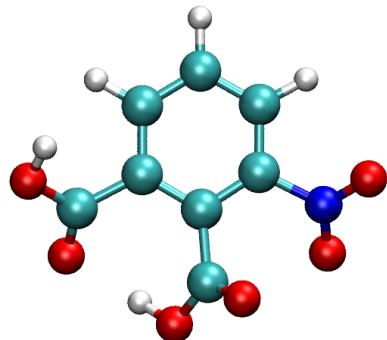
482.027	1240.32	1647.08
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Different

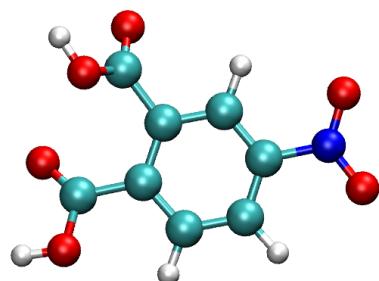


# FireTest Número 366

Molecule A 3NFAACi



Molecule B 4NFAACd



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

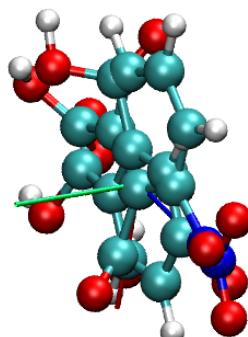
EingenValues - Molecule A

521.475	949.659	1346.18
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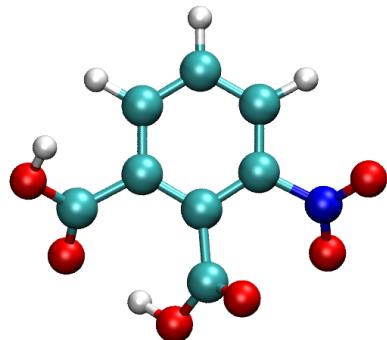
EingenValues - Molecule B

491.663	1231.14	1650.13
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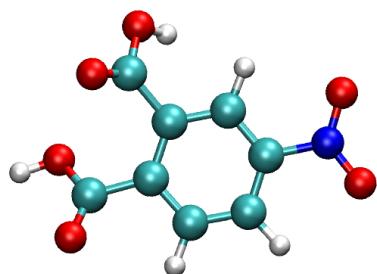
Different



Molecule A 3NFAACi



Molecule B 4NFAACe



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

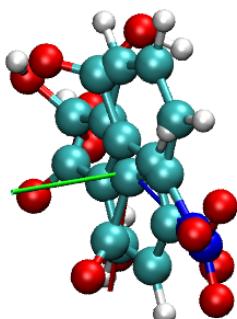
EingenValues - Molecule A

521.475	949.659	1346.18
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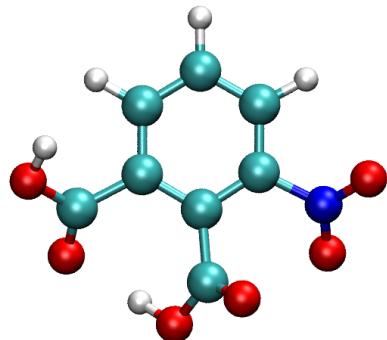
EingenValues - Molecule B

489.011	1233.7	1641.81
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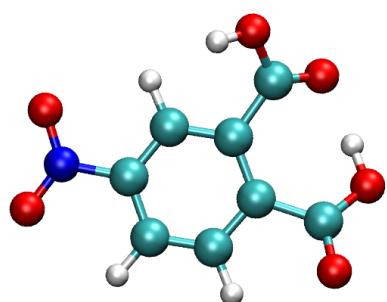
Different



Molecule A 3NFAACi



Molecule B 4NFAACf



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

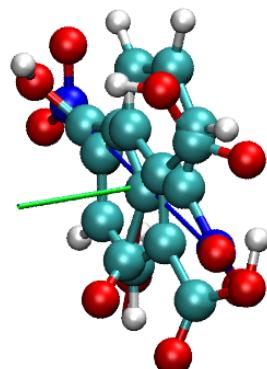
EingenValues - Molecule A

521.475	949.659	1346.18
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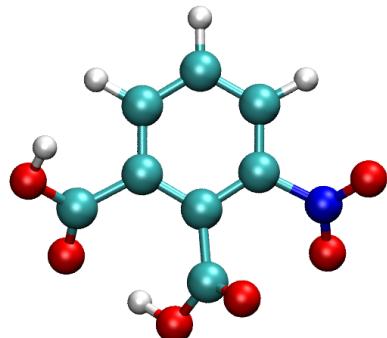
EingenValues - Molecule B

509.668	1219.11	1681.18
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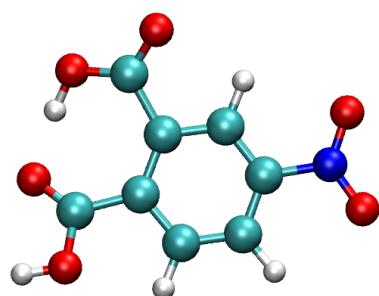
Different



Molecule A 3NFAACi



Molecule B 4NFAACg



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

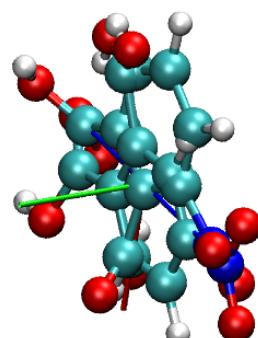
EingenValues - Molecule A

521.475	949.659	1346.18
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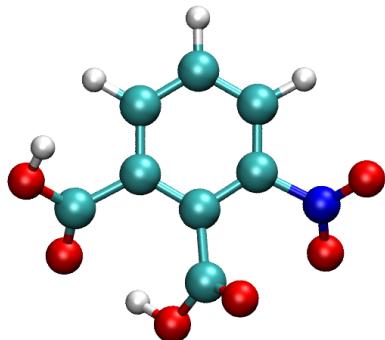
EingenValues - Molecule B

513.751	1208.07	1700.9
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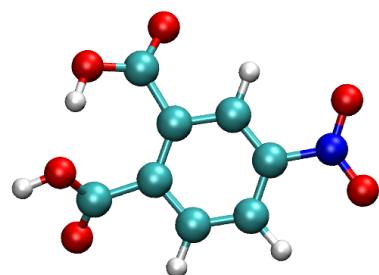
Different



Molecule A 3NFAACi



Molecule B 4NFAACi



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

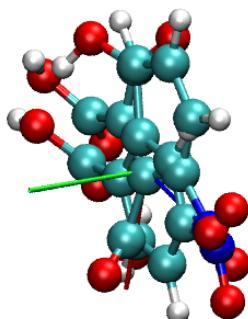
EingenValues - Molecule A

521.475	949.659	1346.18
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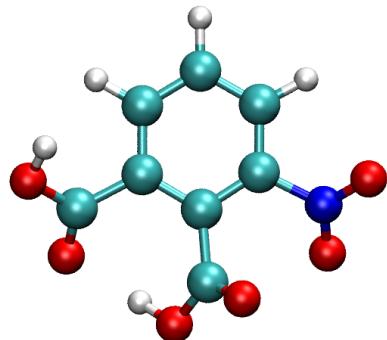
EingenValues - Molecule B

502.409	1232.26	1676.02
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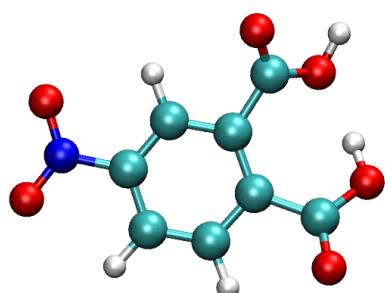
Different



Molecule A 3NFAACi



Molecule B 4NFAACj



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

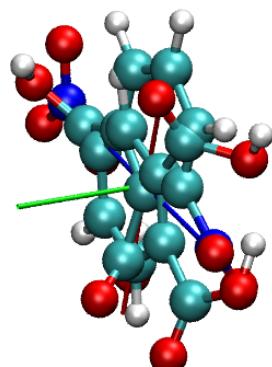
EingenValues - Molecule A

521.475	949.659	1346.18
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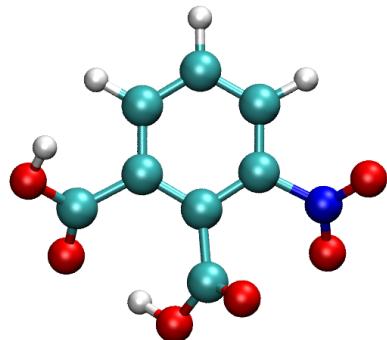
EingenValues - Molecule B

509.897	1225.65	1680.83
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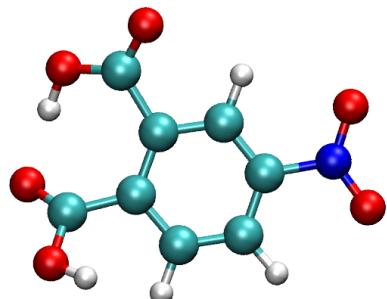
Different



Molecule A 3NFAACi



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

521.487	-1.22943	-2.71042
-1.22943	949.663	1.67006
-2.71042	1.67006	1346.16

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999991	0.00285841	0.00328077
0.00284452	-0.999987	0.00423133
-0.00329282	0.00422196	0.999986

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

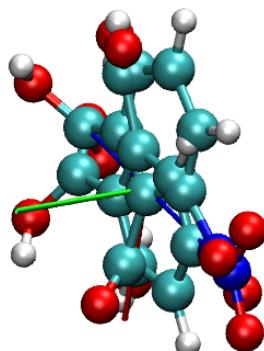
EingenValues - Molecule A

521.475	949.659	1346.18
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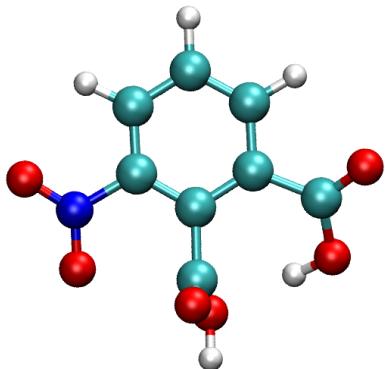
EingenValues - Molecule B

506.607	1222.36	1678.43
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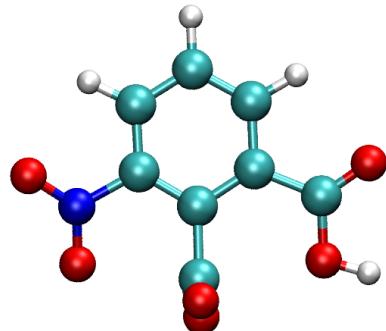
Different



Molecule A 3NFAACj



Molecule B 3NFAACk



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

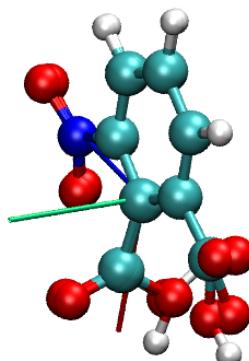
EingenValues - Molecule A

533.726	920.137	1348.3
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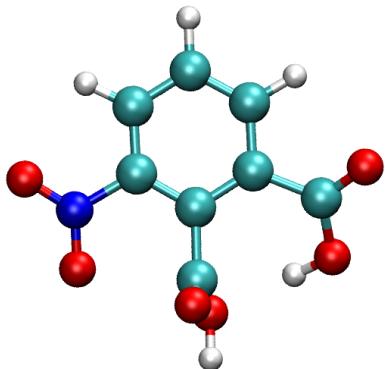
EingenValues - Molecule B

534.81	913.339	1353.78
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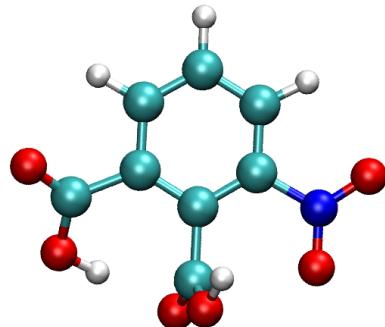
Different



Molecule A 3NFAACj



Molecule B 3NFAACl



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

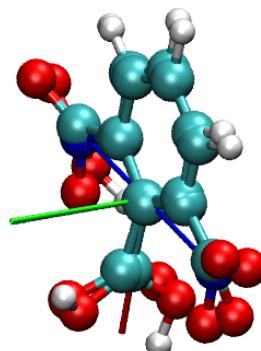
EingenValues - Molecule A

533.726	920.137	1348.3
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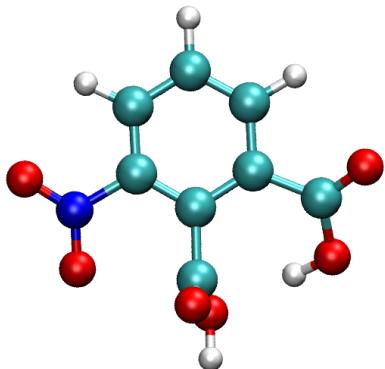
EingenValues - Molecule B

531.691	929.434	1355.4
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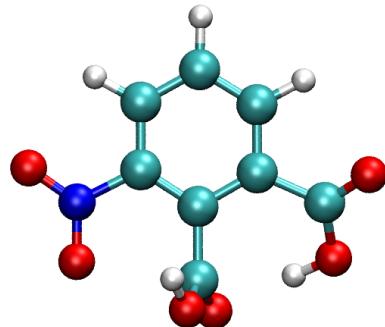
Different



Molecule A 3NFAACj



Molecule B 3NFAACm



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

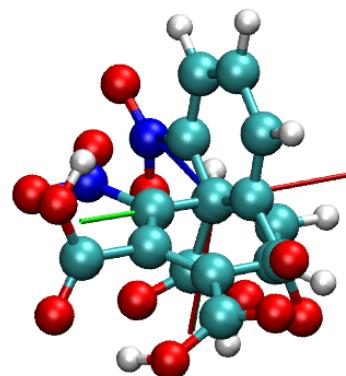
EingenValues - Molecule A

533.726	920.137	1348.3
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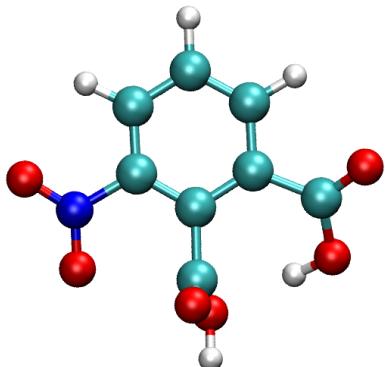
EingenValues - Molecule B

531.698	929.417	1355.4
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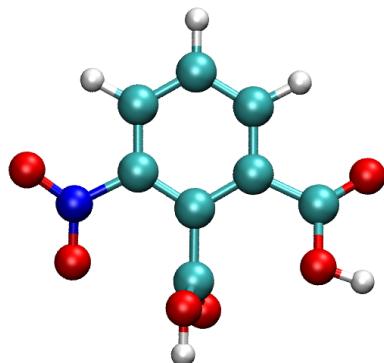
Different



Molecule A 3NFAACj



Molecule B 3NFAACn



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

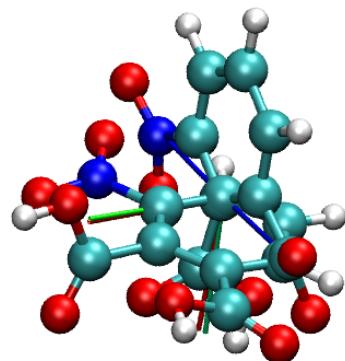
EingenValues - Molecule A

533.726	920.137	1348.3
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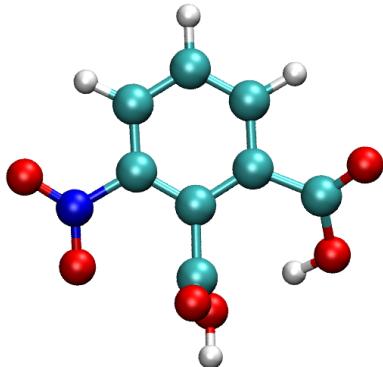
EingenValues - Molecule B

531.43	913.309	1353.35
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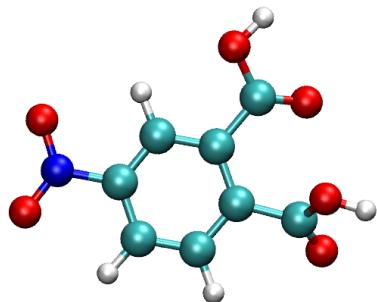
Different



Molecule A 3NFAACj



Molecule B 4NFAACa



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

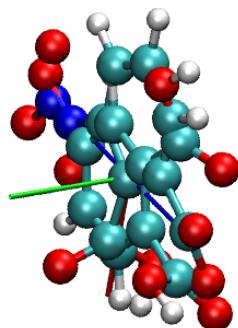
EingenValues - Molecule A

533.726	920.137	1348.3
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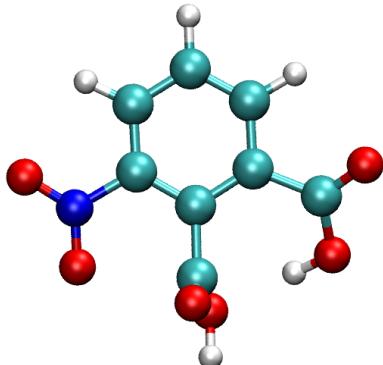
EingenValues - Molecule B

479.363	1242.41	1647.39
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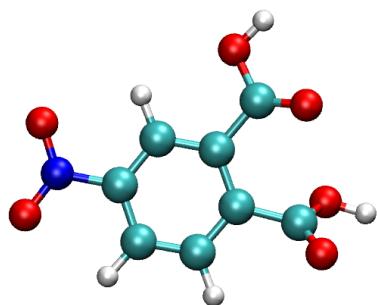
Different



Molecule A 3NFAACj



Molecule B 4NFAACb



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

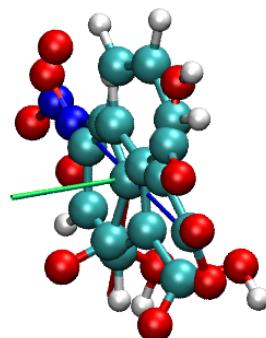
EingenValues - Molecule A

533.726	920.137	1348.3
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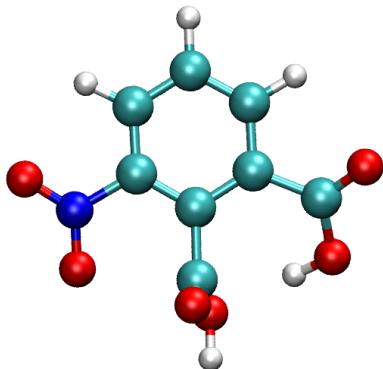
EingenValues - Molecule B

479.308	1242.41	1647.31
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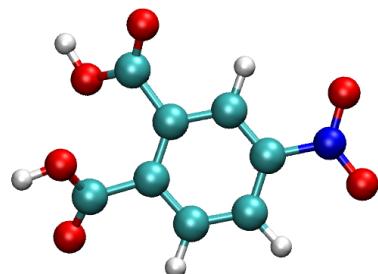
Different



Molecule A 3NFAACj



Molecule B 4NFAACCc



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

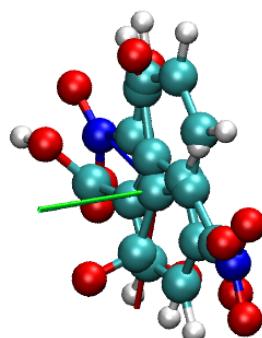
EingenValues - Molecule A

533.726	920.137	1348.3
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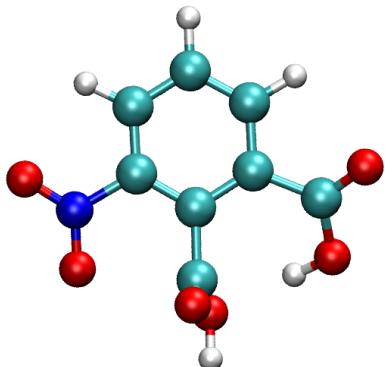
EingenValues - Molecule B

482.027	1240.32	1647.08
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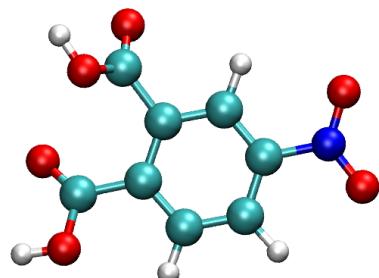
Different



Molecule A 3NFAACj



Molecule B 4NFAACd



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

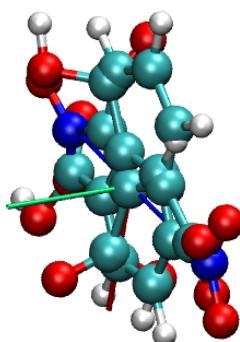
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

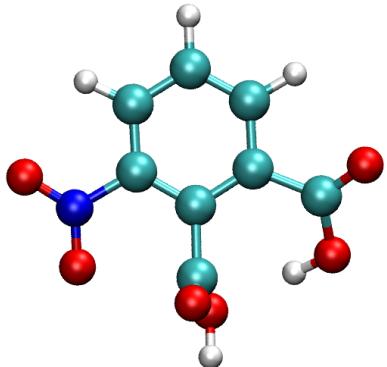
491.663	1231.14	1650.13
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Different

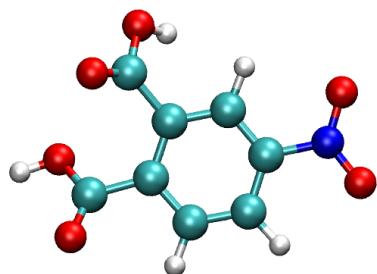


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Molecule A 3NFAACj



Molecule B 4NFAACe



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

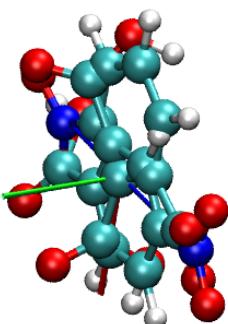
EingenValues - Molecule A

533.726	920.137	1348.3
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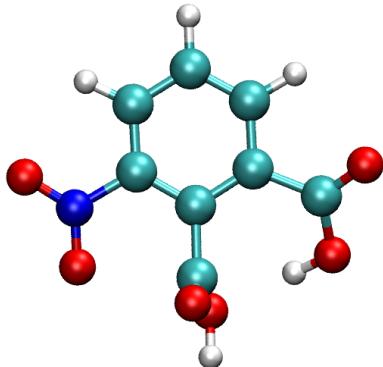
EingenValues - Molecule B

489.011	1233.7	1641.81
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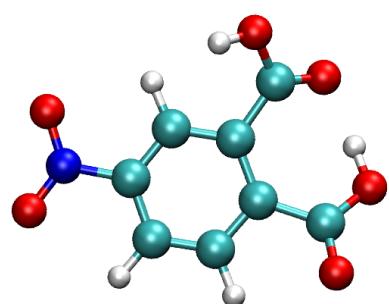
Different



Molecule A 3NFAACj



Molecule B 4NFAACf



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

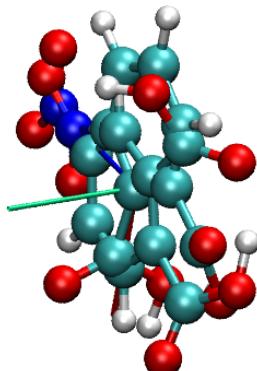
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

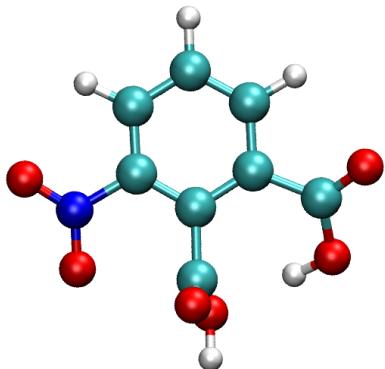
509.668	1219.11	1681.18
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Different

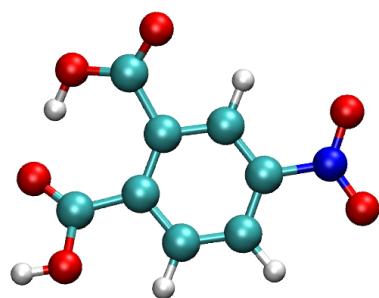


FireTest Número 383

Molecule A 3NFAACj



Molecule B 4NFAACg



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

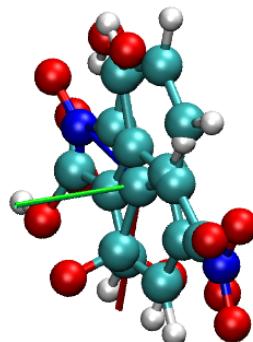
EingenValues - Molecule A

533.726	920.137	1348.3
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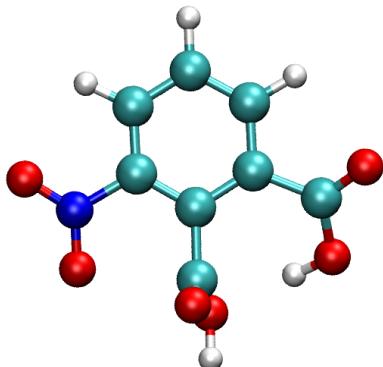
EingenValues - Molecule B

513.751	1208.07	1700.9
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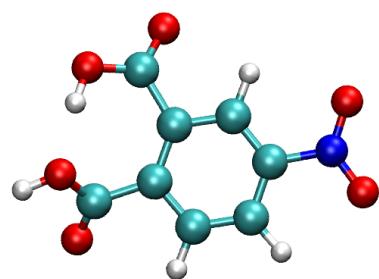
Different



Molecule A 3NFAACj



Molecule B 4NFAACi



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

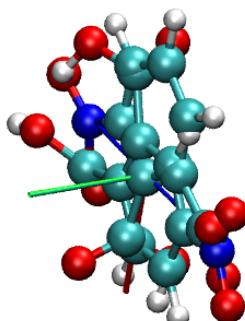
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

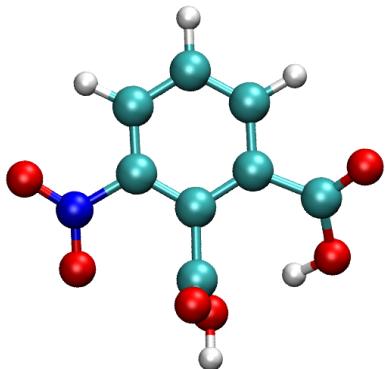
502.409	1232.26	1676.02
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Different

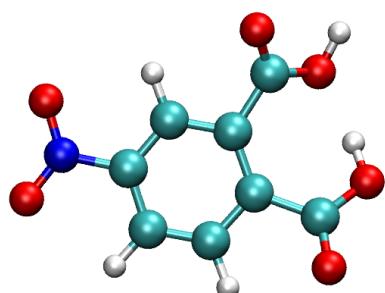


FireTest Número 385

Molecule A 3NFAACj



Molecule B 4NFAACj



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

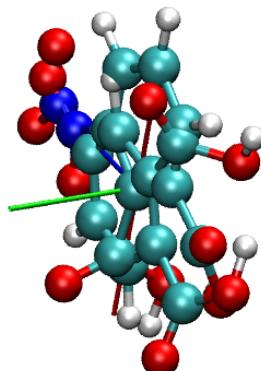
EingenValues - Molecule A

533.726	920.137	1348.3
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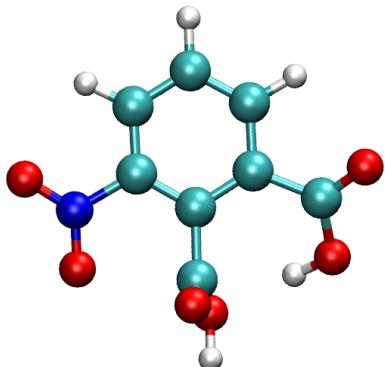
EingenValues - Molecule B

509.897	1225.65	1680.83
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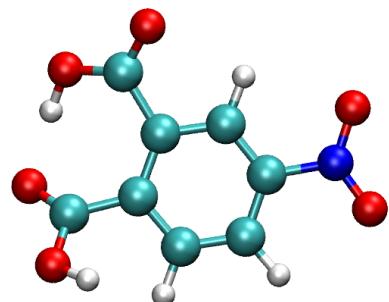
Different



Molecule A 3NFAACj



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

533.789	-4.75521	-1.91525
-4.75521	920.091	2.28449
-1.91525	2.28449	1348.28

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999922	-0.0122929	-0.00231663
0.0122803	-0.99991	0.00539026
-0.00238268	0.00536139	0.999983

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

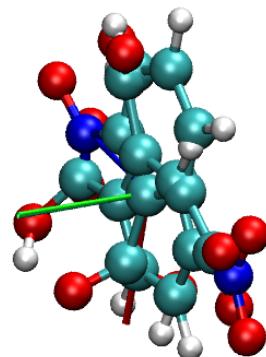
EingenValues - Molecule A

533.726	920.137	1348.3
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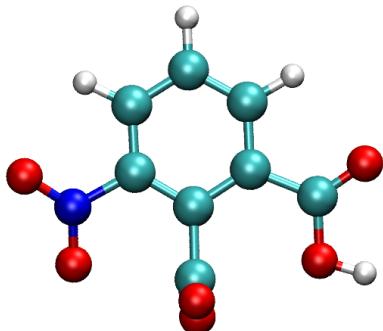
EingenValues - Molecule B

506.607	1222.36	1678.43
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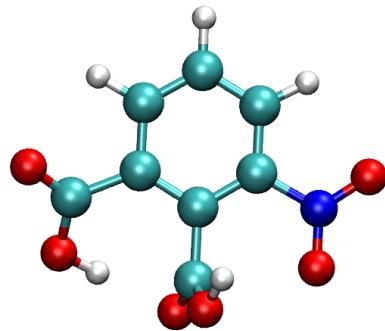
Different



Molecule A 3NFAACk



Molecule B 3NFAACl



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

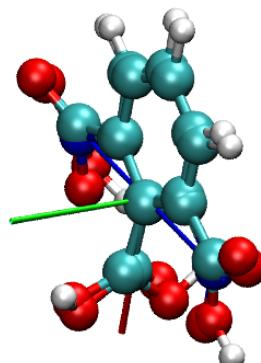
EingenValues - Molecule A

534.81	913.339	1353.78
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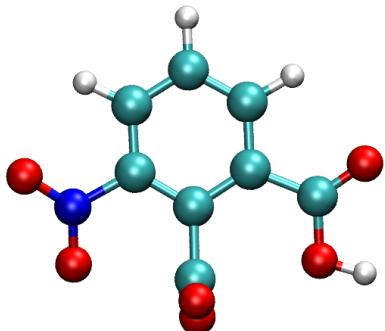
EingenValues - Molecule B

531.691	929.434	1355.4
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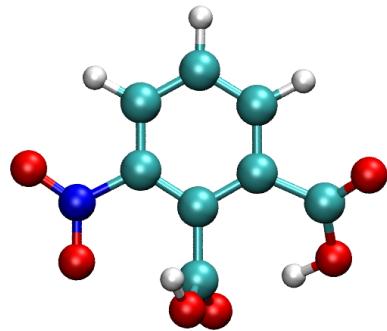
Different



Molecule A 3NFAACk



Molecule B 3NFAACm



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

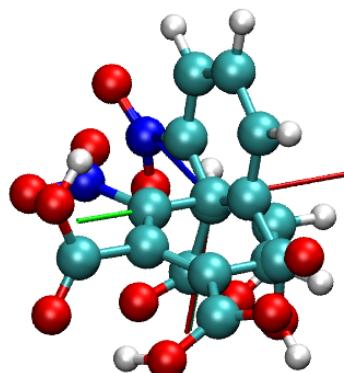
EingenValues - Molecule A

534.81	913.339	1353.78
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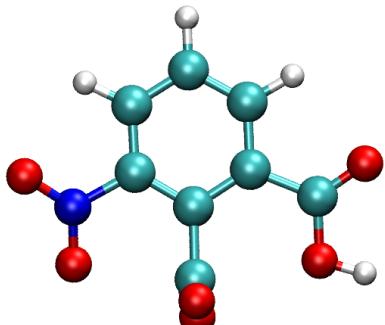
EingenValues - Molecule B

531.698	929.417	1355.4
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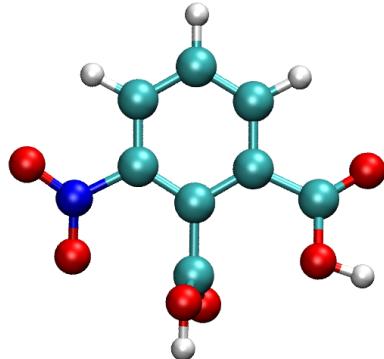
Different



Molecule A 3NFAACk



Molecule B 3NFAACn



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

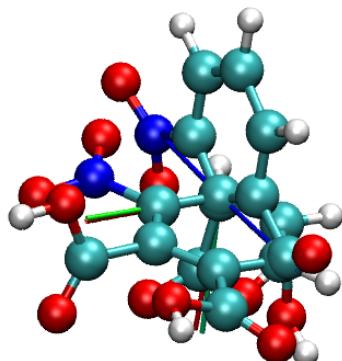
EingenValues - Molecule A

534.81	913.339	1353.78
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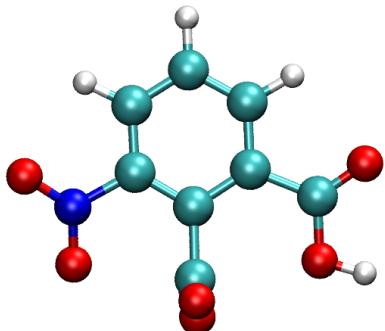
EingenValues - Molecule B

531.43	913.309	1353.35
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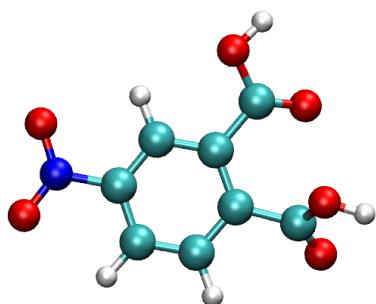
Different



Molecule A 3NFAACk



Molecule B 4NFAACa



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

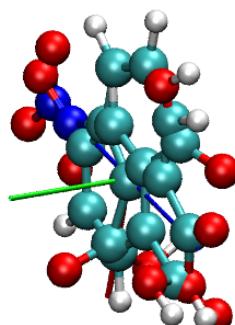
EingenValues - Molecule A

534.81	913.339	1353.78
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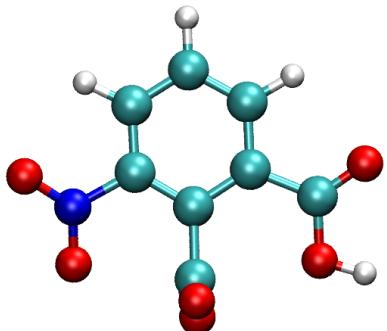
EingenValues - Molecule B

479.363	1242.41	1647.39
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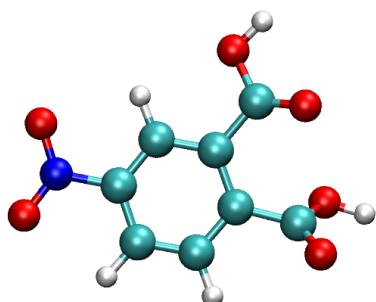
Different



Molecule A 3NFAACk



Molecule B 4NFAACb



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

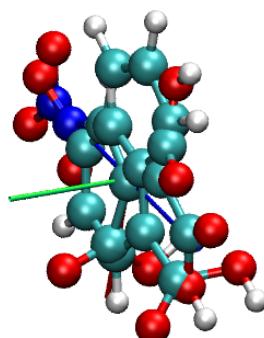
EingenValues - Molecule A

534.81	913.339	1353.78
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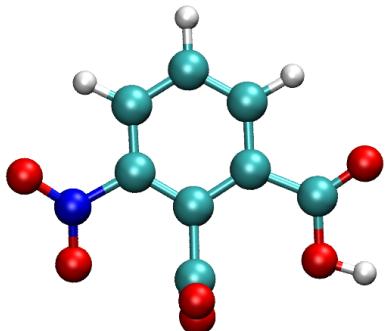
EingenValues - Molecule B

479.308	1242.41	1647.31
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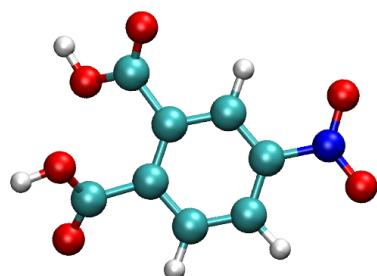
Different



Molecule A 3NFAACk



Molecule B 4NFAACC



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

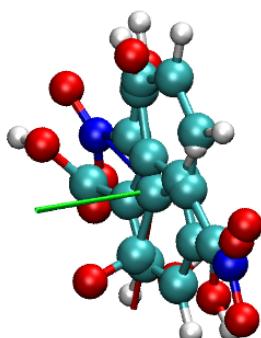
EingenValues - Molecule A

534.81	913.339	1353.78
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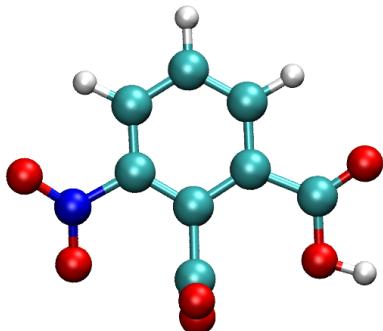
EingenValues - Molecule B

482.027	1240.32	1647.08
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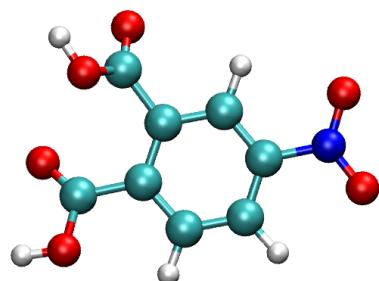
Different



Molecule A 3NFAACk



Molecule B 4NFAACd



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

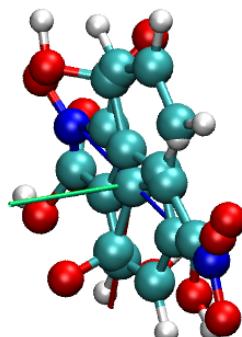
EingenValues - Molecule A

534.81	913.339	1353.78
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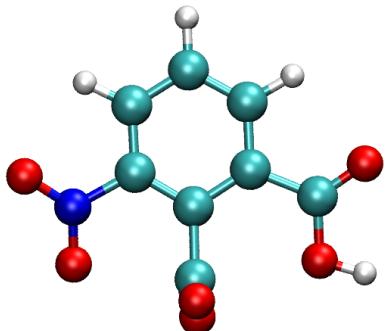
EingenValues - Molecule B

491.663	1231.14	1650.13
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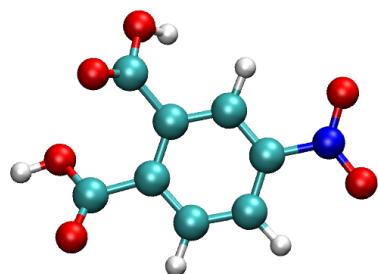
Different



Molecule A 3NFAACk



Molecule B 4NFAACe



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

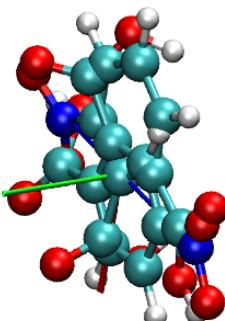
EingenValues - Molecule A

534.81	913.339	1353.78
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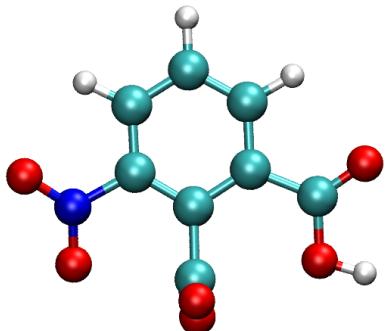
EingenValues - Molecule B

489.011	1233.7	1641.81
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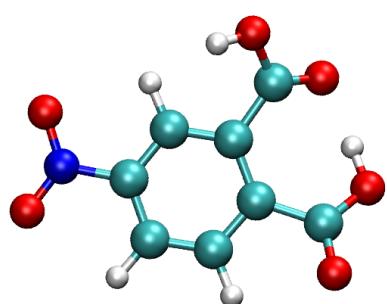
Different



Molecule A 3NFAACk



Molecule B 4NFAACf



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

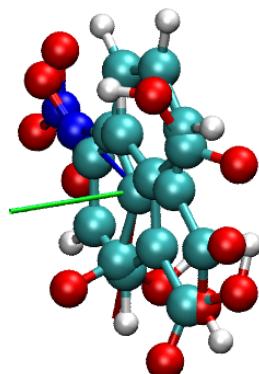
EingenValues - Molecule A

534.81	913.339	1353.78
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EingenValues - Molecule B

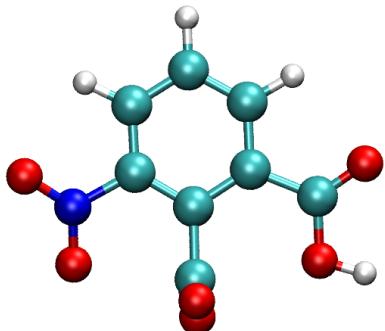
509.668	1219.11	1681.18
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Different

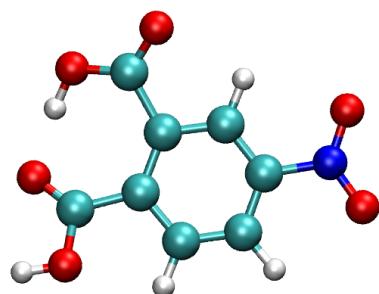


FireTest Número 396

Molecule A 3NFAACk



Molecule B 4NFAACg



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

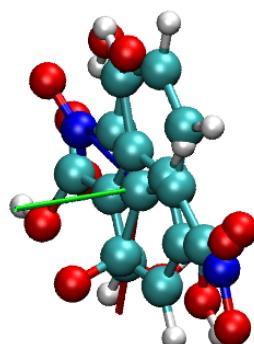
EingenValues - Molecule A

534.81	913.339	1353.78
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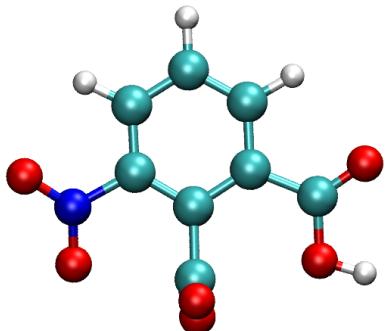
EingenValues - Molecule B

513.751	1208.07	1700.9
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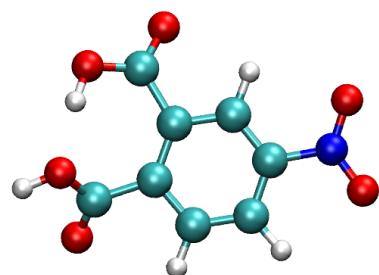
Different



Molecule A 3NFAACk



Molecule B 4NFAACi



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

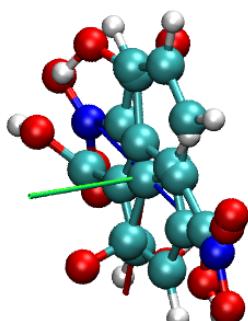
EingenValues - Molecule A

534.81	913.339	1353.78
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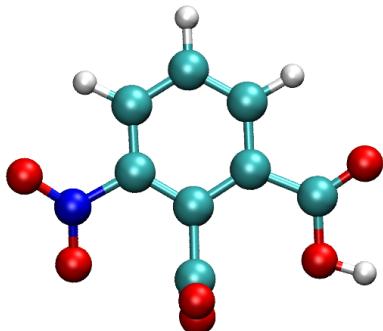
EingenValues - Molecule B

502.409	1232.26	1676.02
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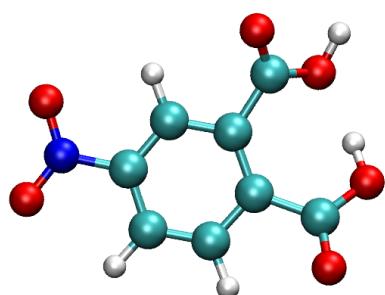
Different



Molecule A 3NFAACk



Molecule B 4NFAACj



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

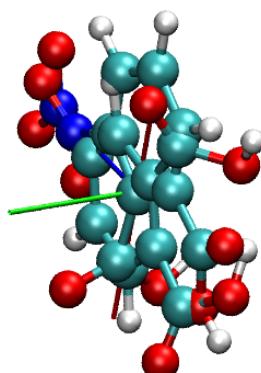
EingenValues - Molecule A

534.81	913.339	1353.78
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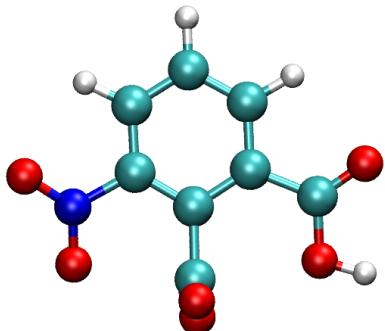
EingenValues - Molecule B

509.897	1225.65	1680.83
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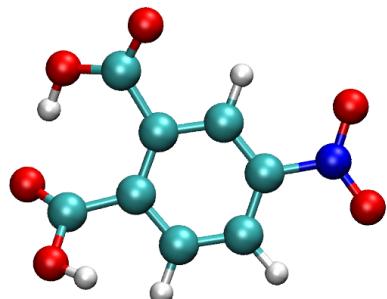
Different



Molecule A 3NFAACk



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

534.899	-5.81418	-0.270063
-5.81418	913.263	2.4519
-0.270063	2.4519	1353.77

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999882	-0.0153593	-0.00028374
0.0153575	-0.999867	0.00557573
-0.000369342	0.00557072	0.999984

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

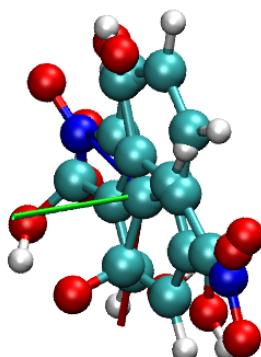
EingenValues - Molecule A

534.81	913.339	1353.78
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EingenValues - Molecule B

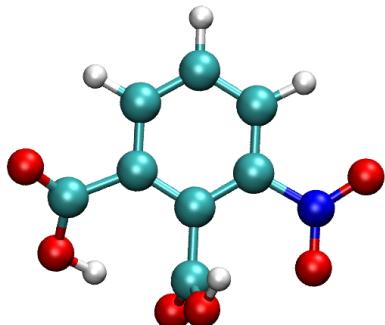
506.607	1222.36	1678.43
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Different

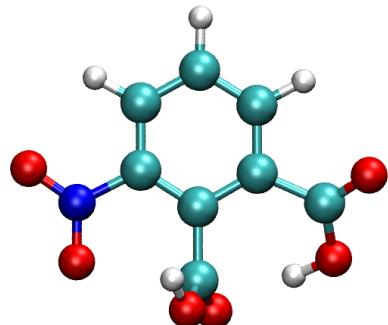


# FireTest Número 400

Molecule A 3NFAACl



Molecule B 3NFAACm



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

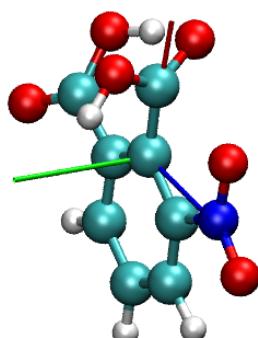
EingenValues - Molecule A

531.691	929.434	1355.4
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EingenValues - Molecule B

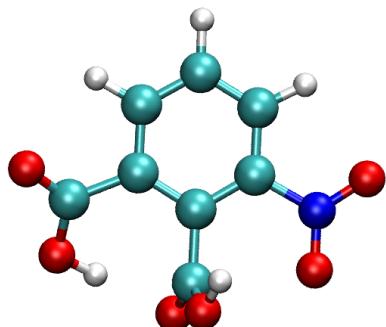
531.698	929.417	1355.4
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Enantiomers

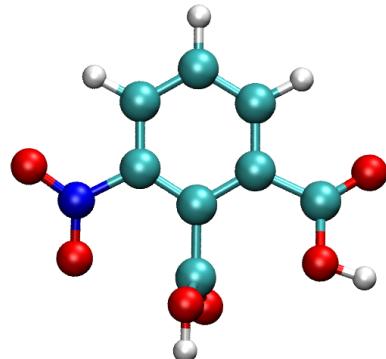


FireTest Número 401

Molecule A 3NFAACl



Molecule B 3NFAACn



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

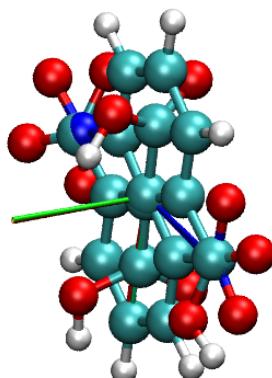
EingenValues - Molecule A

531.691	929.434	1355.4
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EingenValues - Molecule B

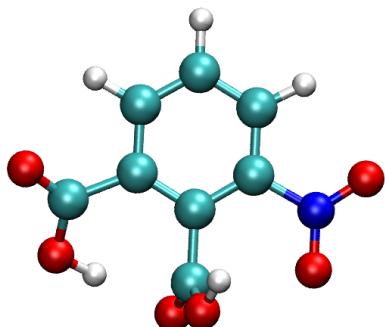
531.43	913.309	1353.35
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Different

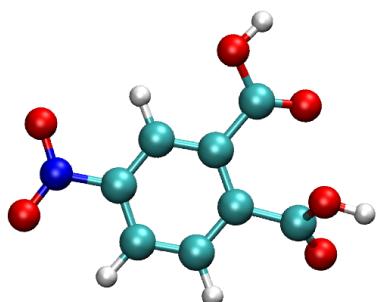


FireTest Número 402

Molecule A 3NFAACl



Molecule B 4NFAACa



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

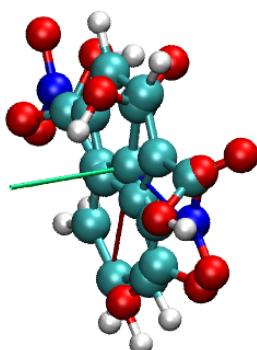
EingenValues - Molecule A

531.691	929.434	1355.4
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EingenValues - Molecule B

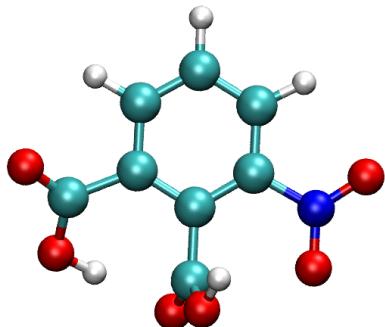
479.363	1242.41	1647.39
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Different

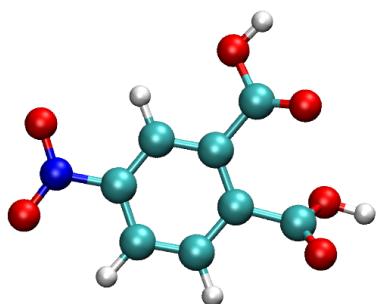


FireTest Número 403

Molecule A 3NFAACl



Molecule B 4NFAACb



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

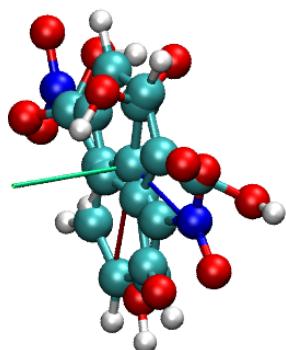
EingenValues - Molecule A

531.691	929.434	1355.4
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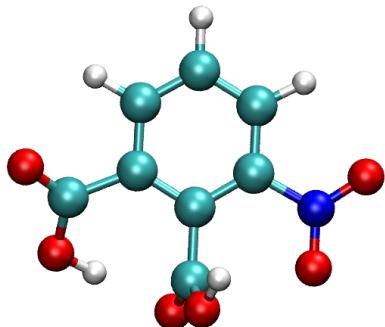
EingenValues - Molecule B

479.308	1242.41	1647.31
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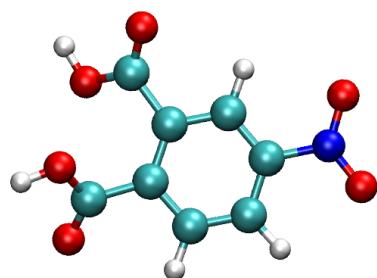
Different



Molecule A 3NFAACl



Molecule B 4NFAACCc



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

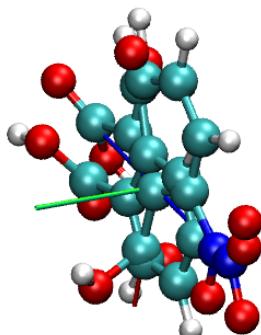
EingenValues - Molecule A

531.691	929.434	1355.4
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EingenValues - Molecule B

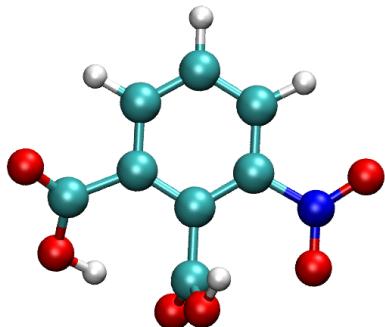
482.027	1240.32	1647.08
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Different

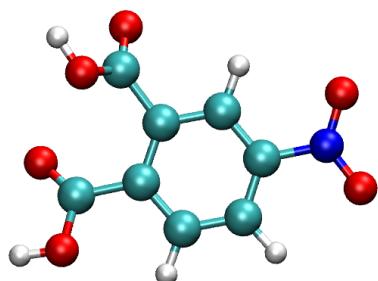


FireTest Número 405

Molecule A 3NFAACl



Molecule B 4NFAACd



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

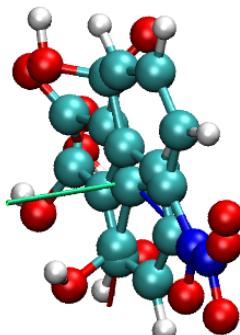
EingenValues - Molecule A

531.691	929.434	1355.4
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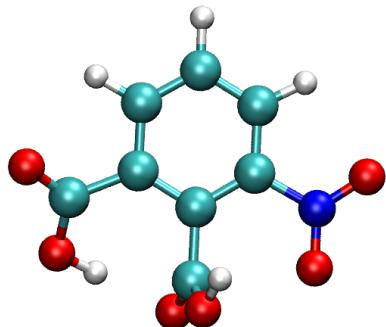
EingenValues - Molecule B

491.663	1231.14	1650.13
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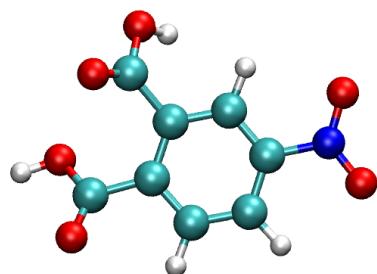
Different



Molecule A 3NFAACl



Molecule B 4NFAACe



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

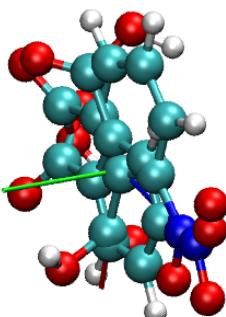
EingenValues - Molecule A

531.691	929.434	1355.4
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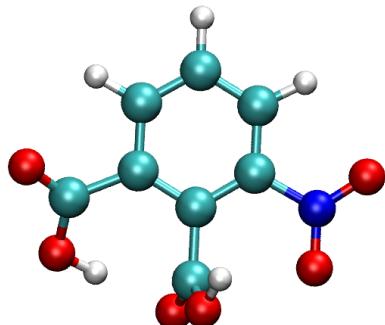
EingenValues - Molecule B

489.011	1233.7	1641.81
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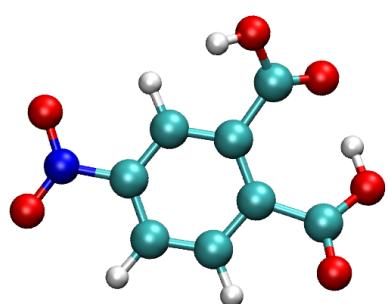
Different



Molecule A 3NFAACl



Molecule B 4NFAACf



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

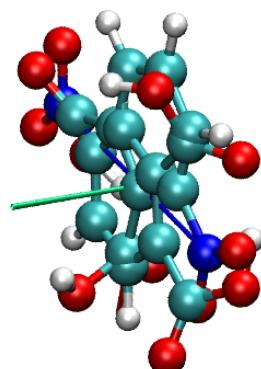
EingenValues - Molecule A

531.691	929.434	1355.4
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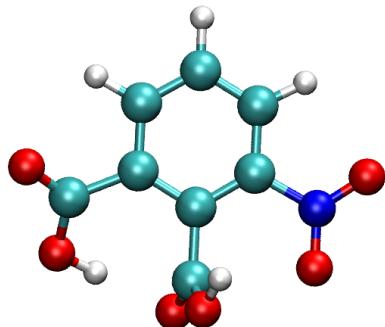
EingenValues - Molecule B

509.668	1219.11	1681.18
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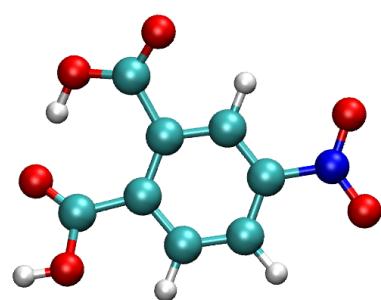
Different



Molecule A 3NFAACl



Molecule B 4NFAACg



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

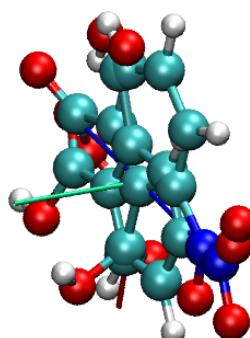
EingenValues - Molecule A

531.691	929.434	1355.4
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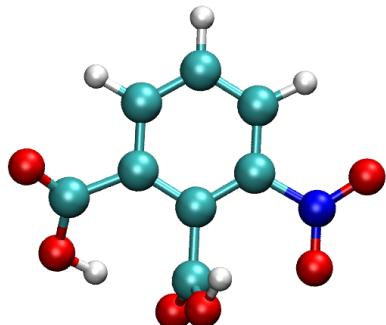
EingenValues - Molecule B

513.751	1208.07	1700.9
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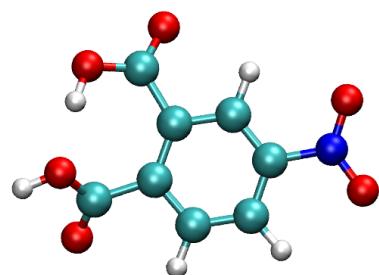
Different



Molecule A 3NFAACl



Molecule B 4NFAACl



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

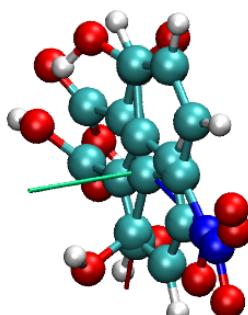
EingenValues - Molecule A

531.691	929.434	1355.4
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EingenValues - Molecule B

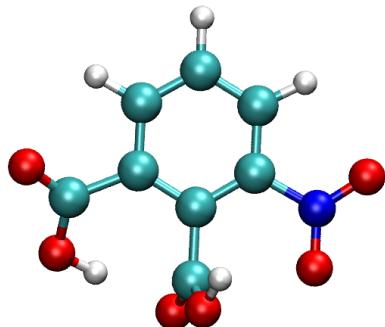
502.409	1232.26	1676.02
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Different

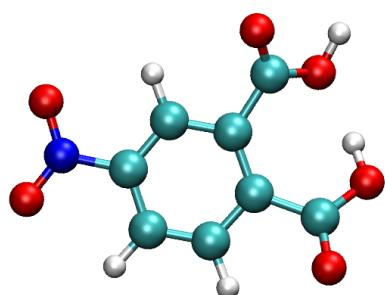


# FireTest Número 410

Molecule A 3NFAACl



Molecule B 4NFAACj



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

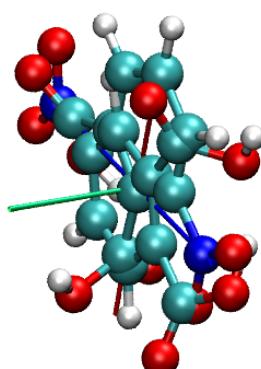
EigenValues - Molecule A

531.691	929.434	1355.4
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EigenValues - Molecule B

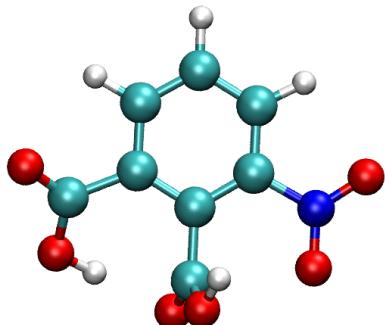
509.897	1225.65	1680.83
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Different

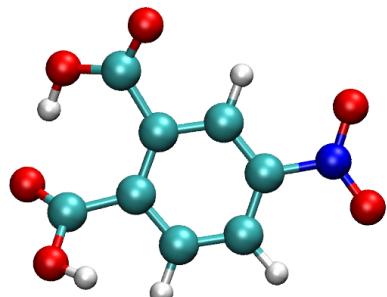


# FireTest Número 411

Molecule A 3NFAACl



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

531.723	3.03424	2.73426
3.03424	929.418	-1.84284
2.73426	-1.84284	1355.39

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999965	-0.00764413	-0.00333648
-0.00765838	-0.999962	-0.00427708
0.00330366	-0.00430248	0.999985

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

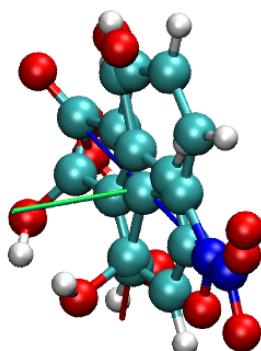
EingenValues - Molecule A

531.691	929.434	1355.4
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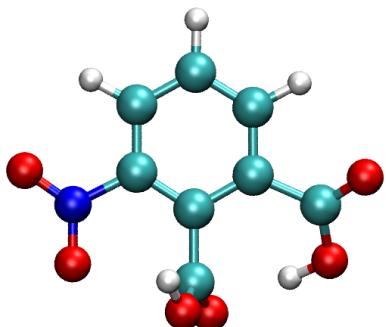
EingenValues - Molecule B

506.607	1222.36	1678.43
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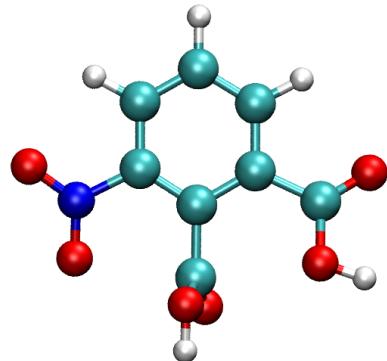
Different



Molecule A 3NFAACm



Molecule B 3NFAACn



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

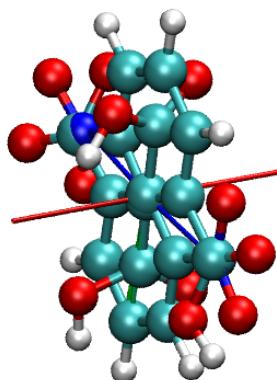
EingenValues - Molecule A

531.698	929.417	1355.4
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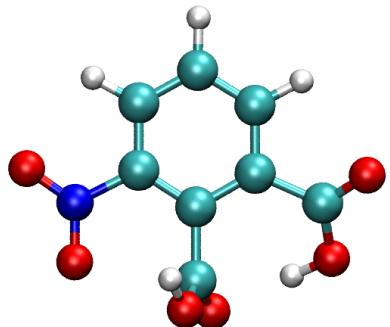
EingenValues - Molecule B

531.43	913.309	1353.35
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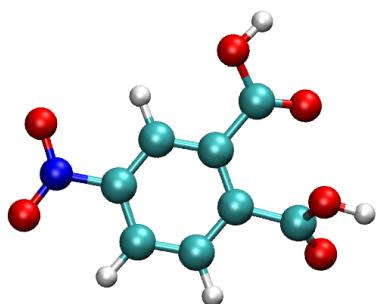
Different



Molecule A 3NFAACm



Molecule B 4NFAACa



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

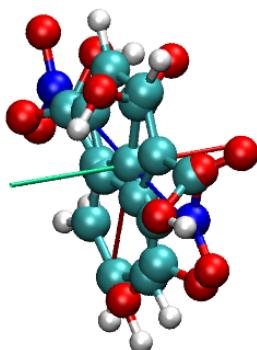
EingenValues - Molecule A

531.698	929.417	1355.4
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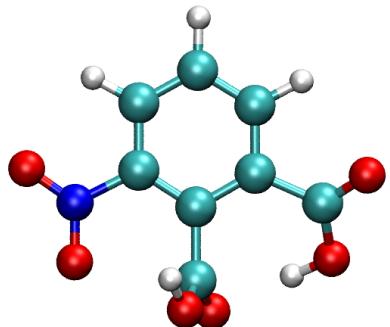
EingenValues - Molecule B

479.363	1242.41	1647.39
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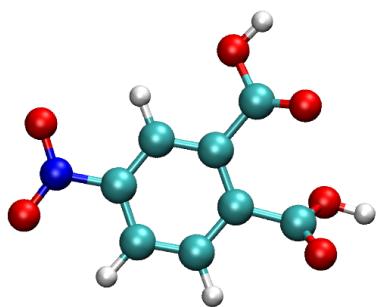
Different



Molecule A 3NFAACm



Molecule B 4NFAACb



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

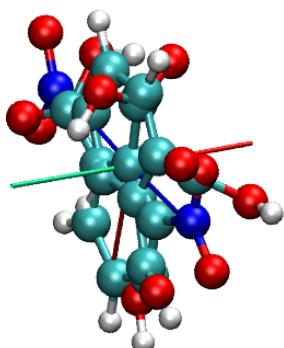
EingenValues - Molecule A

531.698	929.417	1355.4
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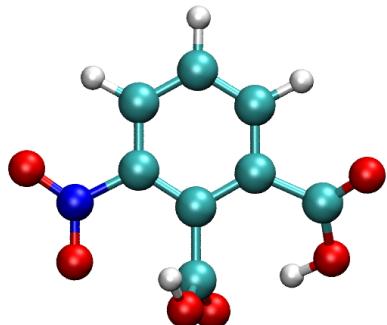
EingenValues - Molecule B

479.308	1242.41	1647.31
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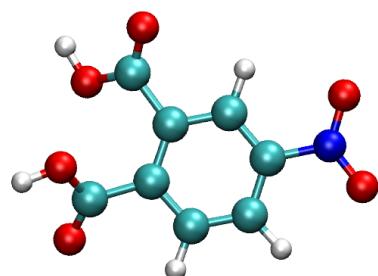
Different



Molecule A 3NFAACm



Molecule B 4NFAACCc



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

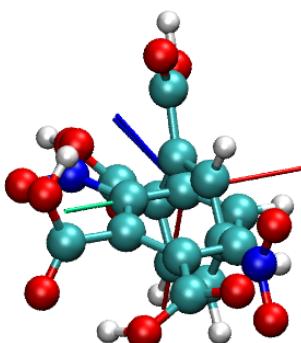
EingenValues - Molecule A

531.698	929.417	1355.4
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EingenValues - Molecule B

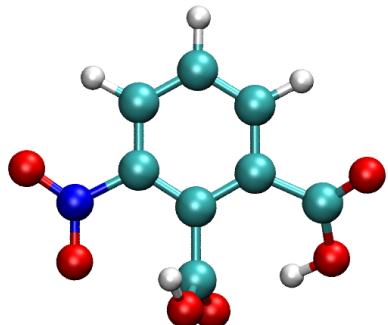
482.027	1240.32	1647.08
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Different

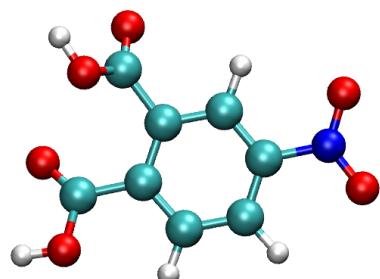


FireTest Número 416

Molecule A 3NFAACm



Molecule B 4NFAACd



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

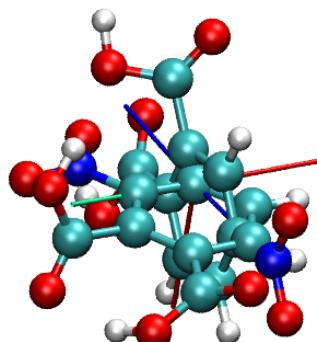
EingenValues - Molecule A

531.698	929.417	1355.4
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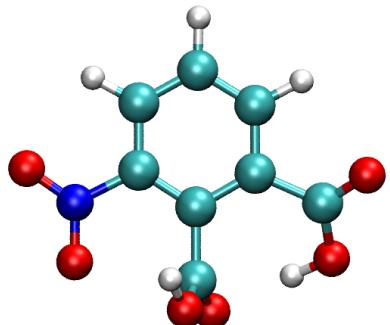
EingenValues - Molecule B

491.663	1231.14	1650.13
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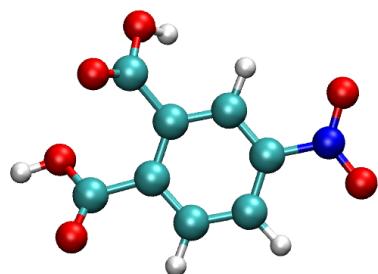
Different



Molecule A 3NFAACm



Molecule B 4NFAACe



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

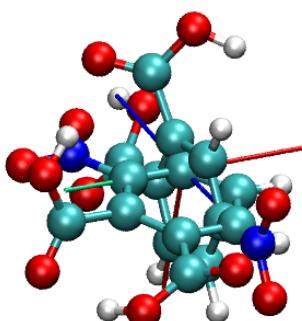
EingenValues - Molecule A

531.698	929.417	1355.4
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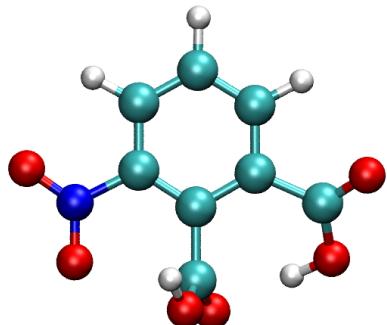
EingenValues - Molecule B

489.011	1233.7	1641.81
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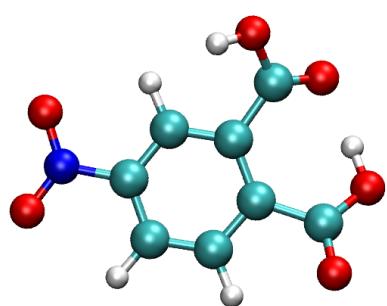
Different



Molecule A 3NFAACm



Molecule B 4NFAACf



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

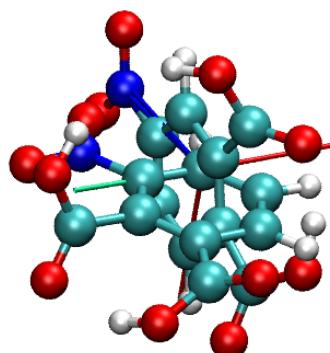
EingenValues - Molecule A

531.698	929.417	1355.4
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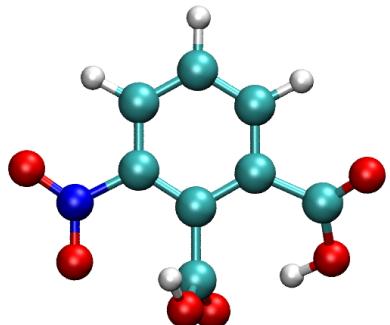
EingenValues - Molecule B

509.668	1219.11	1681.18
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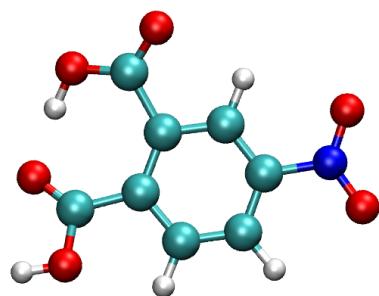
Different



Molecule A 3NFAACm



Molecule B 4NFAACg



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

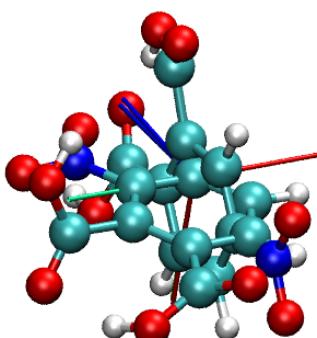
EingenValues - Molecule A

531.698	929.417	1355.4
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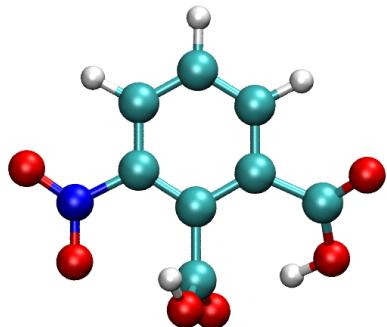
EingenValues - Molecule B

513.751	1208.07	1700.9
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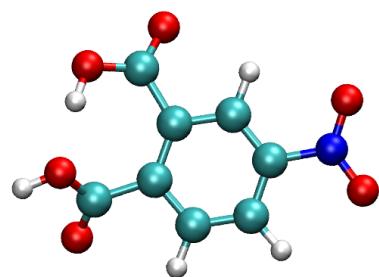
Different



Molecule A 3NFAACm



Molecule B 4NFAACi



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

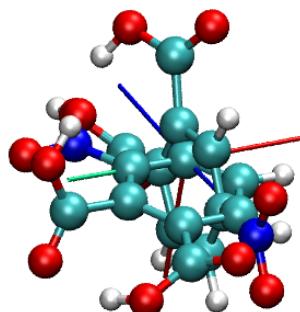
EingenValues - Molecule A

531.698	929.417	1355.4
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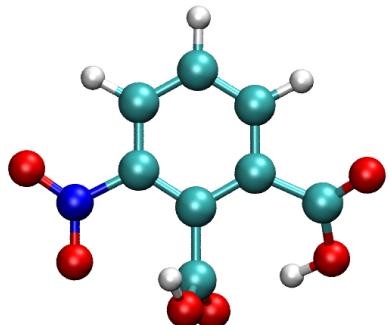
EingenValues - Molecule B

502.409	1232.26	1676.02
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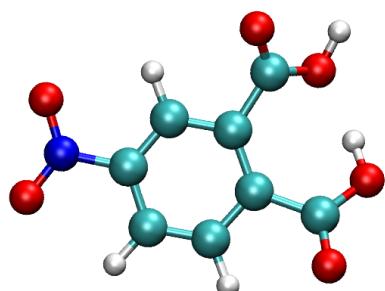
Different



Molecule A 3NFAACm



Molecule B 4NFAACj



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

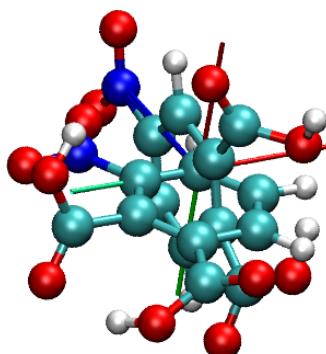
EingenValues - Molecule A

531.698	929.417	1355.4
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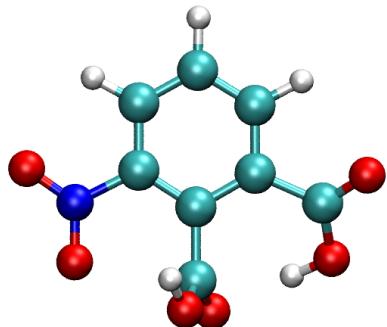
EingenValues - Molecule B

509.897	1225.65	1680.83
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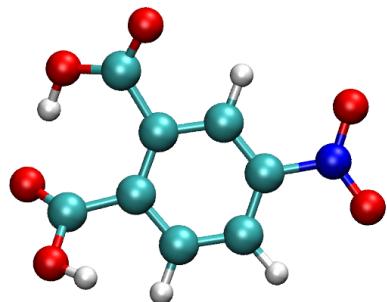
Different



Molecule A 3NFAACm



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

532.546	13.7854	-15.4626
13.7854	1354.87	11.5786
-15.4626	11.5786	929.101

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999075	0.0172851	-0.0393769
0.0398168	0.0258942	-0.998871
-0.016246	-0.999515	-0.0265584

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

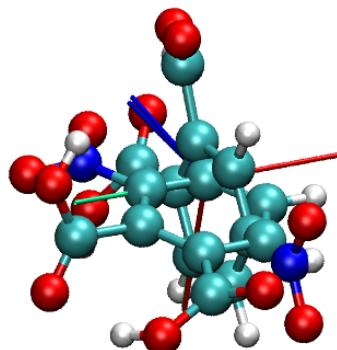
EingenValues - Molecule A

531.698	929.417	1355.4
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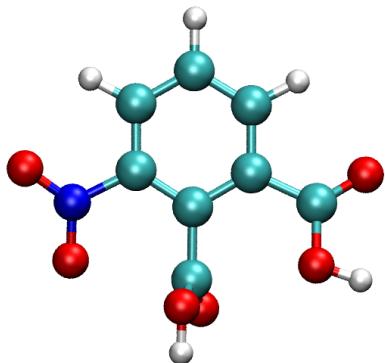
EingenValues - Molecule B

506.607	1222.36	1678.43
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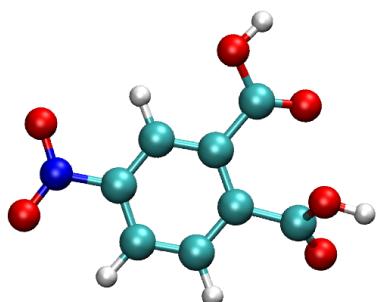
Different



Molecule A 3NFAACn



Molecule B 4NFAACa



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

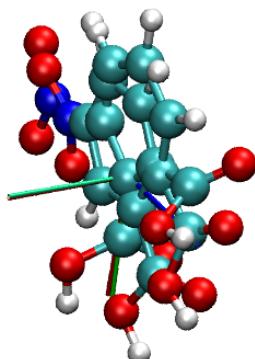
EingenValues - Molecule A

531.43	913.309	1353.35
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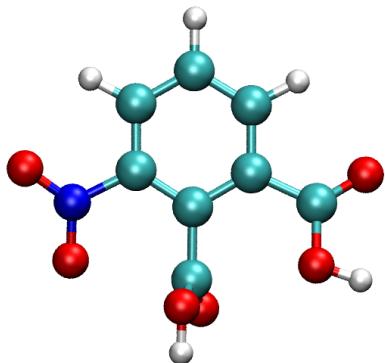
EingenValues - Molecule B

479.363	1242.41	1647.39
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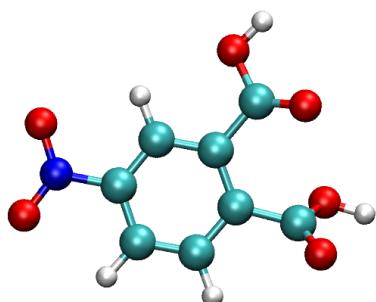
Different



Molecule A 3NFAACn



Molecule B 4NFAACb



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

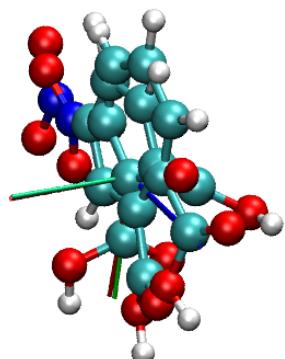
EingenValues - Molecule A

531.43	913.309	1353.35
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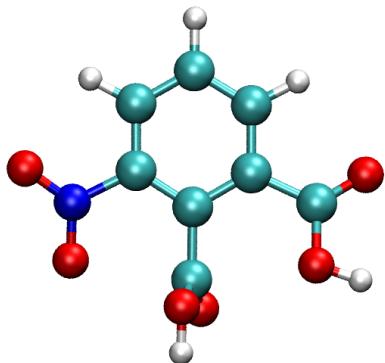
EingenValues - Molecule B

479.308	1242.41	1647.31
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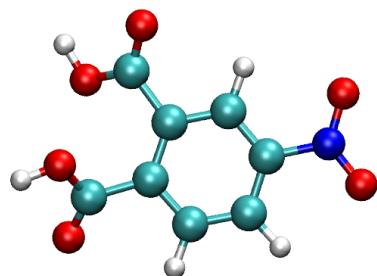
Different



Molecule A 3NFAACn



Molecule B 4NFAACC



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

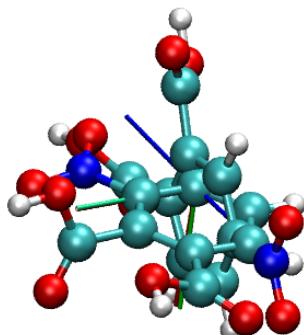
EingenValues - Molecule A

531.43	913.309	1353.35
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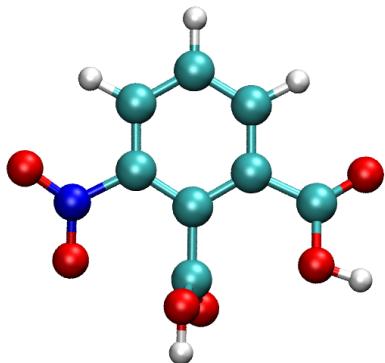
EingenValues - Molecule B

482.027	1240.32	1647.08
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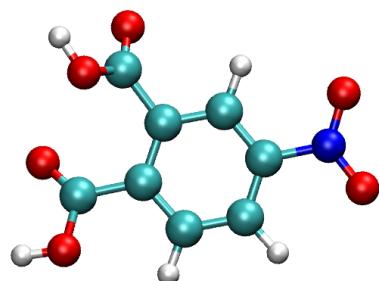
Different



Molecule A 3NFAACn



Molecule B 4NFAACd



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

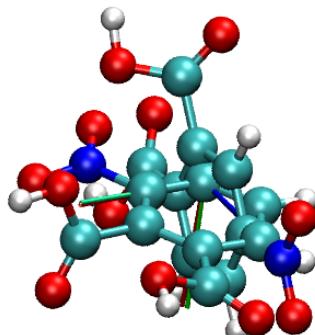
EingenValues - Molecule A

531.43	913.309	1353.35
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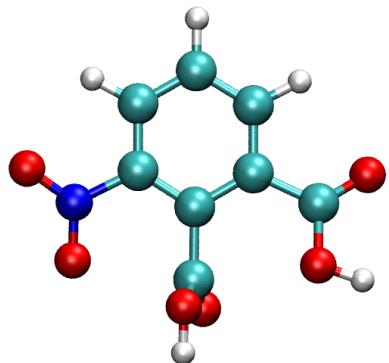
EingenValues - Molecule B

491.663	1231.14	1650.13
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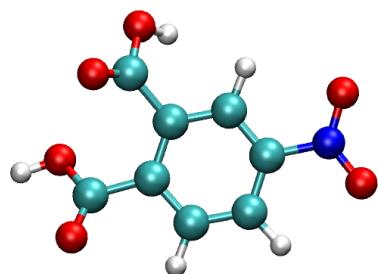
Different



Molecule A 3NFAACn



Molecule B 4NFAACe



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

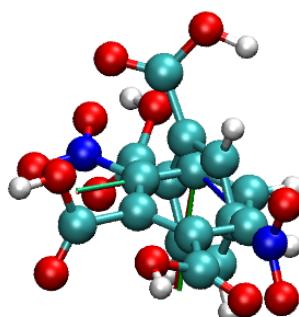
EingenValues - Molecule A

531.43	913.309	1353.35
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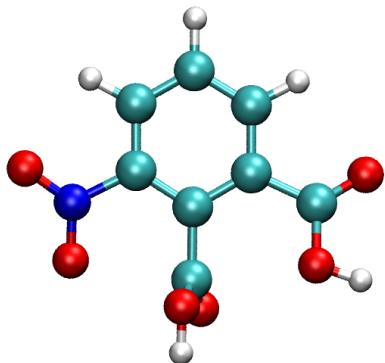
EingenValues - Molecule B

489.011	1233.7	1641.81
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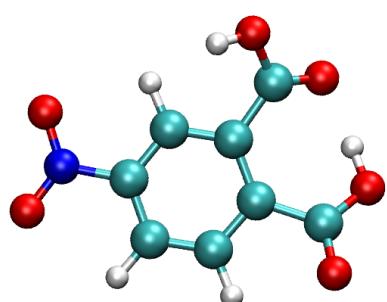
Different



Molecule A 3NFAACn



Molecule B 4NFAACf



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

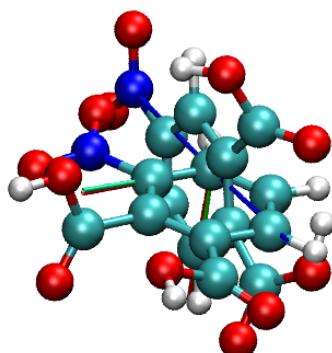
EingenValues - Molecule A

531.43	913.309	1353.35
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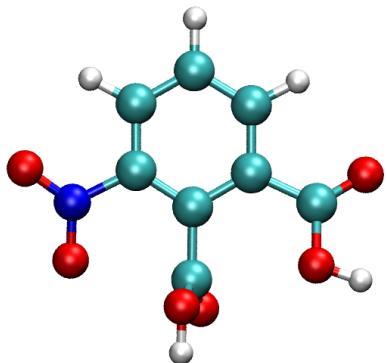
EingenValues - Molecule B

509.668	1219.11	1681.18
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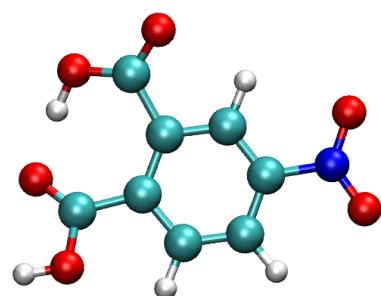
Different



Molecule A 3NFAACn



Molecule B 4NFAACg



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

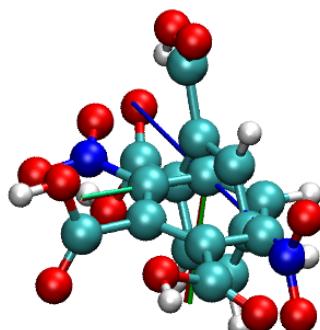
EingenValues - Molecule A

531.43	913.309	1353.35
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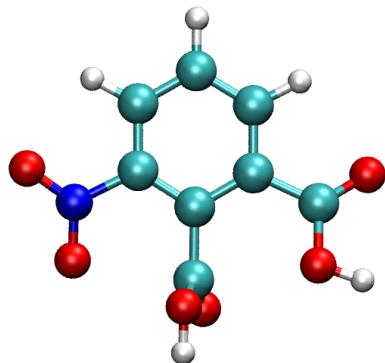
EingenValues - Molecule B

513.751	1208.07	1700.9
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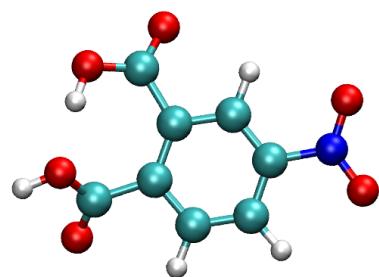
Different



Molecule A 3NFAACn



Molecule B 4NFAACi



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

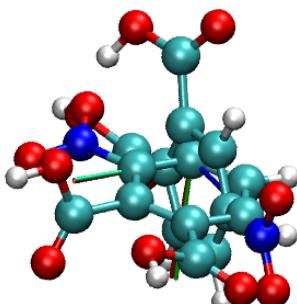
EingenValues - Molecule A

531.43	913.309	1353.35
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EingenValues - Molecule B

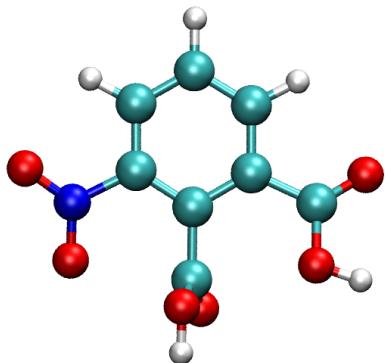
502.409	1232.26	1676.02
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Different

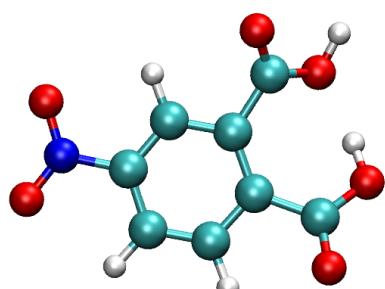


FireTest Número 431

Molecule A 3NFAACn



Molecule B 4NFAACj



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

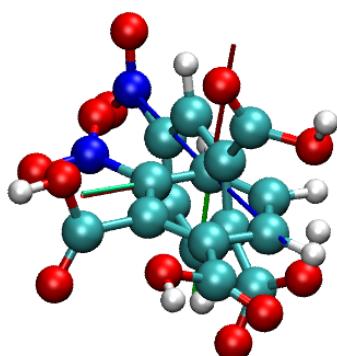
EingenValues - Molecule A

531.43	913.309	1353.35
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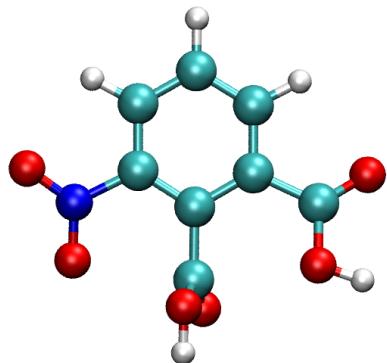
EingenValues - Molecule B

509.897	1225.65	1680.83
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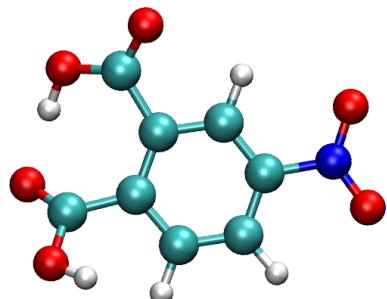
Different



Molecule A 3NFAACn



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

531.896	3.78027	-13.1151
3.78027	1353.2	-7.47403
-13.1151	-7.47403	912.989

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999403	-0.00428573	0.0342679
0.0341891	-0.0172718	-0.999266
0.00487445	0.999842	-0.017115

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

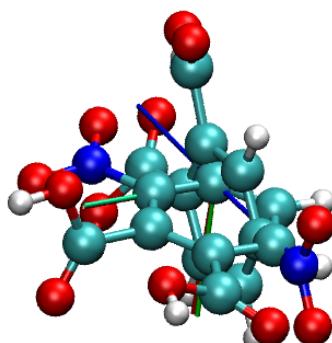
EingenValues - Molecule A

531.43	913.309	1353.35
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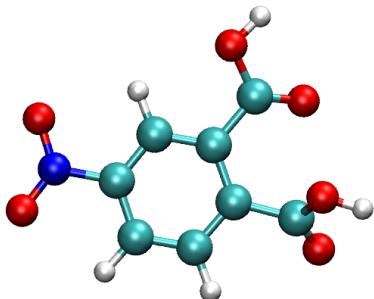
EingenValues - Molecule B

506.607	1222.36	1678.43
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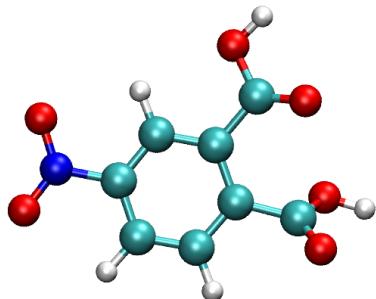
Different



Molecule A 4NFAACa



Molecule B 4NFAACb



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

EingenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EingenVectors - Molecule B

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

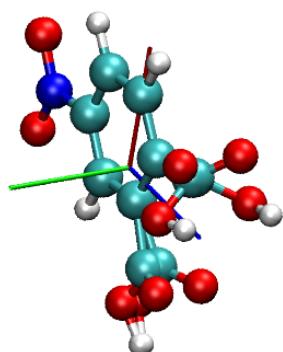
EingenValues - Molecule A

479.363	1242.41	1647.39
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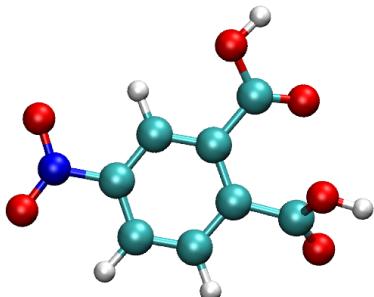
EingenValues - Molecule B

479.308	1242.41	1647.31
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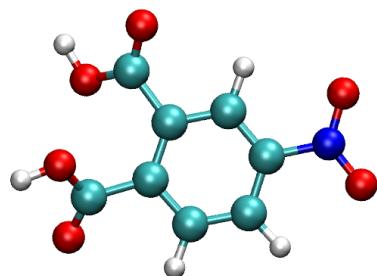
Enantiomers



Molecule A 4NFAACa



Molecule B 4NFAACCc



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

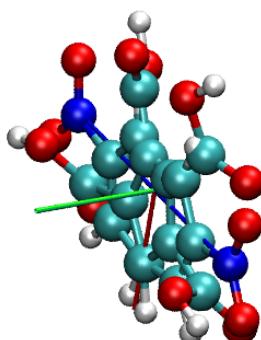
EingenValues - Molecule A

479.363	1242.41	1647.39
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EingenValues - Molecule B

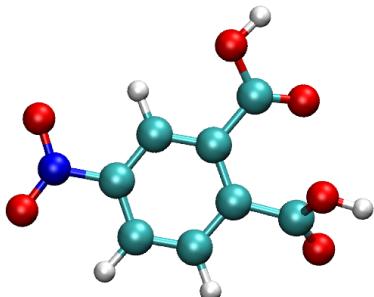
482.027	1240.32	1647.08
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Different

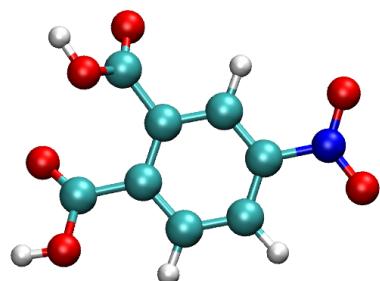


FireTest Número 435

Molecule A 4NFAACa



Molecule B 4NFAACd



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

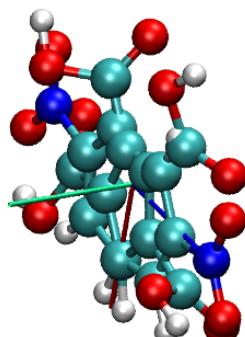
EingenValues - Molecule A

479.363	1242.41	1647.39
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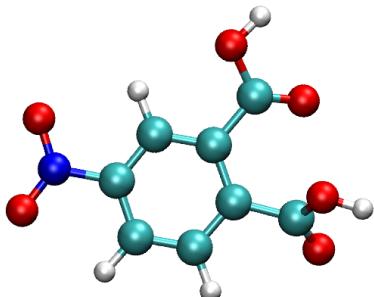
EingenValues - Molecule B

491.663	1231.14	1650.13
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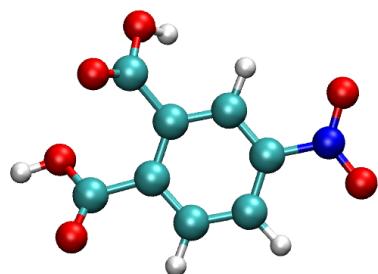
Different



Molecule A 4NFAACa



Molecule B 4NFAACe



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

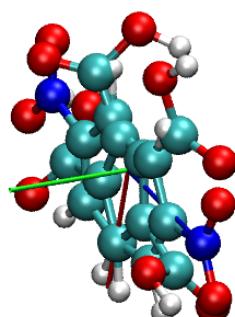
EingenValues - Molecule A

479.363	1242.41	1647.39
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EingenValues - Molecule B

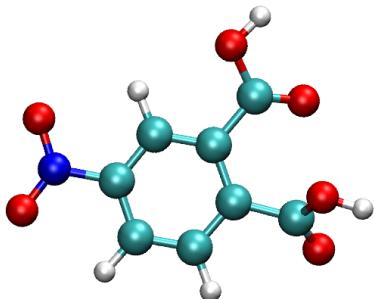
489.011	1233.7	1641.81
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Different

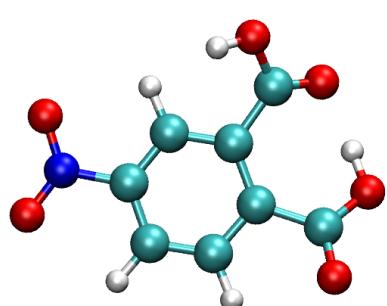


FireTest Número 437

Molecule A 4NFAACa



Molecule B 4NFAACf



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

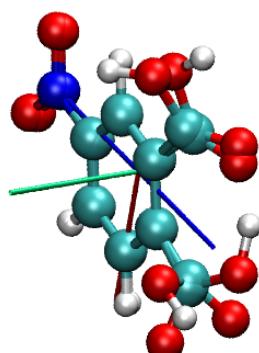
EingenValues - Molecule A

479.363	1242.41	1647.39
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EingenValues - Molecule B

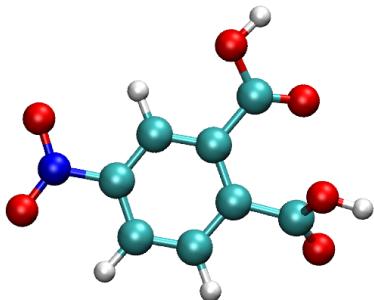
509.668	1219.11	1681.18
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Different

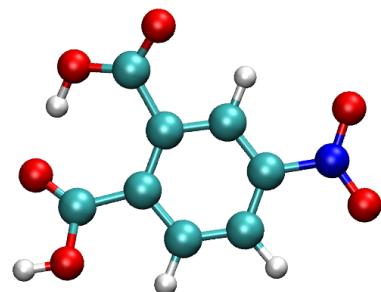


# FireTest Número 438

Molecule A 4NFAACa



Molecule B 4NFAACg



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EigenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EigenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

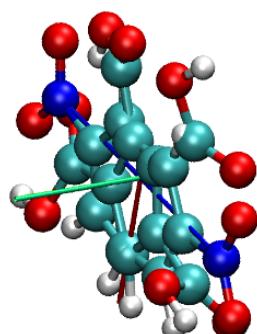
EigenValues - Molecule A

479.363	1242.41	1647.39
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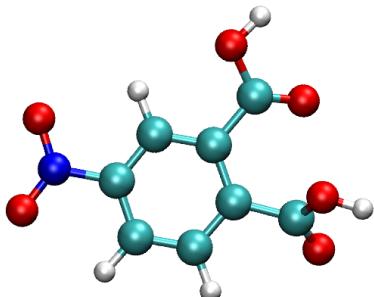
EigenValues - Molecule B

513.751	1208.07	1700.9
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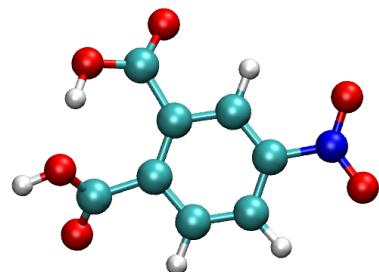
Different



Molecule A 4NFAACa



Molecule B 4NFAACi



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

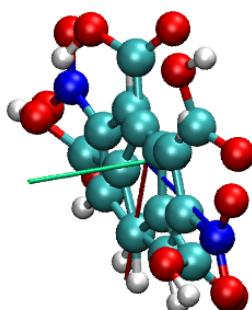
EingenValues - Molecule A

479.363	1242.41	1647.39
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EingenValues - Molecule B

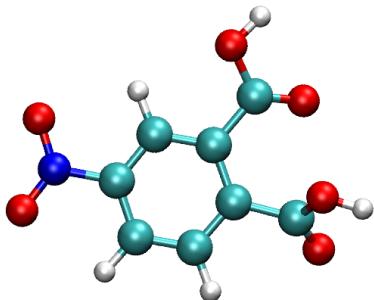
502.409	1232.26	1676.02
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Different

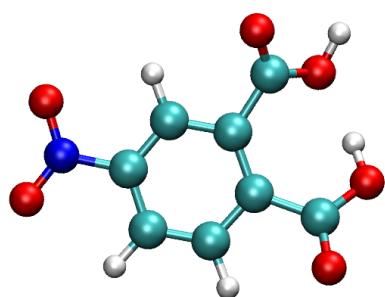


# FireTest Número 440

Molecule A 4NFAACa



Molecule B 4NFAACj



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

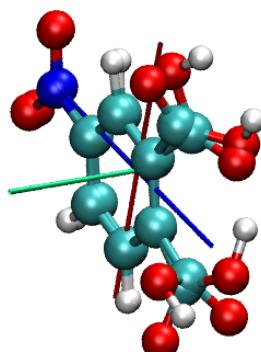
EigenValues - Molecule A

479.363	1242.41	1647.39
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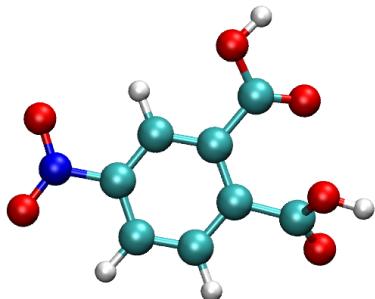
EigenValues - Molecule B

509.897	1225.65	1680.83
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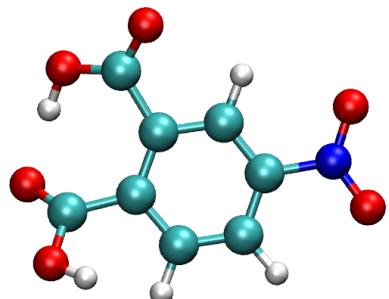
Different



Molecule A 4NFAACa



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

479.392	3.27131	4.22557
3.27131	1242.39	-0.852684
4.22557	-0.852684	1647.37

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999984	-0.00429123	-0.00362083
-0.00429871	-0.999989	-0.0020607
0.00361195	-0.00207623	0.999991

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

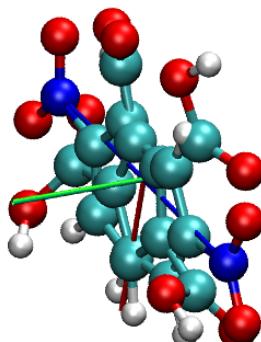
EingenValues - Molecule A

479.363	1242.41	1647.39
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EingenValues - Molecule B

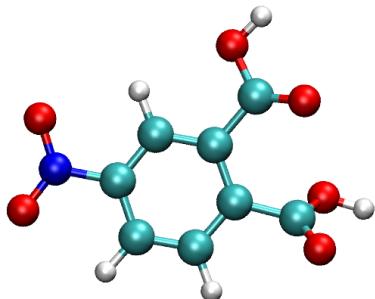
506.607	1222.36	1678.43
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Different

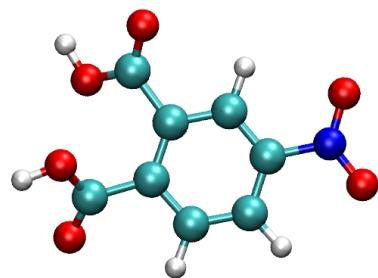


FireTest Número 442

Molecule A 4NFAACb



Molecule B 4NFAACCc



Inertia Tensor - Molecule A

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

Inertia Tensor - Molecule B

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

EingenVectors - Molecule A

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

EingenVectors - Molecule B

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

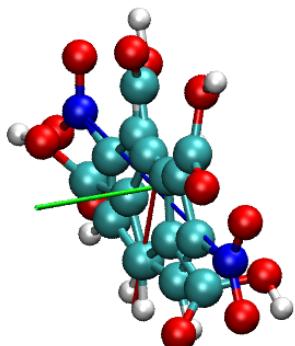
EingenValues - Molecule A

479.308	1242.41	1647.31
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EingenValues - Molecule B

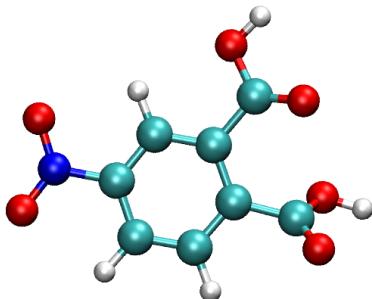
482.027	1240.32	1647.08
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Different

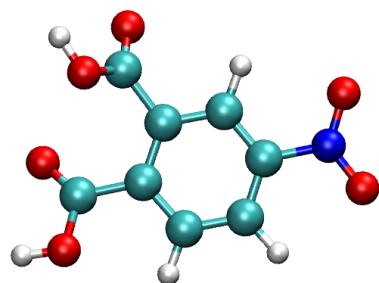


FireTest Número 443

Molecule A 4NFAACb



Molecule B 4NFAACd



Inertia Tensor - Molecule A

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

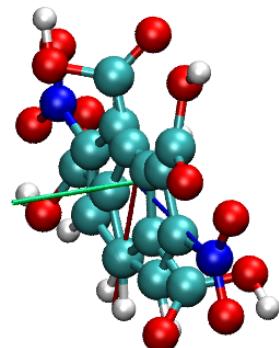
EingenValues - Molecule A

479.308	1242.41	1647.31
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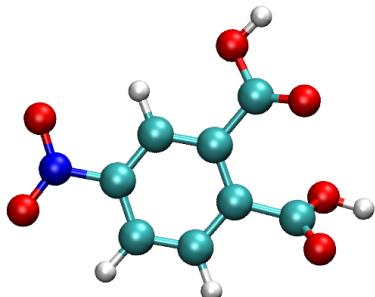
EingenValues - Molecule B

491.663	1231.14	1650.13
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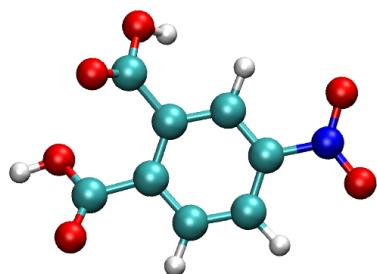
Different



Molecule A 4NFAACb



Molecule B 4NFAACe



Inertia Tensor - Molecule A

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

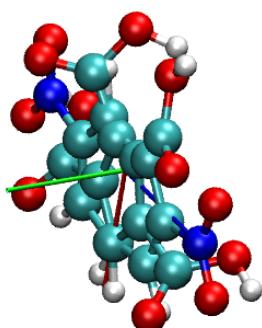
EingenValues - Molecule A

479.308	1242.41	1647.31
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EingenValues - Molecule B

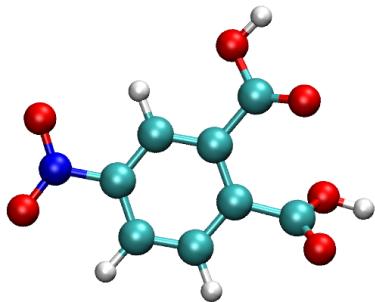
489.011	1233.7	1641.81
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Different

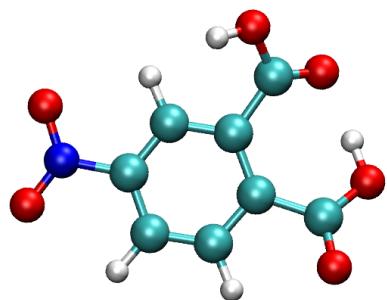


FireTest Número 445

Molecule A 4NFAACb



Molecule B 4NFAACf



Inertia Tensor - Molecule A

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

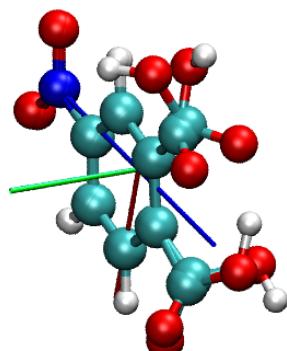
EingenValues - Molecule A

479.308	1242.41	1647.31
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EingenValues - Molecule B

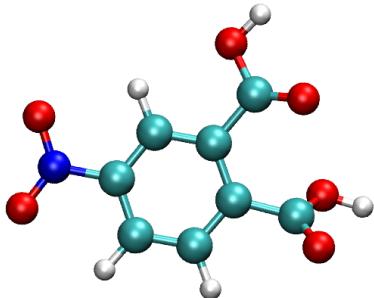
509.668	1219.11	1681.18
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Different

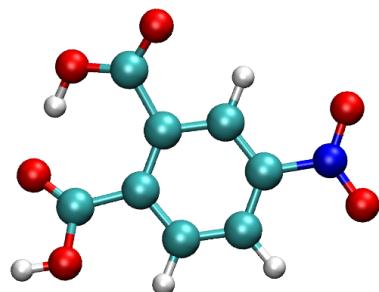


# FireTest Número 446

Molecule A 4NFAACb



Molecule B 4NFAACg



Inertia Tensor - Molecule A

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EigenVectors - Molecule A

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

EigenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

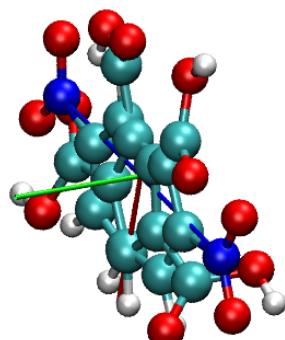
EigenValues - Molecule A

479.308	1242.41	1647.31
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EigenValues - Molecule B

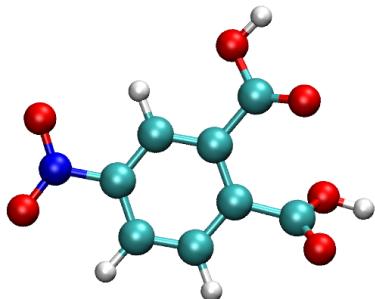
513.751	1208.07	1700.9
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Different

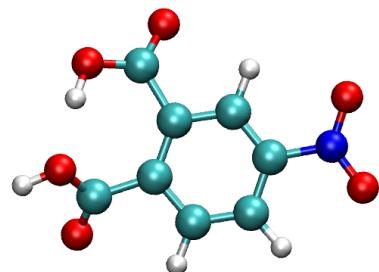


FireTest Número 447

Molecule A 4NFAACb



Molecule B 4NFAACi



Inertia Tensor - Molecule A

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

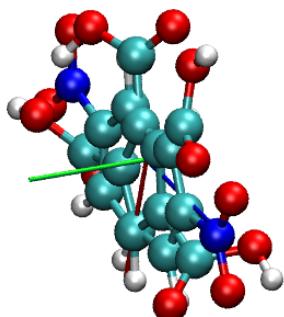
EingenValues - Molecule A

479.308	1242.41	1647.31
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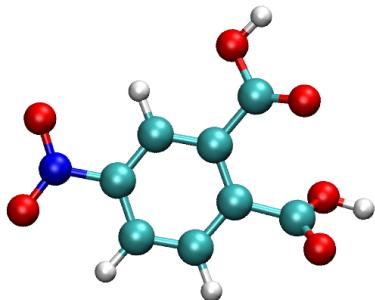
EingenValues - Molecule B

502.409	1232.26	1676.02
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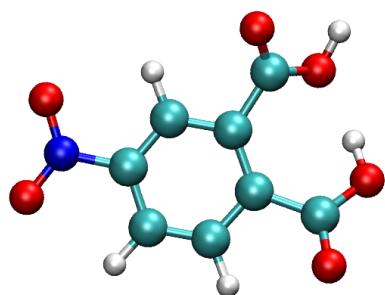
Different



Molecule A 4NFAACb



Molecule B 4NFAACj



Inertia Tensor - Molecule A

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

EingenVectors - Molecule B

-0.9999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

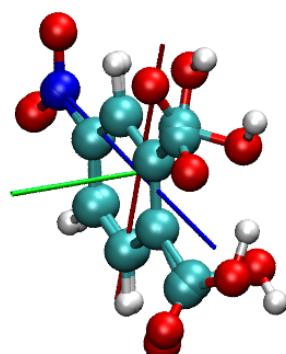
EingenValues - Molecule A

479.308	1242.41	1647.31
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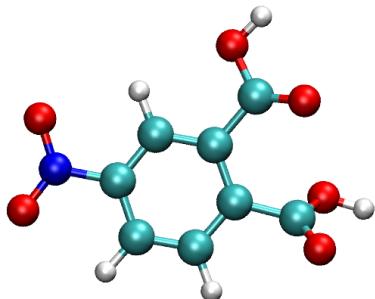
EingenValues - Molecule B

509.897	1225.65	1680.83
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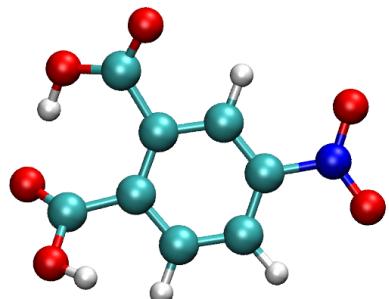
Different



Molecule A 4NFAACb



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

479.338	3.27331	-4.22553
3.27331	1242.4	0.852083
-4.22553	0.852083	1647.3

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999984	-0.00429353	0.00362086
-0.004301	-0.999989	0.00205959
-0.00361198	0.00207513	0.999991

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

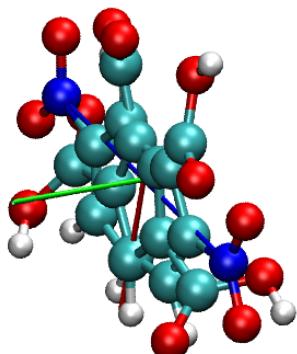
EingenValues - Molecule A

479.308	1242.41	1647.31
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EingenValues - Molecule B

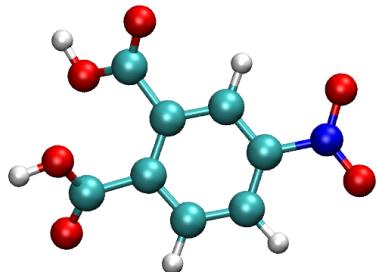
506.607	1222.36	1678.43
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Different

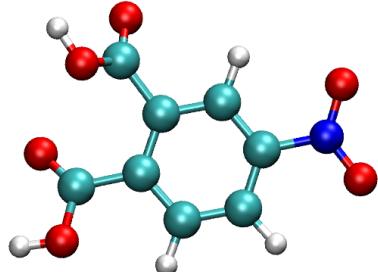


# FireTest Número 450

Molecule A 4NFAACc



Molecule B 4NFAACd



Inertia Tensor - Molecule A

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

Inertia Tensor - Molecule B

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

EingenVectors - Molecule A

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

EingenVectors - Molecule B

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

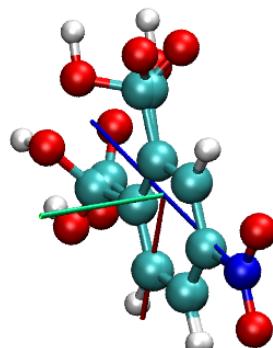
EingenValues - Molecule A

482.027	1240.32	1647.08
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EingenValues - Molecule B

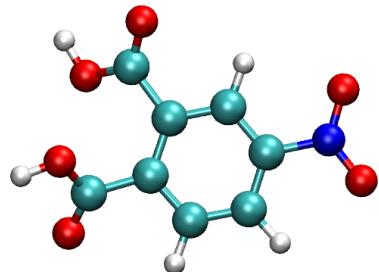
491.663	1231.14	1650.13
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Different

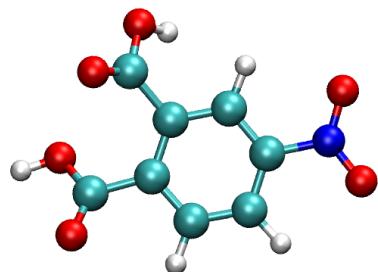


FireTest Número 451

Molecule A 4NFAACc



Molecule B 4NFAACe



Inertia Tensor - Molecule A

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

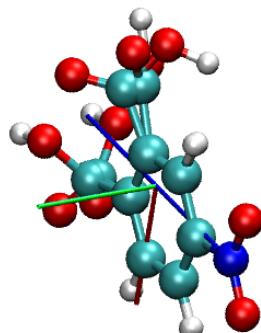
EingenValues - Molecule A

482.027	1240.32	1647.08
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EingenValues - Molecule B

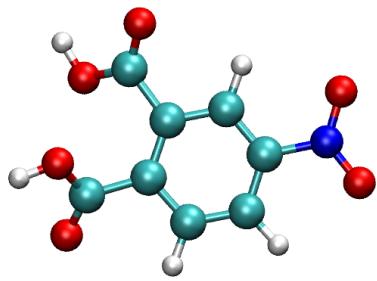
489.011	1233.7	1641.81
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Different

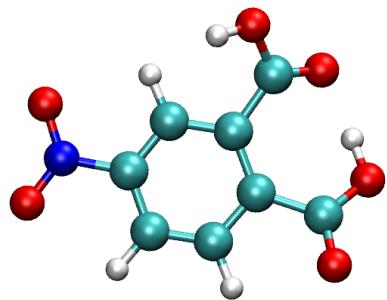


FireTest Número 452

Molecule A 4NFAACc



Molecule B 4NFAACf



Inertia Tensor - Molecule A

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

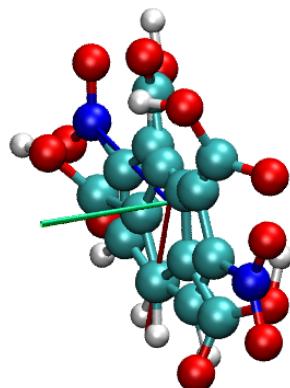
EingenValues - Molecule A

482.027	1240.32	1647.08
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EingenValues - Molecule B

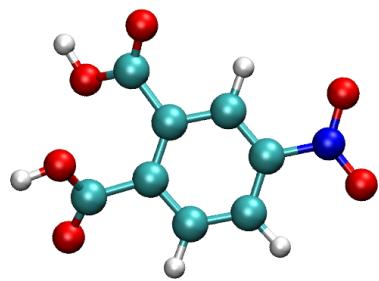
509.668	1219.11	1681.18
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Different

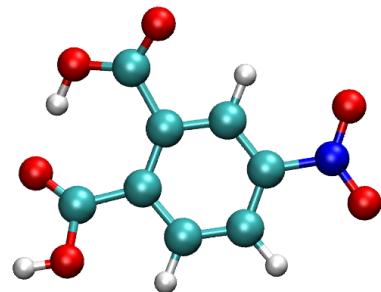


FireTest Número 453

Molecule A 4NFAACc



Molecule B 4NFAACg



Inertia Tensor - Molecule A

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EigenVectors - Molecule A

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

EigenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

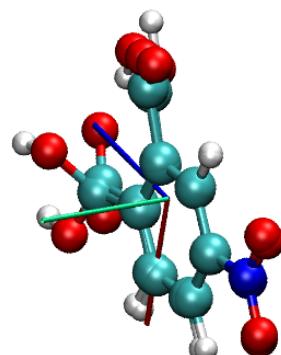
EigenValues - Molecule A

482.027	1240.32	1647.08
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EigenValues - Molecule B

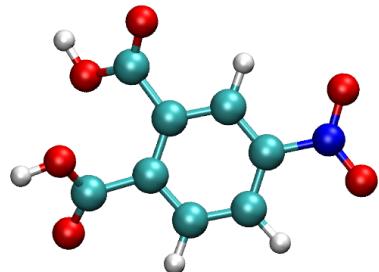
513.751	1208.07	1700.9
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Different

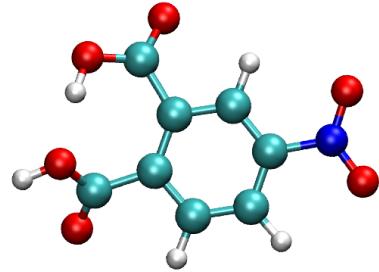


FireTest Número 454

Molecule A 4NFAACc



Molecule B 4NFAACi



Inertia Tensor - Molecule A

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

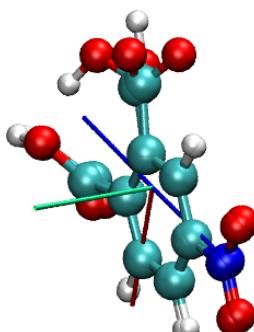
EingenValues - Molecule A

482.027	1240.32	1647.08
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EingenValues - Molecule B

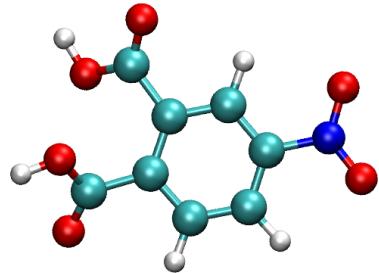
502.409	1232.26	1676.02
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Different

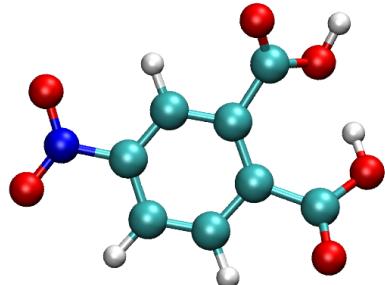


FireTest Número 455

Molecule A 4NFAACc



Molecule B 4NFAACj



Inertia Tensor - Molecule A

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

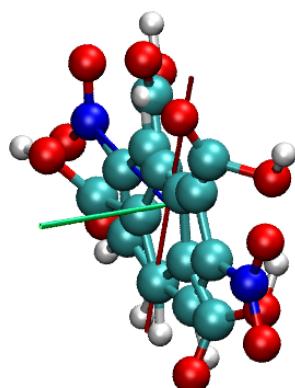
EigenValues - Molecule A

482.027	1240.32	1647.08
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EigenValues - Molecule B

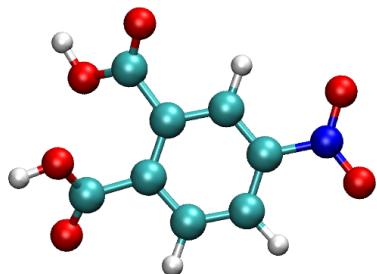
509.897	1225.65	1680.83
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Different

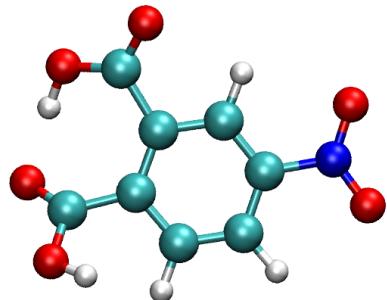


FireTest Número 456

Molecule A 4NFAACc



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

482.067	-5.39474	-1.35857
-5.39474	1240.3	-2.54035
-1.35857	-2.54035	1647.06

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999974	-0.00711826	-0.0011816
0.00712547	-0.999955	-0.00622156
-0.00113726	-0.00622982	0.99998

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

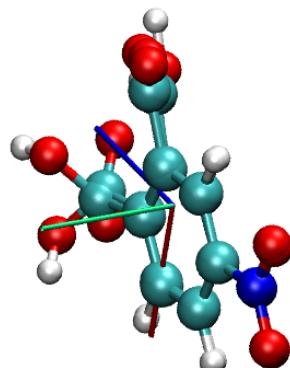
EingenValues - Molecule A

482.027	1240.32	1647.08
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EingenValues - Molecule B

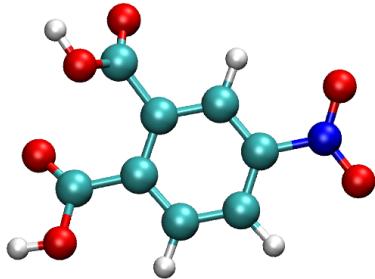
506.607	1222.36	1678.43
---------	---------	---------

Different

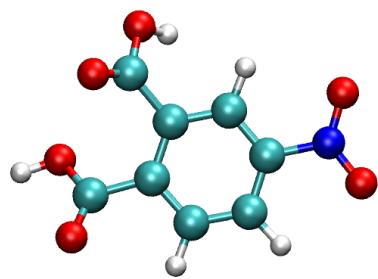


FireTest Número 457

Molecule A 4NFAACd



Molecule B 4NFAACe



Inertia Tensor - Molecule A

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

Inertia Tensor - Molecule B

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

EingenVectors - Molecule A

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

EingenVectors - Molecule B

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

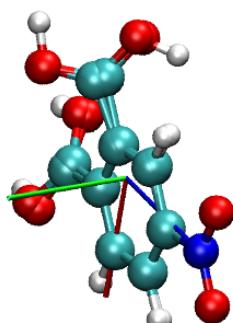
EingenValues - Molecule A

491.663	1231.14	1650.13
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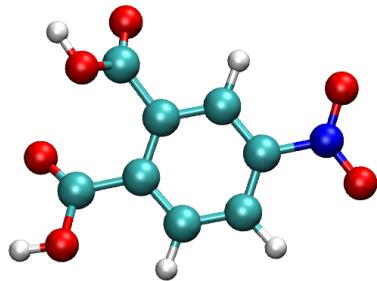
EingenValues - Molecule B

489.011	1233.7	1641.81
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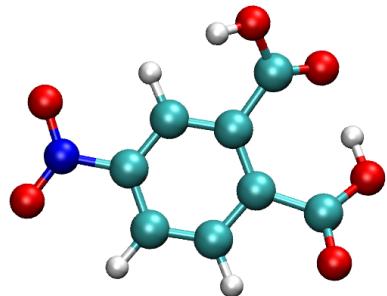
Different



Molecule A 4NFAACd



Molecule B 4NFAACf



Inertia Tensor - Molecule A

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

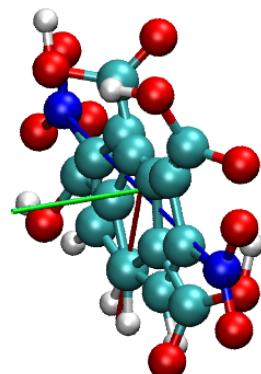
EingenValues - Molecule A

491.663	1231.14	1650.13
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EingenValues - Molecule B

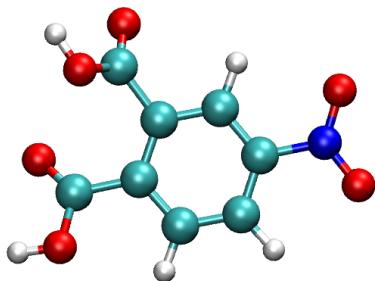
509.668	1219.11	1681.18
---------	---------	---------

Different

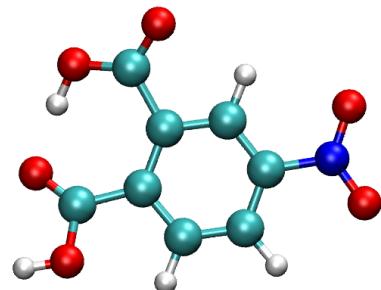


FireTest Número 459

Molecule A 4NFAACd



Molecule B 4NFAACg



Inertia Tensor - Molecule A

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EigenVectors - Molecule A

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

EigenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

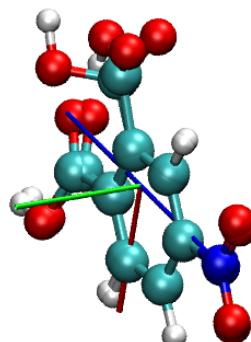
EigenValues - Molecule A

491.663	1231.14	1650.13
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EigenValues - Molecule B

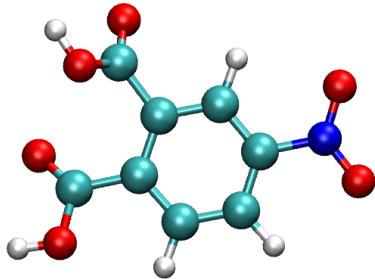
513.751	1208.07	1700.9
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Different

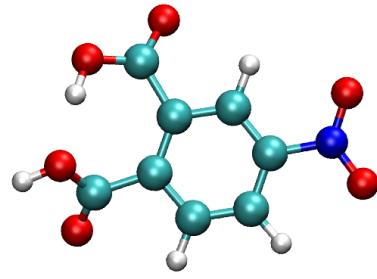


FireTest Número 460

Molecule A 4NFAACd



Molecule B 4NFAACi



Inertia Tensor - Molecule A

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

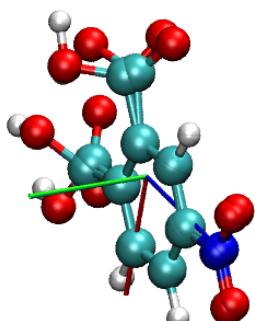
EingenValues - Molecule A

491.663	1231.14	1650.13
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EingenValues - Molecule B

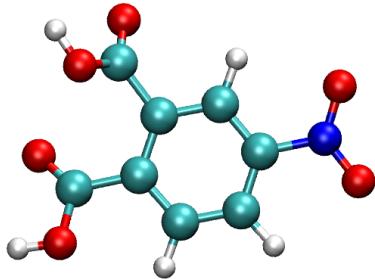
502.409	1232.26	1676.02
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Different

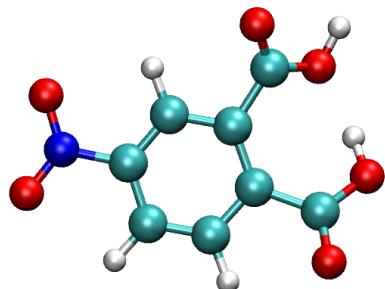


FireTest Número 461

Molecule A 4NFAACd



Molecule B 4NFAACj



Inertia Tensor - Molecule A

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

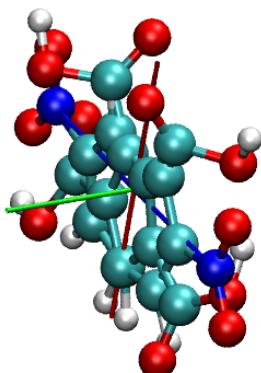
EigenValues - Molecule A

491.663	1231.14	1650.13
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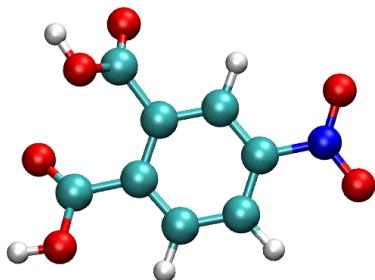
EigenValues - Molecule B

509.897	1225.65	1680.83
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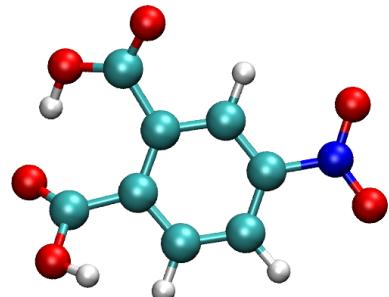
Different



Molecule A 4NFAACd



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

491.672	0.24486	-3.10016
0.24486	1231.15	2.19965
-3.10016	2.19965	1650.11

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999996	-0.000339081	0.00267677
-0.000353124	-0.999986	0.00524747
-0.00267495	0.0052484	0.999983

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

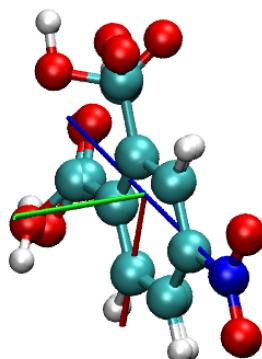
EingenValues - Molecule A

491.663	1231.14	1650.13
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EingenValues - Molecule B

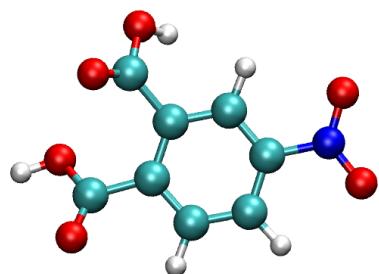
506.607	1222.36	1678.43
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Different

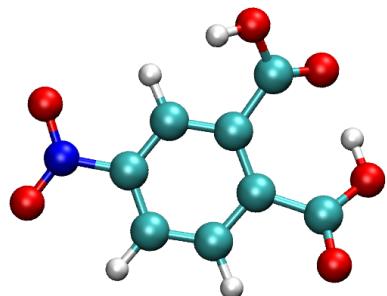


FireTest Número 463

Molecule A 4NFAACe



Molecule B 4NFAACf



Inertia Tensor - Molecule A

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

Inertia Tensor - Molecule B

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

EingenVectors - Molecule A

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

EingenVectors - Molecule B

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

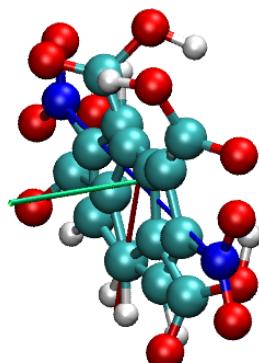
EingenValues - Molecule A

489.011	1233.7	1641.81
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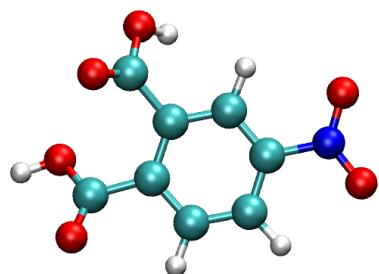
EingenValues - Molecule B

509.668	1219.11	1681.18
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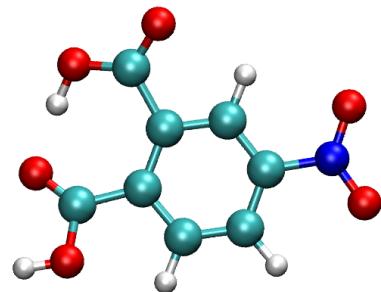
Different



Molecule A 4NFAACe



Molecule B 4NFAACg



Inertia Tensor - Molecule A

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

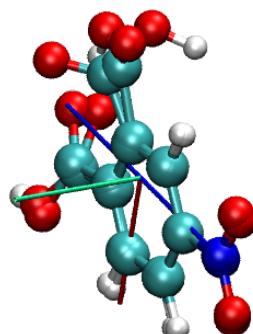
EingenValues - Molecule A

489.011	1233.7	1641.81
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EingenValues - Molecule B

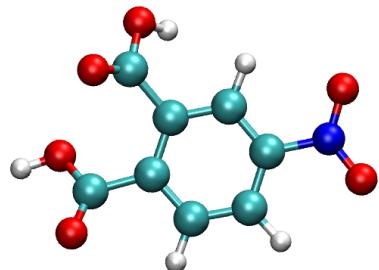
513.751	1208.07	1700.9
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Different

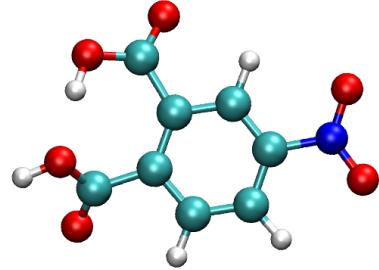


FireTest Número 465

Molecule A 4NFAACe



Molecule B 4NFAACi



Inertia Tensor - Molecule A

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

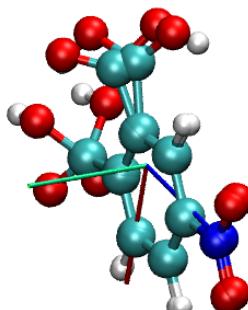
EingenValues - Molecule A

489.011	1233.7	1641.81
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EingenValues - Molecule B

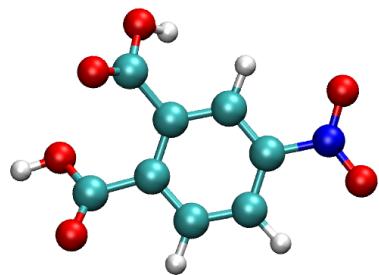
502.409	1232.26	1676.02
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Different

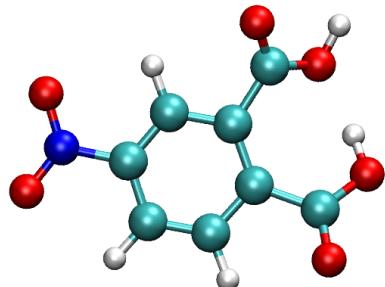


# FireTest Número 466

Molecule A 4NFAACe



Molecule B 4NFAACj



Inertia Tensor - Molecule A

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

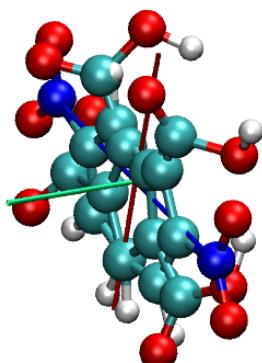
EigenValues - Molecule A

489.011	1233.7	1641.81
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EigenValues - Molecule B

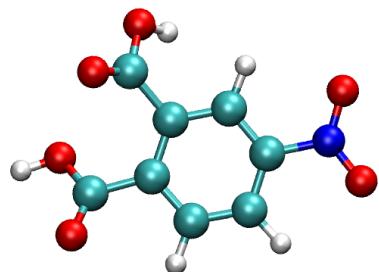
509.897	1225.65	1680.83
---------	---------	---------

Different

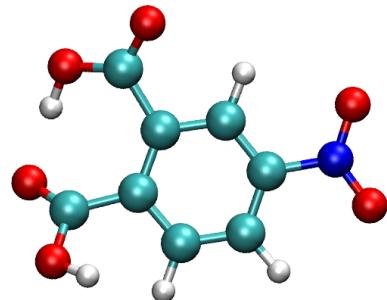


FireTest Número 467

Molecule A 4NFAACe



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

489.025	-0.430035	3.98876
-0.430035	1233.71	-2.06505
3.98876	-2.06505	1641.79

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999994	0.000567863	-0.00345908
0.000550336	-0.999987	-0.00506565
0.00346192	-0.00506372	0.999981

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

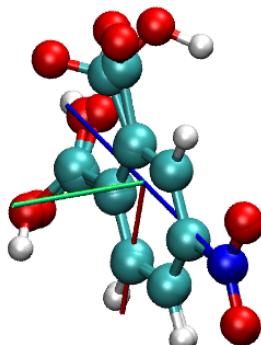
EingenValues - Molecule A

489.011	1233.7	1641.81
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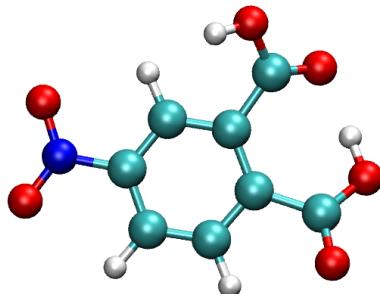
EingenValues - Molecule B

506.607	1222.36	1678.43
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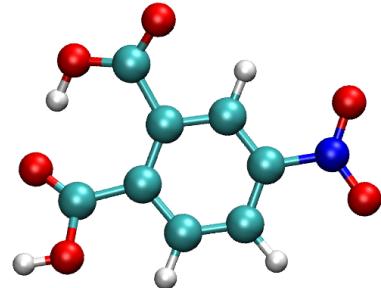
Different



Molecule A 4NFAACf



Molecule B 4NFAACg



Inertia Tensor - Molecule A

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

Inertia Tensor - Molecule B

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

EingenVectors - Molecule A

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

EingenVectors - Molecule B

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

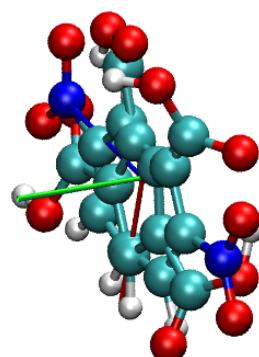
EingenValues - Molecule A

509.668	1219.11	1681.18
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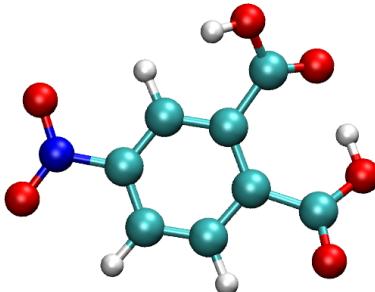
EingenValues - Molecule B

513.751	1208.07	1700.9
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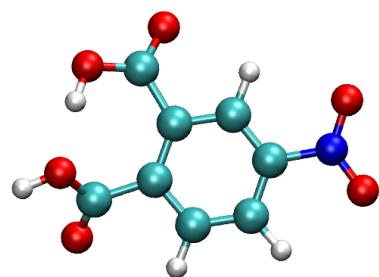
Different



Molecule A 4NFAACf



Molecule B 4NFAACi



Inertia Tensor - Molecule A

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

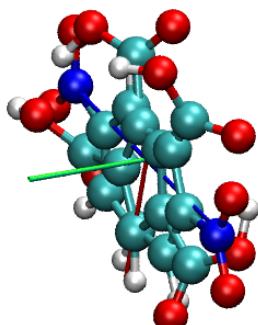
EingenValues - Molecule A

509.668	1219.11	1681.18
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EingenValues - Molecule B

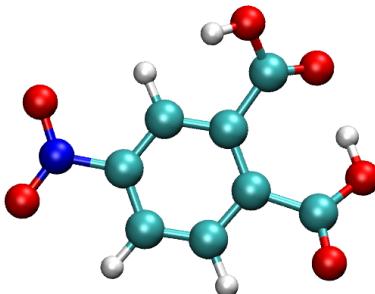
502.409	1232.26	1676.02
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Different

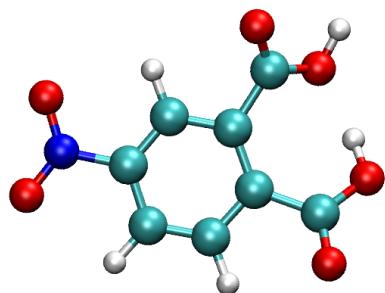


FireTest Número 470

Molecule A 4NFAACf



Molecule B 4NFAACj



Inertia Tensor - Molecule A

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

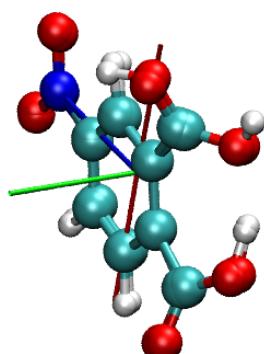
EigenValues - Molecule A

509.668	1219.11	1681.18
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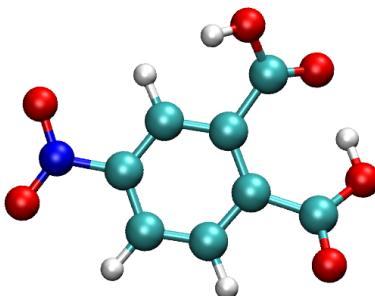
EigenValues - Molecule B

509.897	1225.65	1680.83
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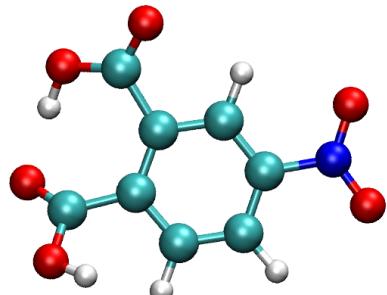
Different



Molecule A 4NFAACf



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

509.683	2.80651	-1.91422
2.80651	1219.11	2.66132
-1.91422	2.66132	1681.17

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999991	0.00396206	-0.00164298
-0.00397143	-0.999976	0.0057431
-0.00162019	0.00574957	0.999982

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

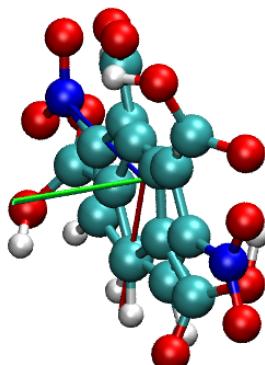
EingenValues - Molecule A

509.668	1219.11	1681.18
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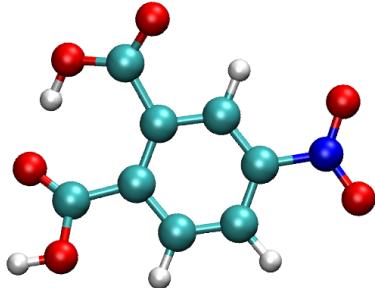
EingenValues - Molecule B

506.607	1222.36	1678.43
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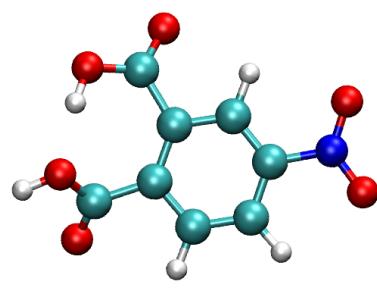
Different



Molecule A 4NFAACg



Molecule B 4NFAACi



Inertia Tensor - Molecule A

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

Inertia Tensor - Molecule B

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

EingenVectors - Molecule A

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

EingenVectors - Molecule B

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

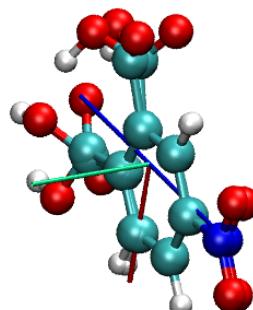
EingenValues - Molecule A

513.751	1208.07	1700.9
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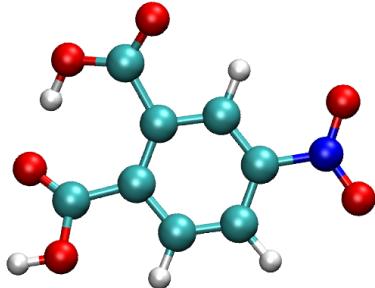
EingenValues - Molecule B

502.409	1232.26	1676.02
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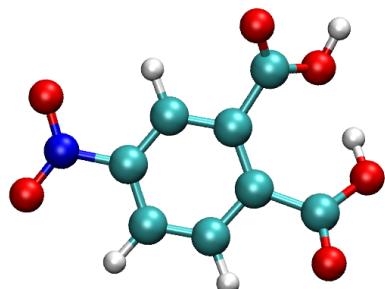
Different



Molecule A 4NFAACg



Molecule B 4NFAACj



Inertia Tensor - Molecule A

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EingenVectors - Molecule A

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

EingenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

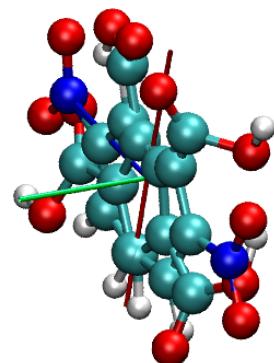
EingenValues - Molecule A

513.751	1208.07	1700.9
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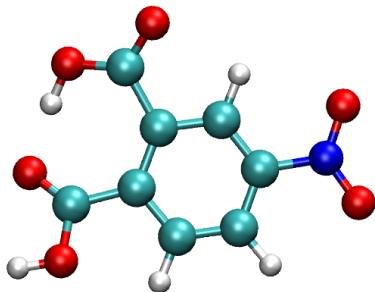
EingenValues - Molecule B

509.897	1225.65	1680.83
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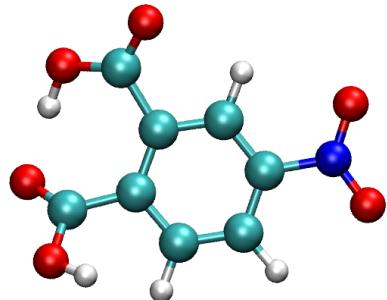
Different



Molecule A 4NFAACg



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

513.78	4.51917	0.266555
4.51917	1208.04	-1.18628
0.266555	-1.18628	1700.9

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999979	0.00650929	0.000231034
-0.00650983	-0.999976	-0.00240351
0.000215383	-0.00240496	0.999997

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

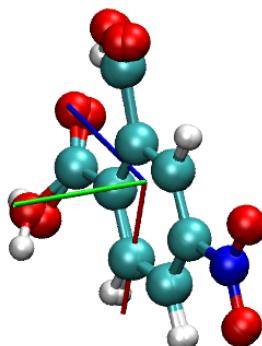
EingenValues - Molecule A

513.751	1208.07	1700.9
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EingenValues - Molecule B

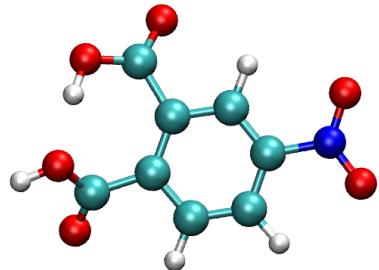
506.607	1222.36	1678.43
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Different

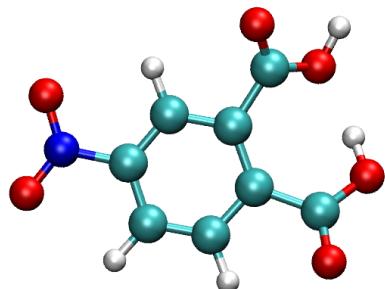


FireTest Número 475

Molecule A 4NFAACi



Molecule B 4NFAACj



Inertia Tensor - Molecule A

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

Inertia Tensor - Molecule B

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

EigenVectors - Molecule A

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

EigenVectors - Molecule B

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

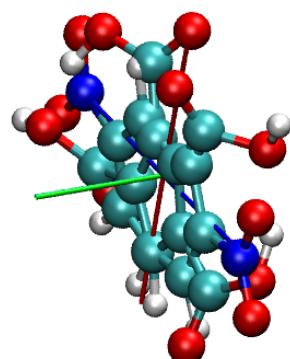
EigenValues - Molecule A

502.409	1232.26	1676.02
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EigenValues - Molecule B

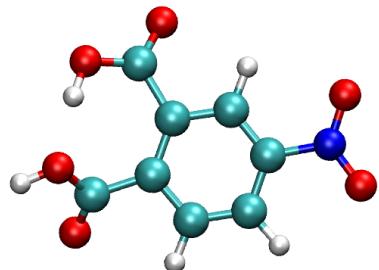
509.897	1225.65	1680.83
---------	---------	---------

Different

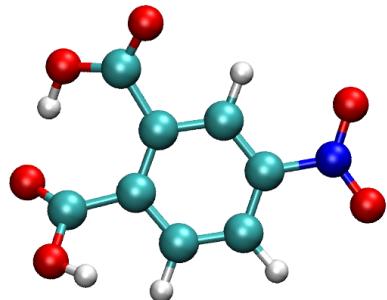


FireTest Número 476

Molecule A 4NFAACi



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

502.43	-0.602691	-4.86988
-0.602691	1232.26	0.407295
-4.86988	0.407295	1676

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

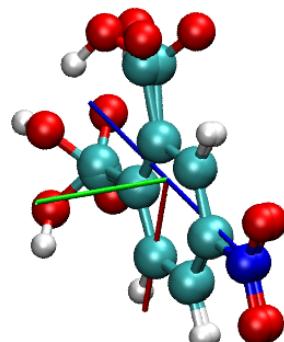
EingenValues - Molecule A

502.409	1232.26	1676.02
---------	---------	---------

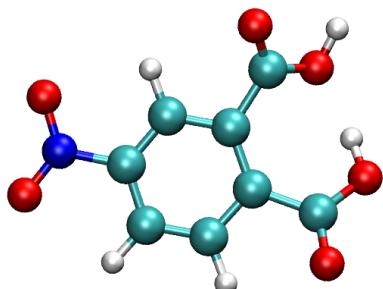
EingenValues - Molecule B

506.607	1222.36	1678.43
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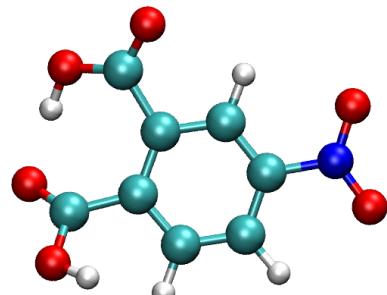
Different



Molecule A 4NFAACj



Molecule B 4NFAACl-3



Inertia Tensor - Molecule A

510.047	9.97005	-3.6306
9.97005	1225.52	-0.981092
-3.6306	-0.981092	1680.82

Inertia Tensor - Molecule B

506.608	0.709539	-0.555426
0.709539	1222.37	-2.84005
-0.555426	-2.84005	1678.41

EingenVectors - Molecule A

-0.999898	0.0139264	-0.00308865
0.0139195	0.999901	0.00226627
-0.00311991	-0.00222305	0.999993

EingenVectors - Molecule B

-0.999999	0.000989428	-0.000471595
-0.000986471	-0.99998	-0.00622856
-0.000477748	-0.00622809	0.99998

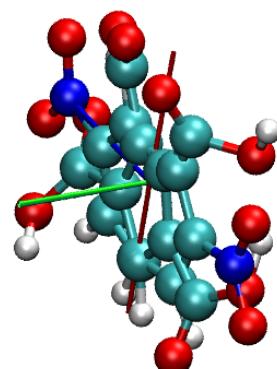
EingenValues - Molecule A

509.897	1225.65	1680.83
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EingenValues - Molecule B

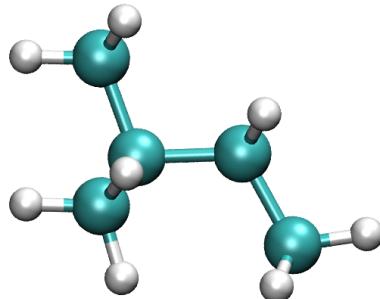
506.607	1222.36	1678.43
---------	---------	---------

Different



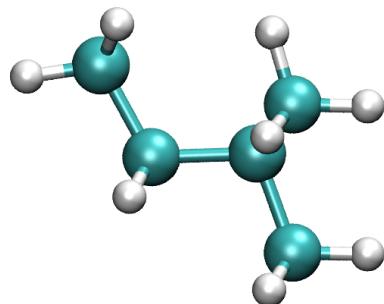
IsomerC6H14 Número 478

Molecule A 2,2-dimethyl-butane.out.G09



Molecule B

2,2-dimethyl-butane.out.G09.inversion



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

EingenVectors - Molecule A

-0.869274	0.494331	0
0.494331	0.869274	0
0	0	1

EingenVectors - Molecule B

-0.869273	0.494332	0
0.494332	0.869273	0
0	0	1

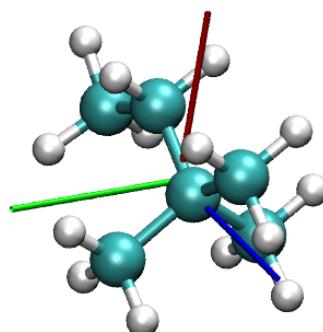
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

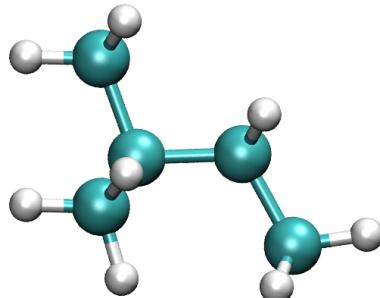
118.684	204.724	205.419
---------	---------	---------

Enantiomers

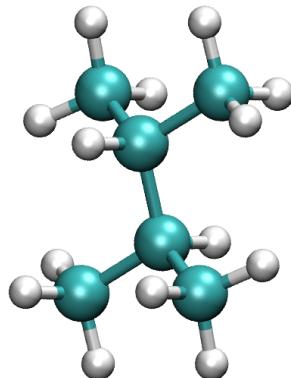


IsomerC6H14 Número 479

Molecule A 2,2-dimethyl-butane\_out\_G09



Molecule B 2,3-dimethyl-butane\_out\_G09



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

EingenVectors - Molecule A

-0.869274	0.494331	0
0.494331	0.869274	0
0	0	1

EingenVectors - Molecule B

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

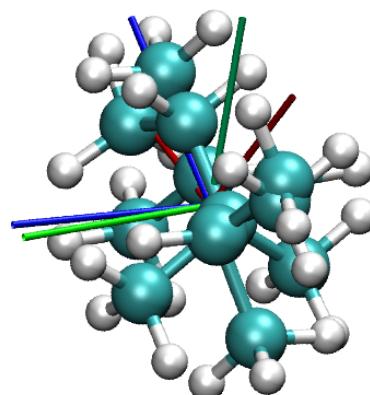
EingenValues - Molecule A

118.683	204.724	205.419
---------	---------	---------

EingenValues - Molecule B

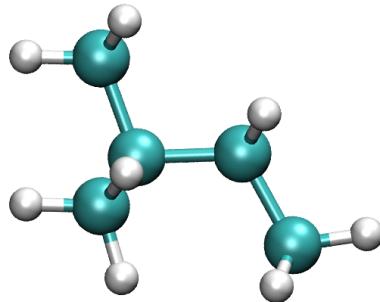
120.611	177.08	272.075
---------	--------	---------

Different



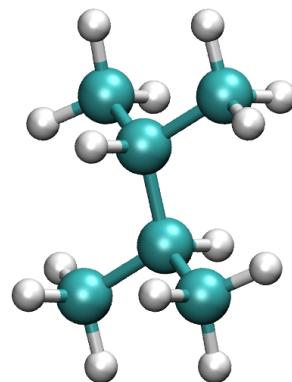
IsomerC6H14 Número 480

Molecule A 2,2-dimethyl-butane.out.G09



Molecule B

2,3-dimethyl-butane.out.G09.inversion



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

EingenVectors - Molecule A

-0.869274	0.494331	0
0.494331	0.869274	0
0	0	1

EingenVectors - Molecule B

-0.112875	-0.993609	0
0	0	1
0.993609	-0.112875	-0

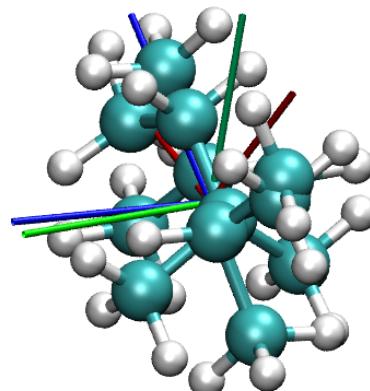
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

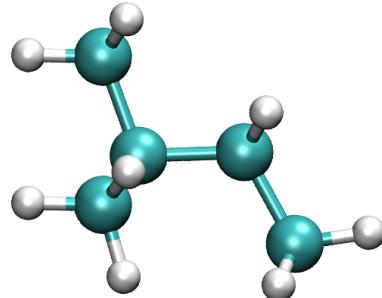
120.611	177.08	272.076
---------	--------	---------

Different

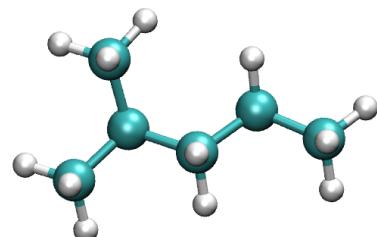


IsomerC6H14 Número 481

Molecule A 2,2-dimethyl-butane\_out\_G09



Molecule B 2-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

76.7701	-0.234564	-0.159008
-0.234564	299.061	-0.102167
-0.159008	-0.102167	347.557

EingenVectors - Molecule A

-0.869274	0.494331	0
0.494331	0.869274	0
0	0	1

EingenVectors - Molecule B

-0.999999	-0.00105548	-0.000587604
-0.00105671	0.999997	0.00210321
-0.000585382	-0.00210383	0.999998

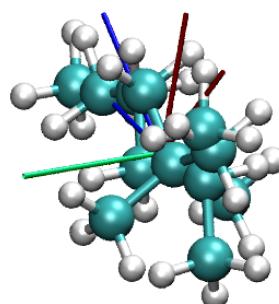
EingenValues - Molecule A

118.683	204.724	205.419
---------	---------	---------

EingenValues - Molecule B

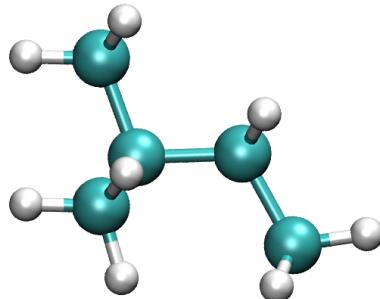
76.7698	299.061	347.558
---------	---------	---------

Different



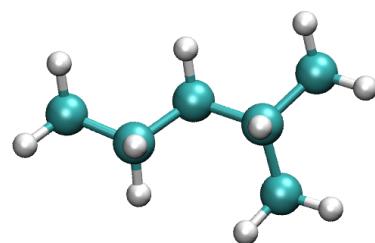
IsomerC6H14 Número 482

Molecule A 2,2-dimethyl-butane\_out\_G09



Molecule B

2-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

$$\begin{vmatrix} 76.7702 & -0.234595 & -0.158982 \\ -0.234595 & 299.061 & -0.102162 \\ -0.158982 & -0.102162 & 347.558 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869274 & 0.494331 & 0 \\ 0.494331 & 0.869274 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999999 & -0.00105562 & -0.000587505 \\ -0.00105685 & 0.999997 & 0.00210312 \\ -0.000585284 & -0.00210374 & 0.999998 \end{vmatrix}$$

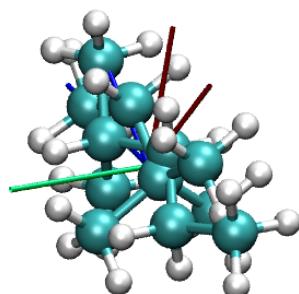
EingenValues - Molecule A

$$\begin{vmatrix} 118.683 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

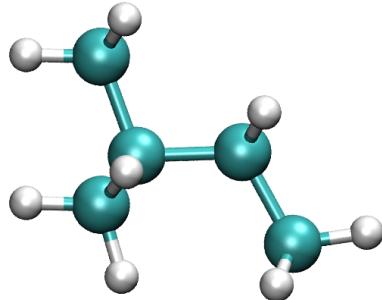
$$\begin{vmatrix} 76.7699 & 299.061 & 347.558 \end{vmatrix}$$

Different

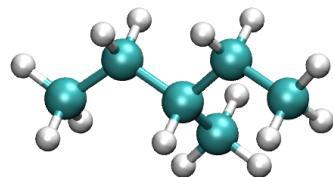


IsomerC6H14 Número 483

Molecule A 2,2-dimethyl-butane\_out\_G09



Molecule B 3-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

294.318	21.9352	0
21.9352	302.288	0
0	0	77.8079

EingenVectors - Molecule A

-0.869274	0.494331	0
0.494331	0.869274	0
0	0	1

EingenVectors - Molecule B

0	0	1
-0.767709	0.640799	0
0.640799	0.767709	0

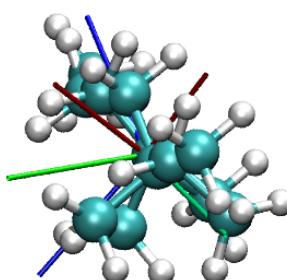
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

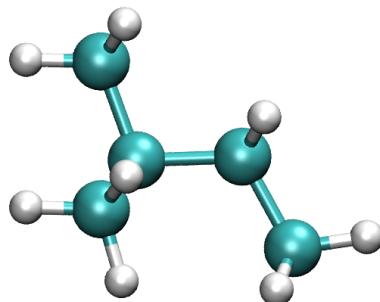
77.8079	276.009	320.597
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Different



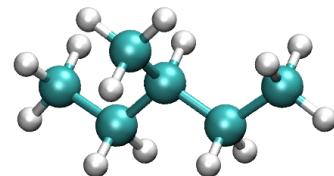
IsomerC6H14 Número 484

Molecule A 2,2-dimethyl-butane\_out\_G09



Molecule B

3-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 294.318 & 21.9353 & 0 \\ 21.9353 & 302.289 & 0 \\ 0 & 0 & 77.8081 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869274 & 0.494331 & 0 \\ 0.494331 & 0.869274 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

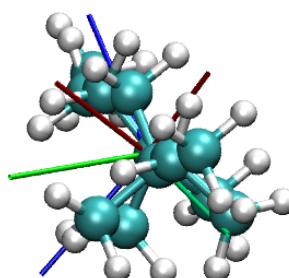
EingenValues - Molecule A

$$\begin{vmatrix} 118.683 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

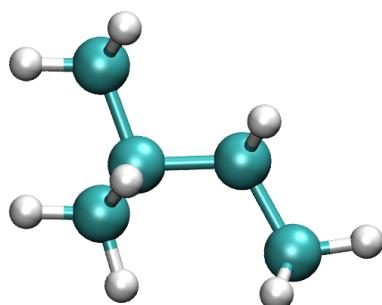
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Different

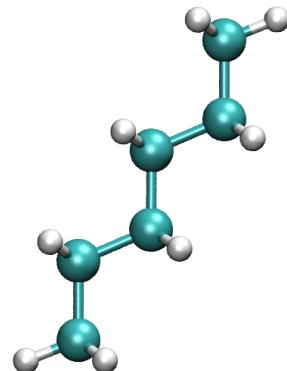


IsomerC6H14 Número 485

Molecule A 2,2-dimethyl-butane\_out\_G09



Molecule B hexane\_out\_G09



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.869274	0.494331	0
0.494331	0.869274	0
0	0	1

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

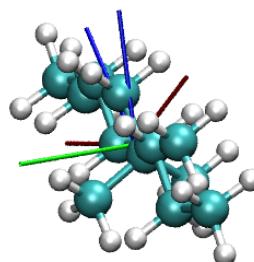
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

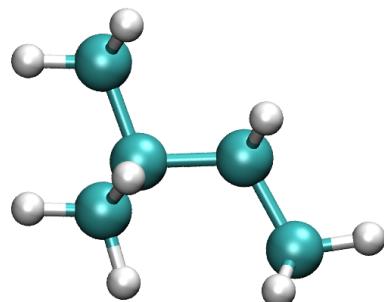
34.6869	449.234	465.177
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Different

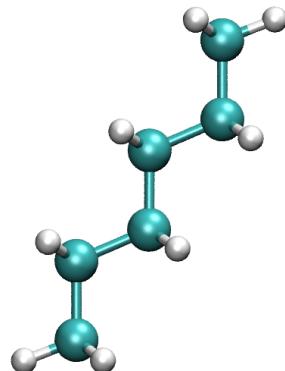


IsomerC6H14 Número 486

Molecule A 2,2-dimethyl-butane\_out\_G09



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

346.245	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.869274	0.494331	0
0.494331	0.869274	0
0	0	1

EingenVectors - Molecule B

-0.498435	-0.866927	0
0.866927	-0.498435	-0
0	0	1

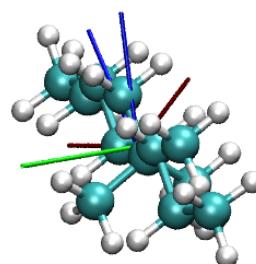
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

34.6868	449.234	465.177
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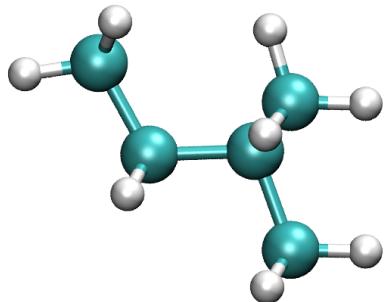
Different



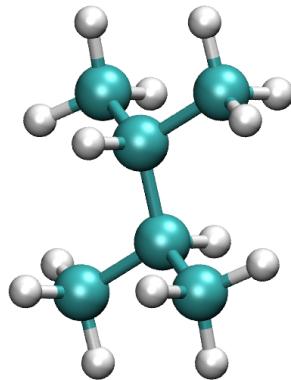
IsomerC6H14 Número 487

Molecule A

2,2-dimethyl-butane\_out\_G09\_inversion



Molecule B 2,3-dimethyl-butane\_out\_G09



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

EingenVectors - Molecule A

-0.869273	0.494332	0
0.494332	0.869273	0
0	0	1

EingenVectors - Molecule B

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

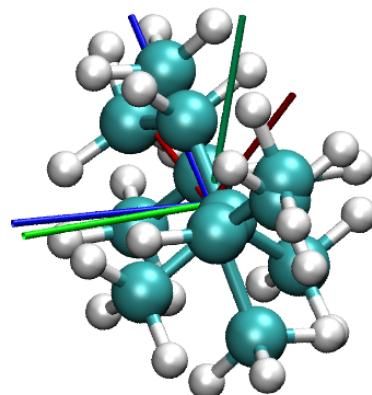
EingenValues - Molecule A

118.684	204.724	205.419
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EingenValues - Molecule B

120.611	177.08	272.075
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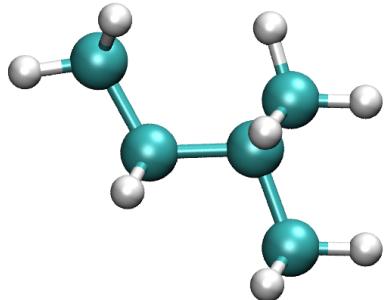
Different



IsomerC6H14 Número 488

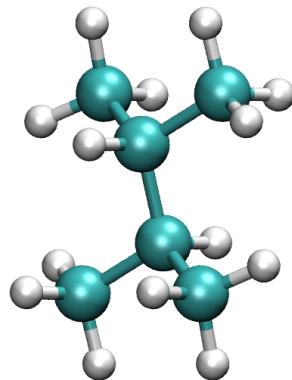
Molecule A

2,2-dimethyl-butane\_out\_G09\_inversion



Molecule B

2,3-dimethyl-butane\_out\_G09\_inversion



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

EingenVectors - Molecule A

-0.869273	0.494332	0
0.494332	0.869273	0
0	0	1

EingenVectors - Molecule B

-0.112875	-0.993609	0
0	0	1
0.993609	-0.112875	-0

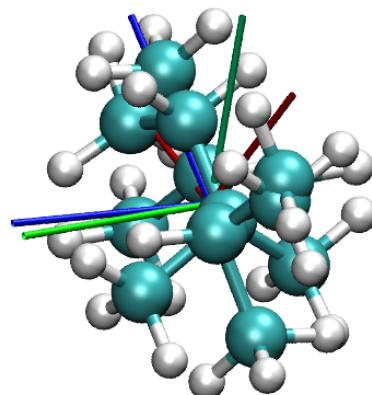
EingenValues - Molecule A

118.684	204.724	205.419
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EingenValues - Molecule B

120.611	177.08	272.076
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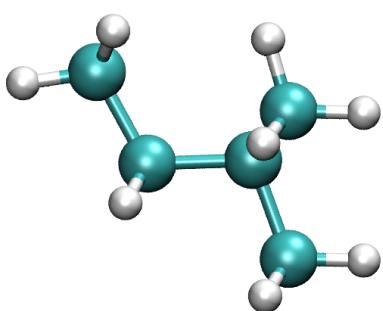
Different



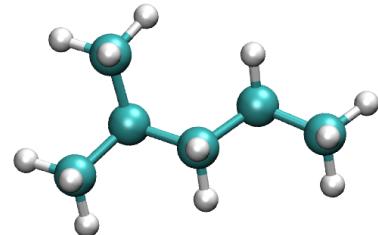
IsomerC6H14 Número 489

Molecule A

2,2-dimethyl-butane\_out\_G09\_inversion



Molecule B 2-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 76.7701 & -0.234564 & -0.159008 \\ -0.234564 & 299.061 & -0.102167 \\ -0.159008 & -0.102167 & 347.557 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869273 & 0.494332 & 0 \\ 0.494332 & 0.869273 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999999 & -0.00105548 & -0.000587604 \\ -0.00105671 & 0.999997 & 0.00210321 \\ -0.000585382 & -0.00210383 & 0.999998 \end{vmatrix}$$

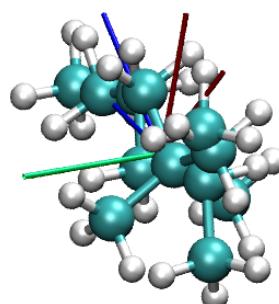
EingenValues - Molecule A

$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 76.7698 & 299.061 & 347.558 \end{vmatrix}$$

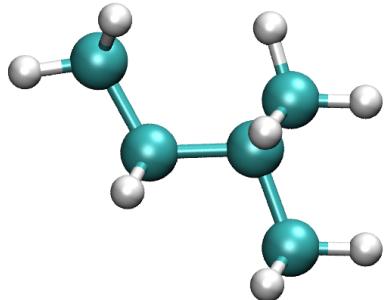
Different



IsomerC6H14 Número 490

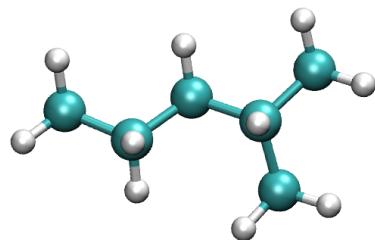
Molecule A

2,2-dimethyl-butane\_out\_G09\_inversion



Molecule B

2-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 76.7702 & -0.234595 & -0.158982 \\ -0.234595 & 299.061 & -0.102162 \\ -0.158982 & -0.102162 & 347.558 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869273 & 0.494332 & 0 \\ 0.494332 & 0.869273 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999999 & -0.00105562 & -0.000587505 \\ -0.00105685 & 0.999997 & 0.00210312 \\ -0.000585284 & -0.00210374 & 0.999998 \end{vmatrix}$$

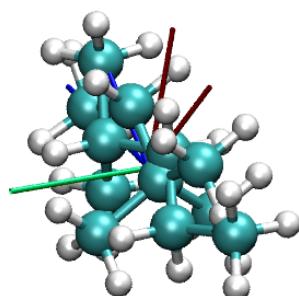
EingenValues - Molecule A

$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 76.7699 & 299.061 & 347.558 \end{vmatrix}$$

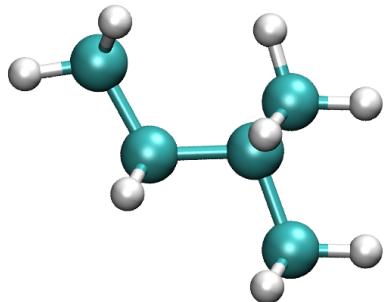
Different



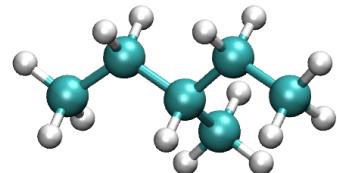
IsomerC6H14 Número 491

Molecule A

2,2-dimethyl-butane\_out\_G09\_inversion



Molecule B 3-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

294.318	21.9352	0
21.9352	302.288	0
0	0	77.8079

EingenVectors - Molecule A

-0.869273	0.494332	0
0.494332	0.869273	0
0	0	1

EingenVectors - Molecule B

0	0	1
-0.767709	0.640799	0
0.640799	0.767709	0

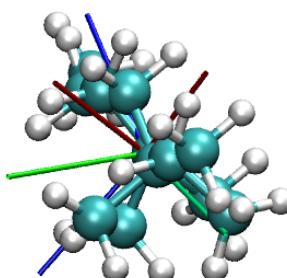
EingenValues - Molecule A

118.684	204.724	205.419
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EingenValues - Molecule B

77.8079	276.009	320.597
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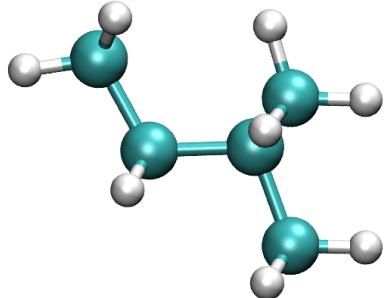
Different



IsomerC6H14 Número 492

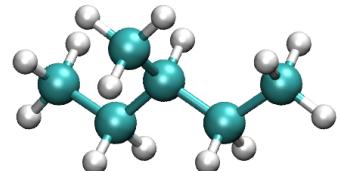
Molecule A

2,2-dimethyl-butane\_out\_G09\_inversion



Molecule B

3-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 294.318 & 21.9353 & 0 \\ 21.9353 & 302.289 & 0 \\ 0 & 0 & 77.8081 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869273 & 0.494332 & 0 \\ 0.494332 & 0.869273 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

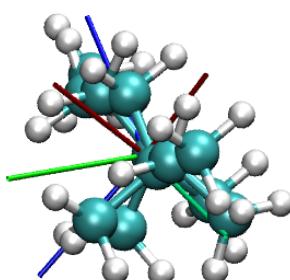
EingenValues - Molecule A

$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

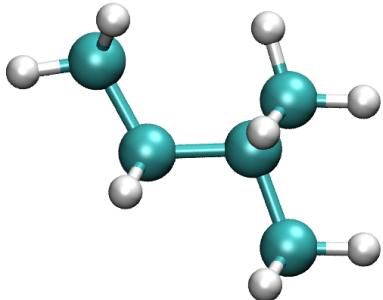
Different



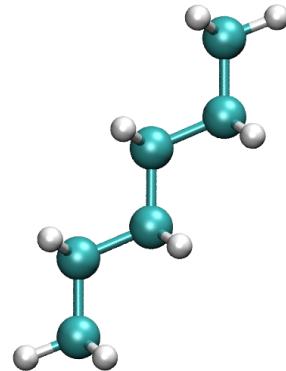
IsomerC6H14 Número 493

Molecule A

2,2-dimethyl-butane\_out\_G09\_inversion



Molecule B hexane\_out\_G09



Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.869273	0.494332	0
0.494332	0.869273	0
0	0	1

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

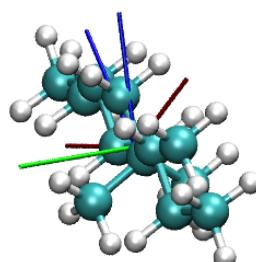
EingenValues - Molecule A

118.684	204.724	205.419
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EingenValues - Molecule B

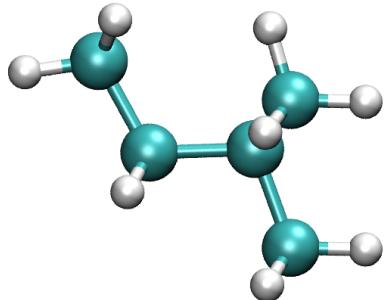
34.6869	449.234	465.177
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Different

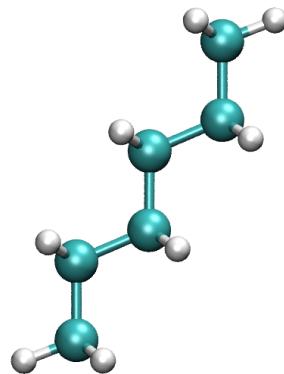


IsomerC6H14 Número 494

Molecule A  
2,2-dimethyl-butane\_out\_G09\_inversion



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 346.245 & -179.129 & 0 \\ -179.129 & 137.676 & 0 \\ 0 & 0 & 465.177 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869273 & 0.494332 & 0 \\ 0.494332 & 0.869273 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.498435 & -0.866927 & 0 \\ 0.866927 & -0.498435 & -0 \\ 0 & 0 & 1 \end{vmatrix}$$

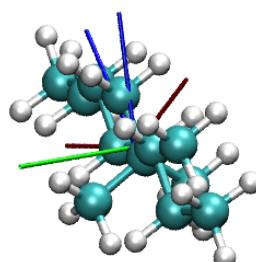
EingenValues - Molecule A

$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

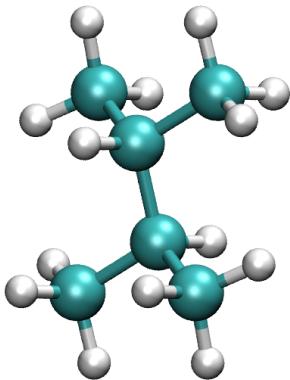
$$\begin{vmatrix} 34.6868 & 449.234 & 465.177 \end{vmatrix}$$

Different



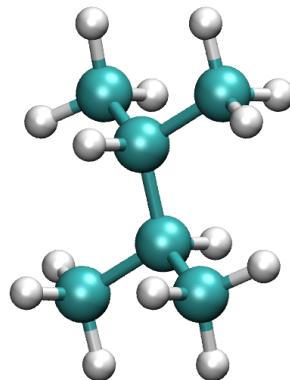
IsomerC6H14 Número 495

Molecule A 2,3-dimethyl-butane.out.G09



Molecule B

2,3-dimethyl-butane.out.G09.inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.112876 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112876 & -0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.112875 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112875 & -0 \end{vmatrix}$$

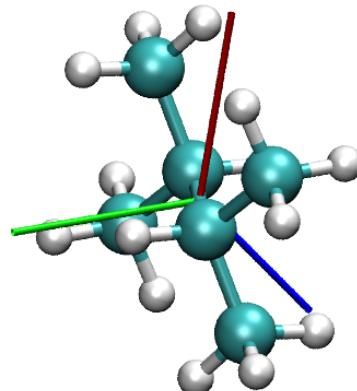
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.075 \end{vmatrix}$$

EingenValues - Molecule B

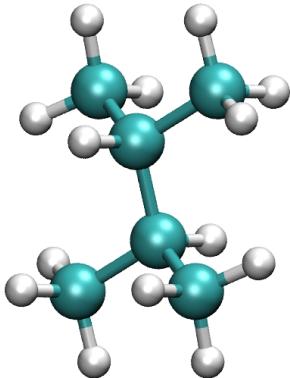
$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

Equal

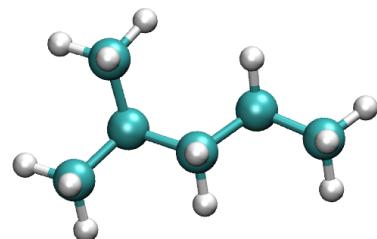


IsomerC6H14 Número 496

Molecule A 2,3-dimethyl-butane\_out\_G09



Molecule B 2-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

Inertia Tensor - Molecule B

76.7701	-0.234564	-0.159008
-0.234564	299.061	-0.102167
-0.159008	-0.102167	347.557

EingenVectors - Molecule A

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

EingenVectors - Molecule B

-0.999999	-0.00105548	-0.000587604
-0.00105671	0.999997	0.00210321
-0.000585382	-0.00210383	0.999998

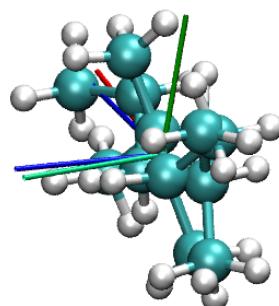
EingenValues - Molecule A

120.611	177.08	272.075
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EingenValues - Molecule B

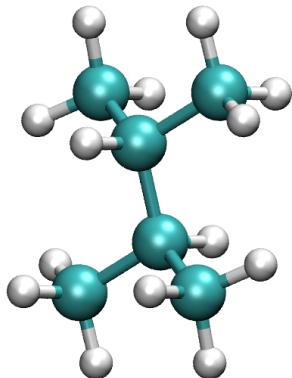
76.7698	299.061	347.558
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Different



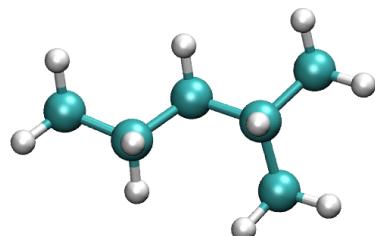
IsomerC6H14 Número 497

Molecule A 2,3-dimethyl-butane\_out\_G09



Molecule B

2-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 76.7702 & -0.234595 & -0.158982 \\ -0.234595 & 299.061 & -0.102162 \\ -0.158982 & -0.102162 & 347.558 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.112876 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112876 & -0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999999 & -0.00105562 & -0.000587505 \\ -0.00105685 & 0.999997 & 0.00210312 \\ -0.000585284 & -0.00210374 & 0.999998 \end{vmatrix}$$

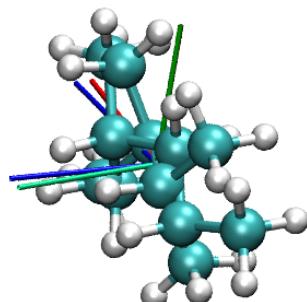
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.075 \end{vmatrix}$$

EingenValues - Molecule B

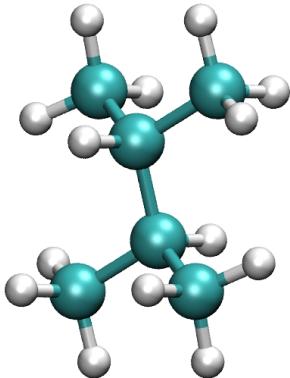
$$\begin{vmatrix} 76.7699 & 299.061 & 347.558 \end{vmatrix}$$

Different

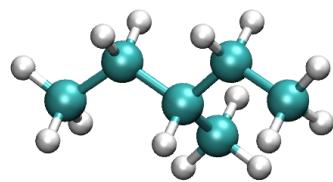


IsomerC6H14 Número 498

Molecule A 2,3-dimethyl-butane\_out\_G09



Molecule B 3-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

Inertia Tensor - Molecule B

294.318	21.9352	0
21.9352	302.288	0
0	0	77.8079

EingenVectors - Molecule A

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

EingenVectors - Molecule B

0	0	1
-0.767709	0.640799	0
0.640799	0.767709	0

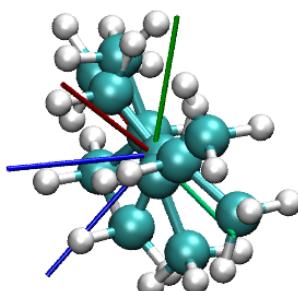
EingenValues - Molecule A

120.611	177.08	272.075
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EingenValues - Molecule B

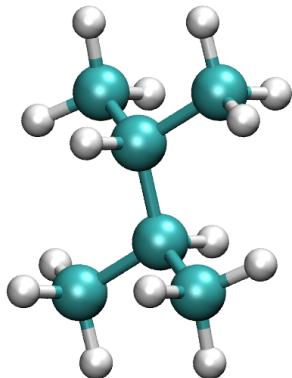
77.8079	276.009	320.597
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Different



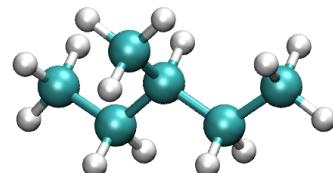
IsomerC6H14 Número 499

Molecule A 2,3-dimethyl-butane\_out\_G09



Molecule B

3-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 294.318 & 21.9353 & 0 \\ 21.9353 & 302.289 & 0 \\ 0 & 0 & 77.8081 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.112876 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112876 & -0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

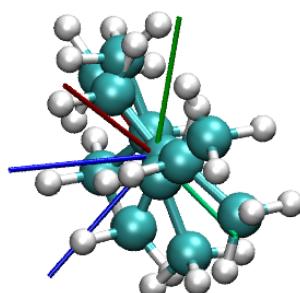
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.075 \end{vmatrix}$$

EingenValues - Molecule B

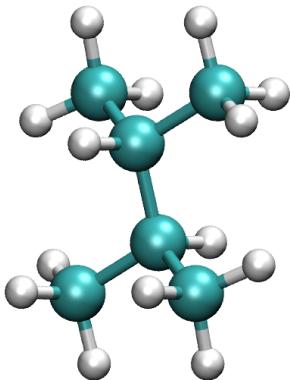
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Different

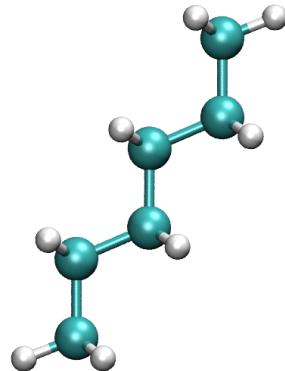


# IsomerC6H14 Número 500

Molecule A 2,3-dimethyl-butane\_out\_G09



Molecule B hexane\_out\_G09



Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

Inertia Tensor - Molecule B

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

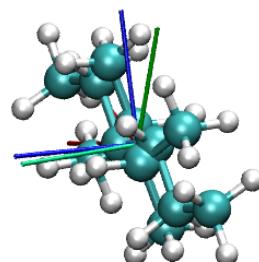
EingenValues - Molecule A

120.611	177.08	272.075
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EingenValues - Molecule B

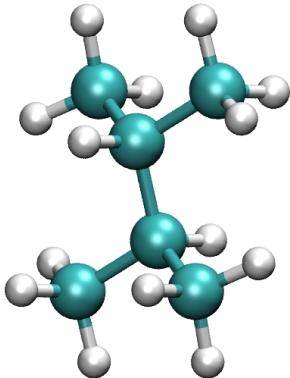
34.6869	449.234	465.177
---------	---------	---------

Different

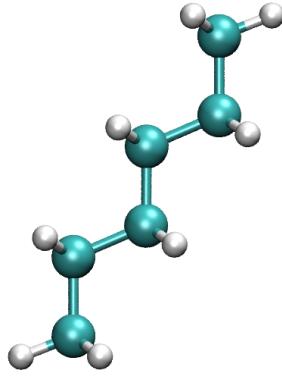


IsomerC6H14 Número 501

Molecule A 2,3-dimethyl-butane\_out\_G09



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

Inertia Tensor - Molecule B

346.245	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

EingenVectors - Molecule B

-0.498435	-0.866927	0
0.866927	-0.498435	-0
0	0	1

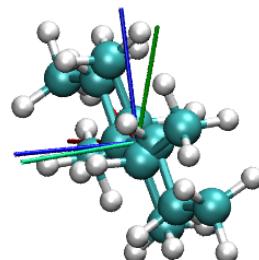
EingenValues - Molecule A

120.611	177.08	272.075
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EingenValues - Molecule B

34.6868	449.234	465.177
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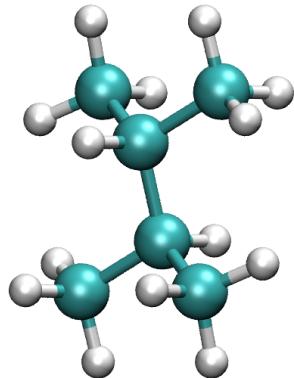
Different



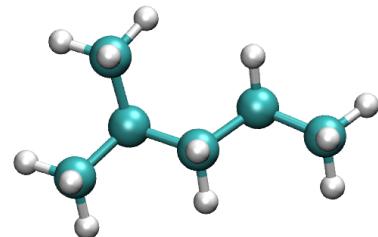
IsomerC6H14 Número 502

Molecule A

2,3-dimethyl-butane\_out\_G09\_inversion



Molecule B 2-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 76.7701 & -0.234564 & -0.159008 \\ -0.234564 & 299.061 & -0.102167 \\ -0.159008 & -0.102167 & 347.557 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.112875 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112875 & -0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999999 & -0.00105548 & -0.000587604 \\ -0.00105671 & 0.999997 & 0.00210321 \\ -0.000585382 & -0.00210383 & 0.999998 \end{vmatrix}$$

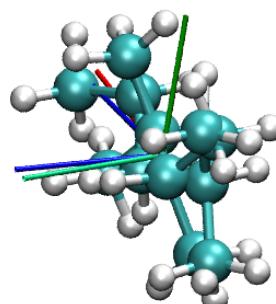
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 76.7698 & 299.061 & 347.558 \end{vmatrix}$$

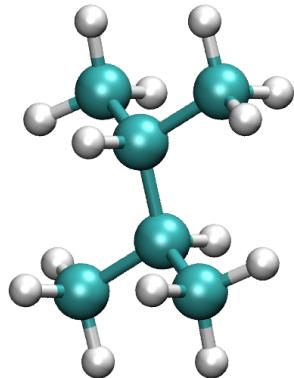
Different



IsomerC6H14 Número 503

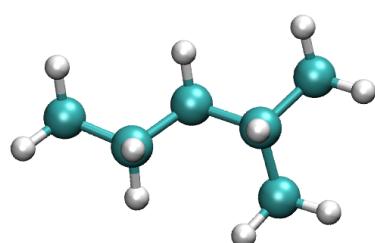
Molecule A

2,3-dimethyl-butane\_out\_G09\_inversion



Molecule B

2-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 76.7702 & -0.234595 & -0.158982 \\ -0.234595 & 299.061 & -0.102162 \\ -0.158982 & -0.102162 & 347.558 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.112875 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112875 & -0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999999 & -0.00105562 & -0.000587505 \\ -0.00105685 & 0.999997 & 0.00210312 \\ -0.000585284 & -0.00210374 & 0.999998 \end{vmatrix}$$

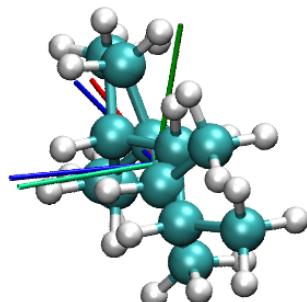
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 76.7699 & 299.061 & 347.558 \end{vmatrix}$$

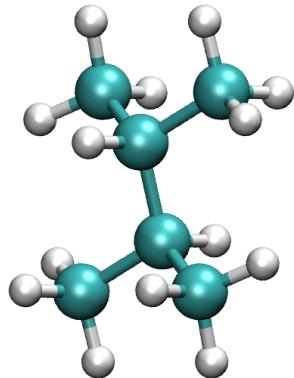
Different



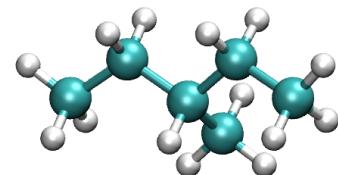
IsomerC6H14 Número 504

Molecule A

2,3-dimethyl-butane\_out\_G09\_inversion



Molecule B 3-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

Inertia Tensor - Molecule B

294.318	21.9352	0
21.9352	302.288	0
0	0	77.8079

EingenVectors - Molecule A

-0.112875	-0.993609	0
0	0	1
0.993609	-0.112875	-0

EingenVectors - Molecule B

0	0	1
-0.767709	0.640799	0
0.640799	0.767709	0

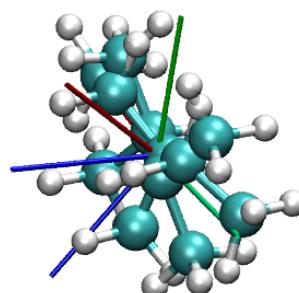
EingenValues - Molecule A

120.611	177.08	272.076
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EingenValues - Molecule B

77.8079	276.009	320.597
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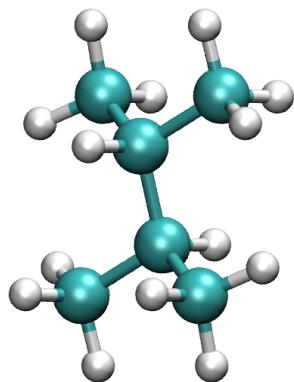
Different



IsomerC6H14 Número 505

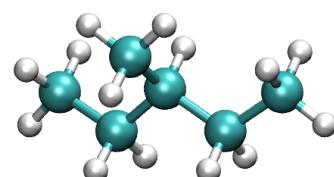
Molecule A

2,3-dimethyl-butane\_out\_G09\_inversion



Molecule B

3-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

Inertia Tensor - Molecule B

294.318	21.9353	0
21.9353	302.289	0
0	0	77.8081

EingenVectors - Molecule A

-0.112875	-0.993609	0
0	0	1
0.993609	-0.112875	-0

EingenVectors - Molecule B

0	0	1
-0.76771	0.640798	0
0.640798	0.76771	0

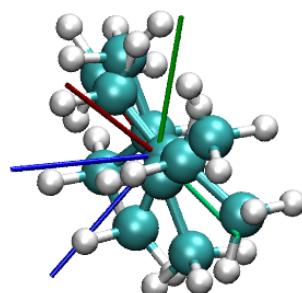
EingenValues - Molecule A

120.611	177.08	272.076
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EingenValues - Molecule B

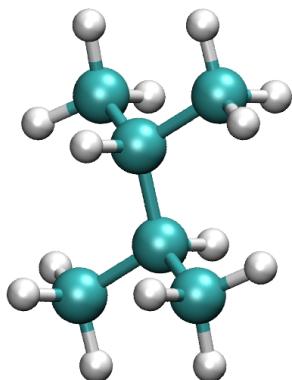
77.8081	276.009	320.598
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Different



IsomerC6H14 Número 506

Molecule A  
2,3-dimethyl-butane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

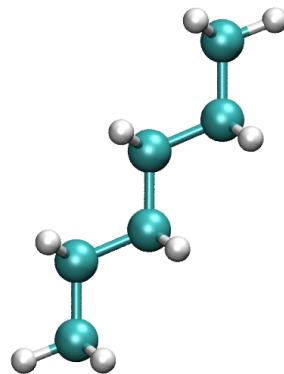
EingenVectors - Molecule A

$$\begin{vmatrix} -0.112875 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112875 & -0 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

Molecule B hexane\_out\_G09



Inertia Tensor - Molecule B

$$\begin{vmatrix} 346.244 & -179.129 & 0 \\ -179.129 & 137.676 & 0 \\ 0 & 0 & 465.177 \end{vmatrix}$$

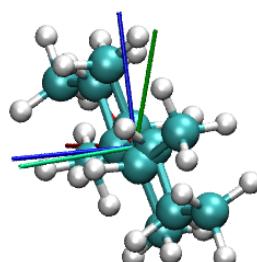
EingenVectors - Molecule B

$$\begin{vmatrix} -0.498436 & -0.866927 & 0 \\ 0.866927 & -0.498436 & -0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenValues - Molecule B

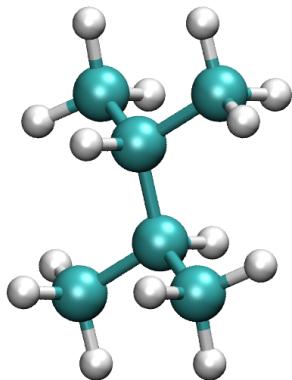
$$\begin{vmatrix} 34.6869 & 449.234 & 465.177 \end{vmatrix}$$

Different

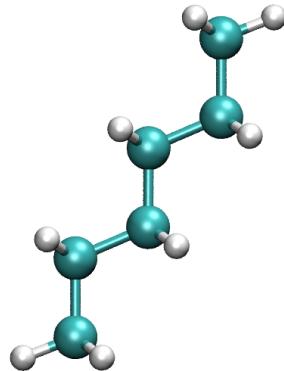


IsomerC6H14 Número 507

Molecule A  
2,3-dimethyl-butane\_out\_G09\_inversion



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 346.245 & -179.129 & 0 \\ -179.129 & 137.676 & 0 \\ 0 & 0 & 465.177 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.112875 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112875 & -0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.498435 & -0.866927 & 0 \\ 0.866927 & -0.498435 & -0 \\ 0 & 0 & 1 \end{vmatrix}$$

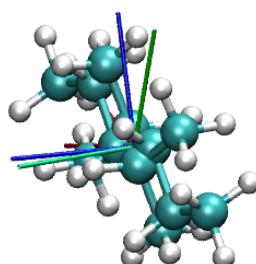
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

EingenValues - Molecule B

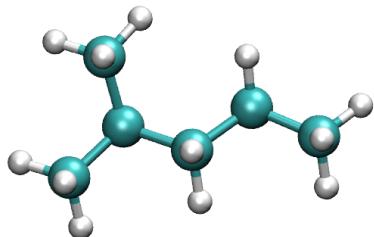
$$\begin{vmatrix} 34.6868 & 449.234 & 465.177 \end{vmatrix}$$

Different



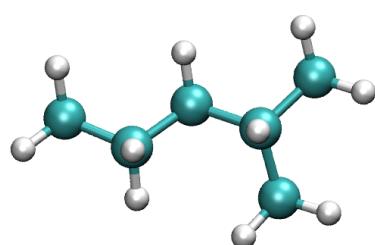
IsomerC6H14 Número 508

Molecule A 2-methyl-pentane\_out\_G09



Molecule B

2-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 76.7701 & -0.234564 & -0.159008 \\ -0.234564 & 299.061 & -0.102167 \\ -0.159008 & -0.102167 & 347.557 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 76.7702 & -0.234595 & -0.158982 \\ -0.234595 & 299.061 & -0.102162 \\ -0.158982 & -0.102162 & 347.558 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.999999 & -0.00105548 & -0.000587604 \\ -0.00105671 & 0.999997 & 0.00210321 \\ -0.000585382 & -0.00210383 & 0.999998 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999999 & -0.00105562 & -0.000587505 \\ -0.00105685 & 0.999997 & 0.00210312 \\ -0.000585284 & -0.00210374 & 0.999998 \end{vmatrix}$$

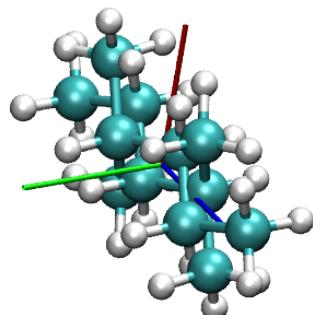
EingenValues - Molecule A

$$\begin{vmatrix} 76.7698 & 299.061 & 347.558 \end{vmatrix}$$

EingenValues - Molecule B

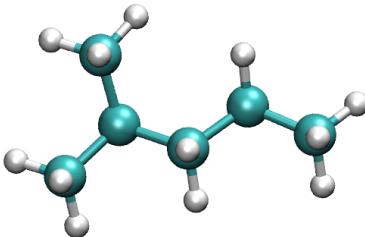
$$\begin{vmatrix} 76.7699 & 299.061 & 347.558 \end{vmatrix}$$

Enantiomers

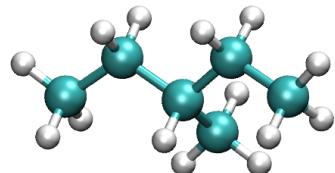


IsomerC6H14 Número 509

Molecule A 2-methyl-pentane\_out\_G09



Molecule B 3-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

76.7701	-0.234564	-0.159008
-0.234564	299.061	-0.102167
-0.159008	-0.102167	347.557

Inertia Tensor - Molecule B

294.318	21.9352	0
21.9352	302.288	0
0	0	77.8079

EingenVectors - Molecule A

-0.999999	-0.00105548	-0.000587604
-0.00105671	0.999997	0.00210321
-0.000585382	-0.00210383	0.999998

EingenVectors - Molecule B

0	0	1
-0.767709	0.640799	0
0.640799	0.767709	0

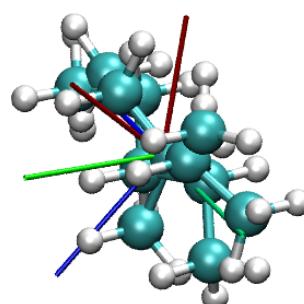
EingenValues - Molecule A

76.7698	299.061	347.558
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EingenValues - Molecule B

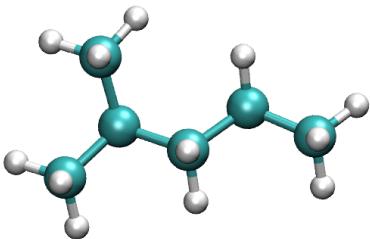
77.8079	276.009	320.597
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Different



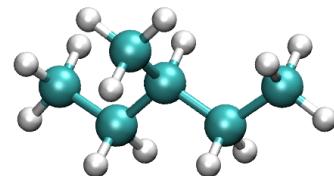
IsomerC6H14 Número 510

Molecule A 2-methyl-pentane\_out\_G09



Molecule B

3-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 76.7701 & -0.234564 & -0.159008 \\ -0.234564 & 299.061 & -0.102167 \\ -0.159008 & -0.102167 & 347.557 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 294.318 & 21.9353 & 0 \\ 21.9353 & 302.289 & 0 \\ 0 & 0 & 77.8081 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.999999 & -0.00105548 & -0.000587604 \\ -0.00105671 & 0.999997 & 0.00210321 \\ -0.000585382 & -0.00210383 & 0.999998 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

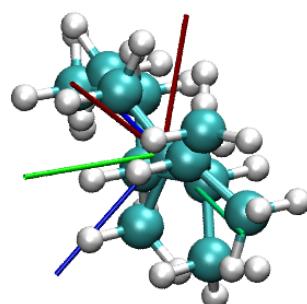
EingenValues - Molecule A

$$\begin{vmatrix} 76.7698 & 299.061 & 347.558 \end{vmatrix}$$

EingenValues - Molecule B

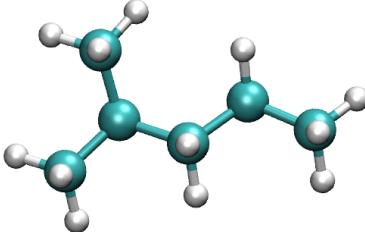
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Different

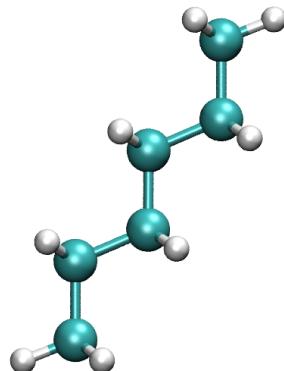


# IsomerC6H14 Número 511

Molecule A 2-methyl-pentane\_out\_G09



Molecule B hexane\_out\_G09



Inertia Tensor - Molecule A

76.7701	-0.234564	-0.159008
-0.234564	299.061	-0.102167
-0.159008	-0.102167	347.557

Inertia Tensor - Molecule B

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.999999	-0.00105548	-0.000587604
-0.00105671	0.999997	0.00210321
-0.000585382	-0.00210383	0.999998

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

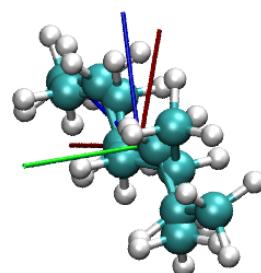
EingenValues - Molecule A

76.7698	299.061	347.558
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EingenValues - Molecule B

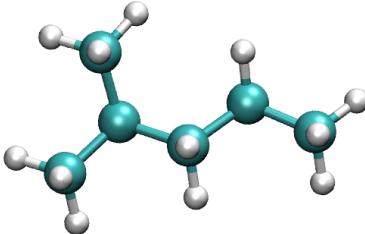
34.6869	449.234	465.177
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Different

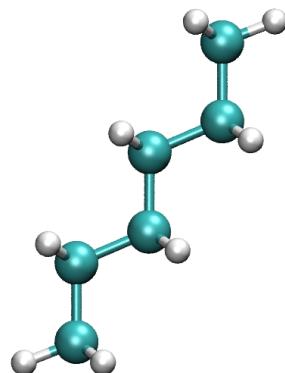


IsomerC6H14 Número 512

Molecule A 2-methyl-pentane\_out\_G09



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A

76.7701	-0.234564	-0.159008
-0.234564	299.061	-0.102167
-0.159008	-0.102167	347.557

Inertia Tensor - Molecule B

346.245	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.999999	-0.00105548	-0.000587604
-0.00105671	0.999997	0.00210321
-0.000585382	-0.00210383	0.999998

EingenVectors - Molecule B

-0.498435	-0.866927	0
0.866927	-0.498435	-0
0	0	1

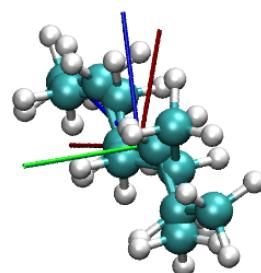
EingenValues - Molecule A

76.7698	299.061	347.558
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EingenValues - Molecule B

34.6868	449.234	465.177
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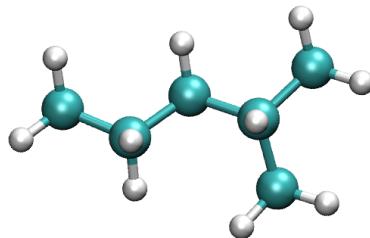
Different



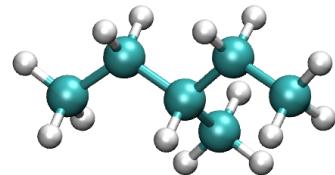
IsomerC6H14 Número 513

Molecule A

2-methyl-pentane\_out\_G09\_inversion



Molecule B 3-methyl-pentane\_out\_G09



Inertia Tensor - Molecule A

76.7702	-0.234595	-0.158982
-0.234595	299.061	-0.102162
-0.158982	-0.102162	347.558

Inertia Tensor - Molecule B

294.318	21.9352	0
21.9352	302.288	0
0	0	77.8079

EigenVectors - Molecule A

-0.999999	-0.00105562	-0.000587505
-0.00105685	0.999997	0.00210312
-0.000585284	-0.00210374	0.999998

EigenVectors - Molecule B

0	0	1
-0.767709	0.640799	0
0.640799	0.767709	0

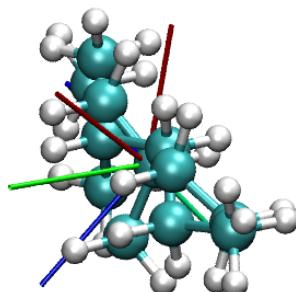
EigenValues - Molecule A

76.7699	299.061	347.558
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EigenValues - Molecule B

77.8079	276.009	320.597
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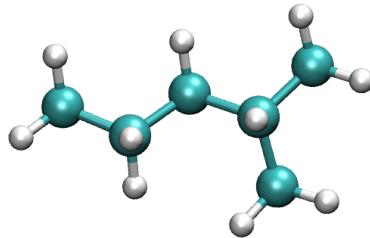
Different



IsomerC6H14 Número 514

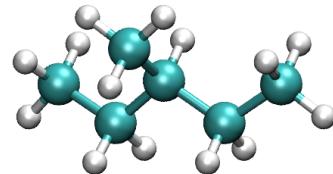
Molecule A

2-methyl-pentane\_out\_G09\_inversion



Molecule B

3-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

76.7702	-0.234595	-0.158982
-0.234595	299.061	-0.102162
-0.158982	-0.102162	347.558

Inertia Tensor - Molecule B

294.318	21.9353	0
21.9353	302.289	0
0	0	77.8081

EingenVectors - Molecule A

-0.999999	-0.00105562	-0.000587505
-0.00105685	0.999997	0.00210312
-0.000585284	-0.00210374	0.999998

EingenVectors - Molecule B

0	0	1
-0.76771	0.640798	0
0.640798	0.76771	0

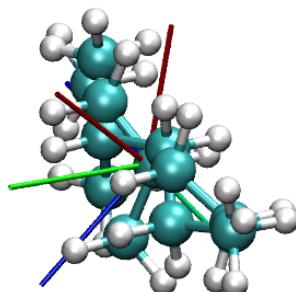
EingenValues - Molecule A

76.7699	299.061	347.558
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EingenValues - Molecule B

77.8081	276.009	320.598
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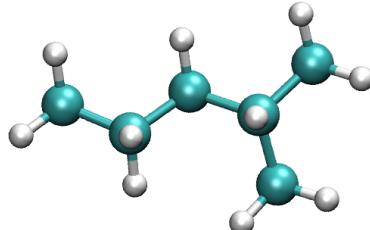
Different



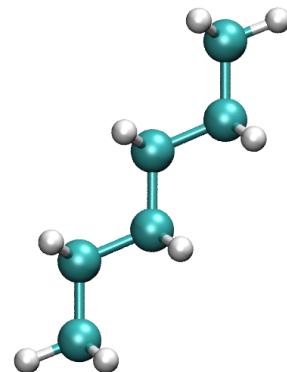
IsomerC6H14 Número 515

Molecule A

2-methyl-pentane\_out\_G09\_inversion



Molecule B hexane\_out\_G09



Inertia Tensor - Molecule A

76.7702	-0.234595	-0.158982
-0.234595	299.061	-0.102162
-0.158982	-0.102162	347.558

Inertia Tensor - Molecule B

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.999999	-0.00105562	-0.000587505
-0.00105685	0.999997	0.00210312
-0.000585284	-0.00210374	0.999998

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

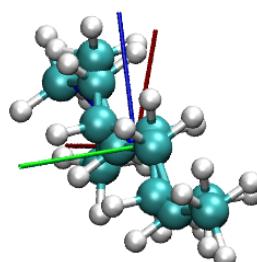
EingenValues - Molecule A

76.7699	299.061	347.558
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EingenValues - Molecule B

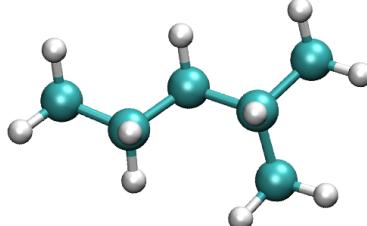
34.6869	449.234	465.177
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Different

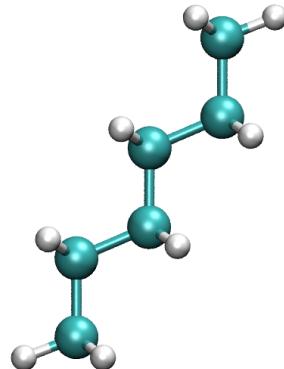


IsomerC6H14 Número 516

Molecule A  
2-methyl-pentane\_out\_G09\_inversion



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A		
76.7702	-0.234595	-0.158982
-0.234595	299.061	-0.102162
-0.158982	-0.102162	347.558

Inertia Tensor - Molecule B		
346.245	-179.129	0
-179.129	137.676	0
0	0	465.177

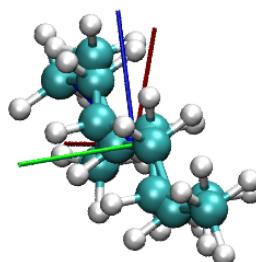
EingenVectors - Molecule A		
-0.999999	-0.00105562	-0.000587505
-0.00105685	0.999997	0.00210312
-0.000585284	-0.00210374	0.999998

EingenVectors - Molecule B		
-0.498435	-0.866927	0
0.866927	-0.498435	-0
0	0	1

EingenValues - Molecule A		
76.7699	299.061	347.558

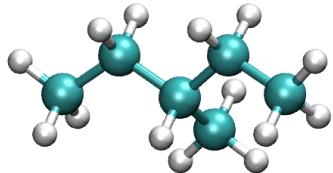
EingenValues - Molecule B		
34.6868	449.234	465.177

Different



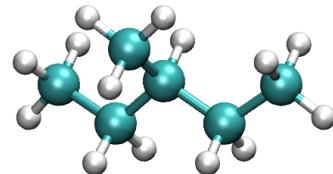
IsomerC6H14 Número 517

Molecule A 3-methyl-pentane\_out\_G09



Molecule B

3-methyl-pentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 294.318 & 21.9352 & 0 \\ 21.9352 & 302.288 & 0 \\ 0 & 0 & 77.8079 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 294.318 & 21.9353 & 0 \\ 21.9353 & 302.289 & 0 \\ 0 & 0 & 77.8081 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.767709 & 0.640799 & 0 \\ 0.640799 & 0.767709 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

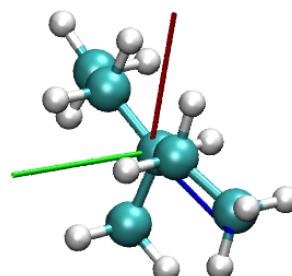
EingenValues - Molecule A

$$\begin{vmatrix} 77.8079 & 276.009 & 320.597 \end{vmatrix}$$

EingenValues - Molecule B

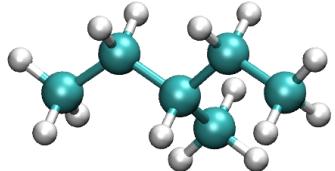
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Equal

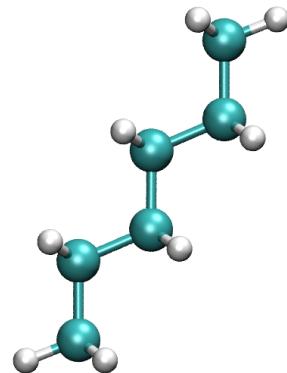


IsomerC6H14 Número 518

Molecule A 3-methyl-pentane\_out\_G09



Molecule B hexane\_out\_G09



Inertia Tensor - Molecule A

294.318	21.9352	0
21.9352	302.288	0
0	0	77.8079

Inertia Tensor - Molecule B

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

0	0	1
-0.767709	0.640799	0
0.640799	0.767709	0

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

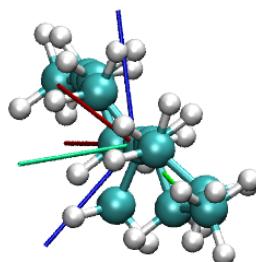
EingenValues - Molecule A

77.8079	276.009	320.597
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EingenValues - Molecule B

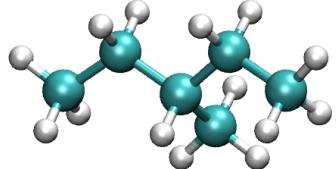
34.6869	449.234	465.177
---------	---------	---------

Different

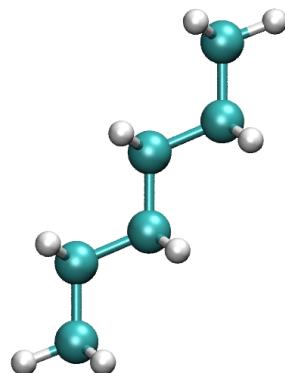


IsomerC6H14 Número 519

Molecule A 3-methyl-pentane\_out\_G09



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A

294.318	21.9352	0
21.9352	302.288	0
0	0	77.8079

Inertia Tensor - Molecule B

346.245	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

0	0	1
-0.767709	0.640799	0
0.640799	0.767709	0

EingenVectors - Molecule B

-0.498435	-0.866927	0
0.866927	-0.498435	-0
0	0	1

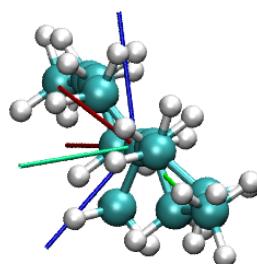
EingenValues - Molecule A

77.8079	276.009	320.597
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EingenValues - Molecule B

34.6868	449.234	465.177
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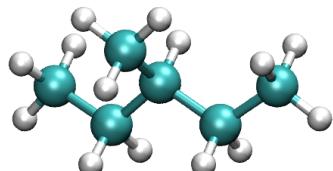
Different



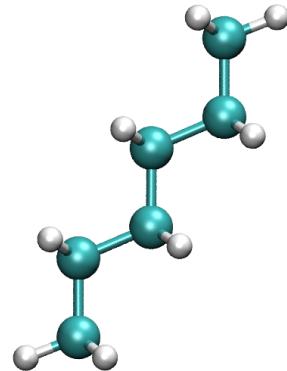
IsomerC6H14 Número 520

Molecule A

3-methyl-pentane\_out\_G09\_inversion



Molecule B hexane\_out\_G09



Inertia Tensor - Molecule A

294.318	21.9353	0
21.9353	302.289	0
0	0	77.8081

Inertia Tensor - Molecule B

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

0	0	1
-0.76771	0.640798	0
0.640798	0.76771	0

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

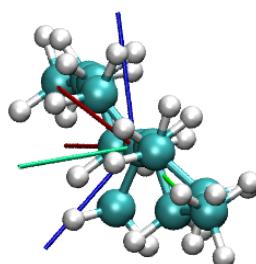
EingenValues - Molecule A

77.8081	276.009	320.598
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EingenValues - Molecule B

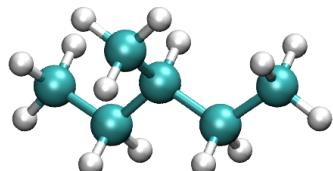
34.6869	449.234	465.177
---------	---------	---------

Different

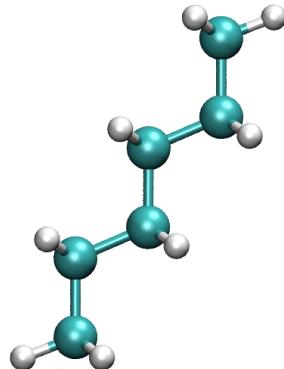


IsomerC6H14 Número 521

Molecule A  
3-methyl-pentane\_out\_G09\_inversion



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A		
294.318	21.9353	0
21.9353	302.289	0
0	0	77.8081

Inertia Tensor - Molecule B		
346.245	-179.129	0
-179.129	137.676	0
0	0	465.177

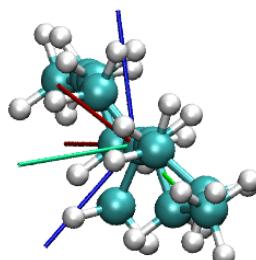
EingenVectors - Molecule A		
0	0	1
-0.76771	0.640798	0
0.640798	0.76771	0

EingenVectors - Molecule B		
-0.498435	-0.866927	0
0.866927	-0.498435	-0
0	0	1

EingenValues - Molecule A		
77.8081	276.009	320.598

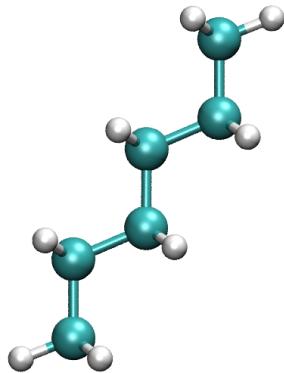
EingenValues - Molecule B		
34.6868	449.234	465.177

Different

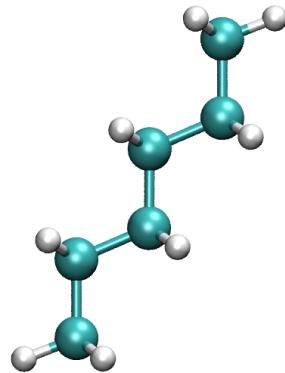


IsomerC6H14 Número 522

Molecule A hexane\_out\_G09



Molecule B hexane\_out\_G09\_inversion



Inertia Tensor - Molecule A

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

Inertia Tensor - Molecule B

346.245	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

EingenVectors - Molecule B

-0.498435	-0.866927	0
0.866927	-0.498435	-0
0	0	1

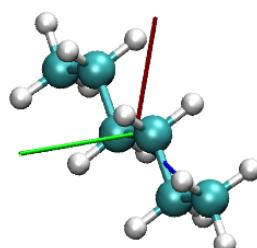
EingenValues - Molecule A

34.6869	449.234	465.177
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EingenValues - Molecule B

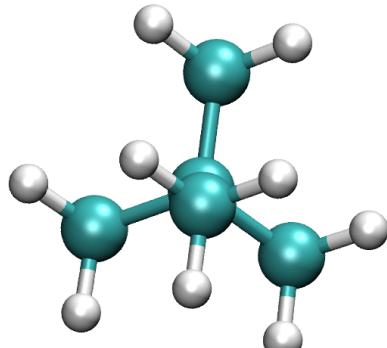
34.6868	449.234	465.177
---------	---------	---------

Equal



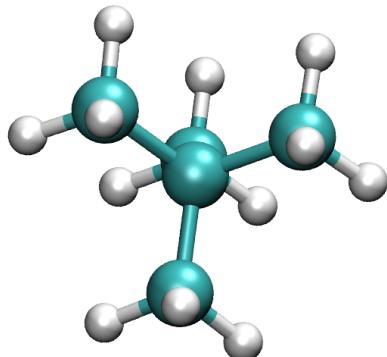
NeoConformation Número 523

Molecule A neopentane\_Symmetry\_out\_G09



Molecule B

neopentane\_Symmetry\_out\_G09\_inversion



Inertia Tensor - Molecule A

114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

Inertia Tensor - Molecule B

114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

EingenVectors - Molecule A

-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B

-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

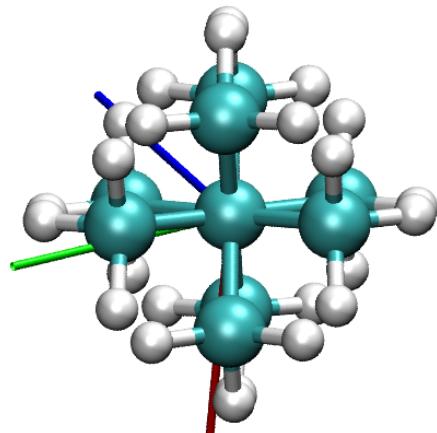
EingenValues - Molecule A

114.662	114.667	114.672
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EingenValues - Molecule B

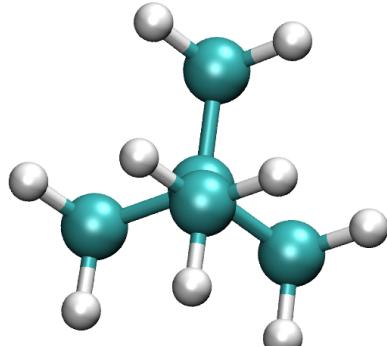
114.662	114.667	114.672
---------	---------	---------

Equal

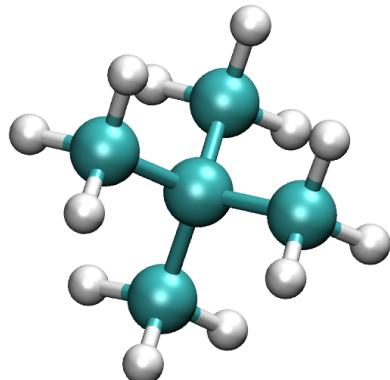


NeoConformation Número 524

Molecule A neopentane\_Symmetry\_out\_G09



Molecule B neopenta-ne\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Inertia Tensor - Molecule A

114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

Inertia Tensor - Molecule B

114.67	0.000461506	0.00322567
0.000461506	114.665	-0.00251676
0.00322567	-0.00251676	114.666

EingenVectors - Molecule A

-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B

0.324711	-0.637189	-0.698965
-0.422625	-0.758878	0.495472
0.846139	-0.134515	0.515708

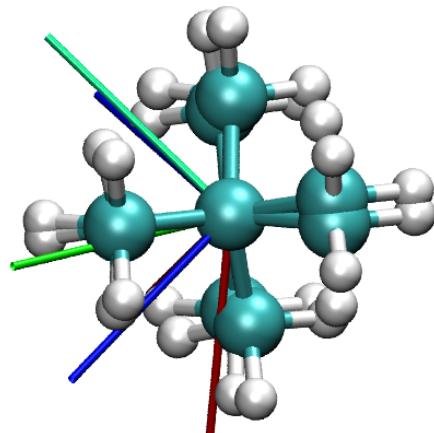
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

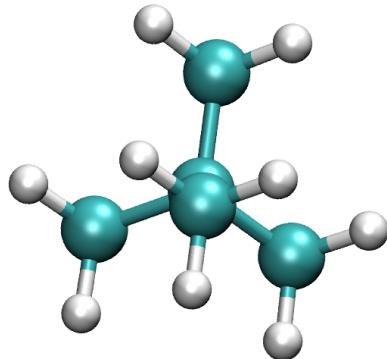
114.662	114.667	114.672
---------	---------	---------

Equal

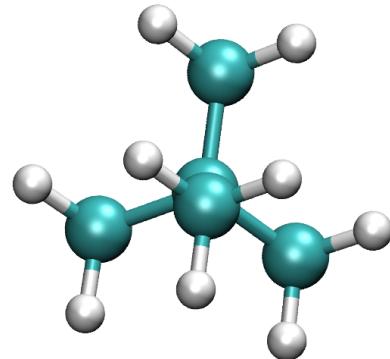


NeoConformation Número 525

Molecule A neopentane\_Symmetry\_out\_G09



Molecule B neopentane\_out\_G09



Inertia Tensor - Molecule A

114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

Inertia Tensor - Molecule B

114.662	0.000172734	0.000184265
0.000172734	114.667	-0.000265353
0.000184265	-0.000265353	114.672

EingenVectors - Molecule A

-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B

-0.999133	0.0364989	0.020046
-0.0375297	-0.997851	-0.053713
0.0180425	-0.0544187	0.998355

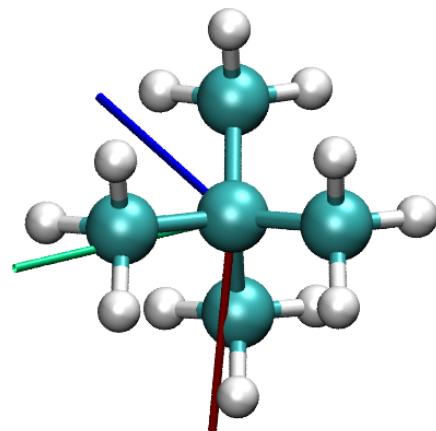
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

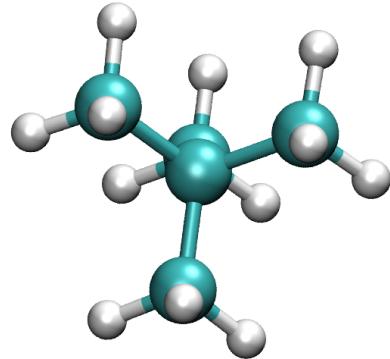
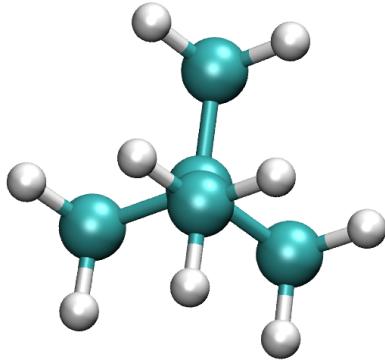
114.662	114.667	114.672
---------	---------	---------

Equal



NeoConformation Número 526

Molecule A neopentane\_Symmetry\_out\_G09 Molecule B neopentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

Inertia Tensor - Molecule B

114.662	0.000171373	0.000184362
0.000171373	114.667	-0.000257766
0.000184362	-0.000257766	114.672

EingenVectors - Molecule A

-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B

-0.99917	0.035564	0.0198547
-0.0365606	-0.997961	-0.0523166
0.0179537	-0.0529991	0.998433

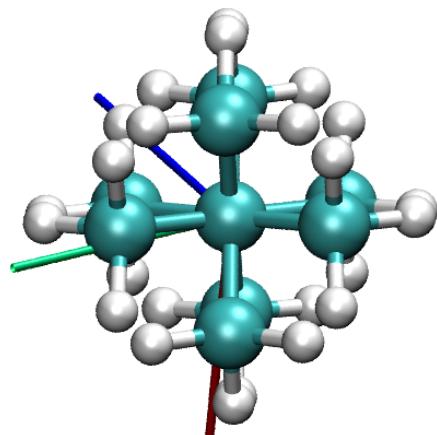
EingenValues - Molecule A

114.662	114.667	114.672
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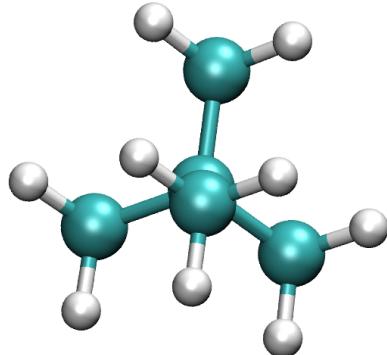
EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

Equal

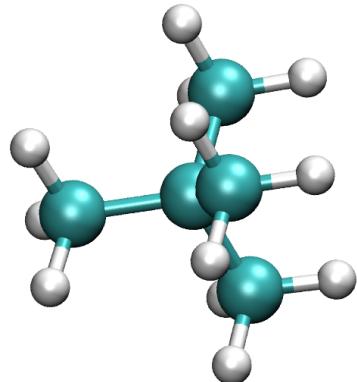


Molecule A neopentane\_Symmetry\_out\_G09



Molecule B

neopentane\_out\_G09\_rot\_x15-y15-z15



Inertia Tensor - Molecule A

114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

Inertia Tensor - Molecule B

114.663	0.00148446	0.00262579
0.00148446	114.666	0.000207396
0.00262579	0.000207396	114.671

EingenVectors - Molecule A

-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B

0.919257	-0.288184	-0.268173
-0.236481	-0.948878	0.209061
0.314712	0.128763	0.940413

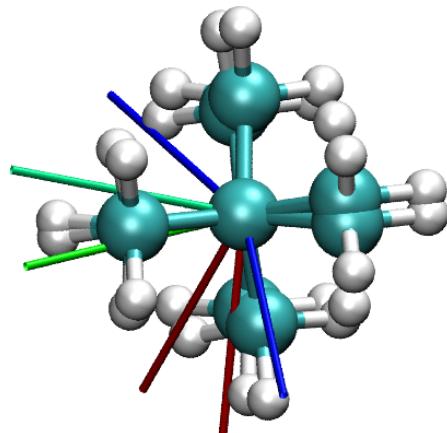
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

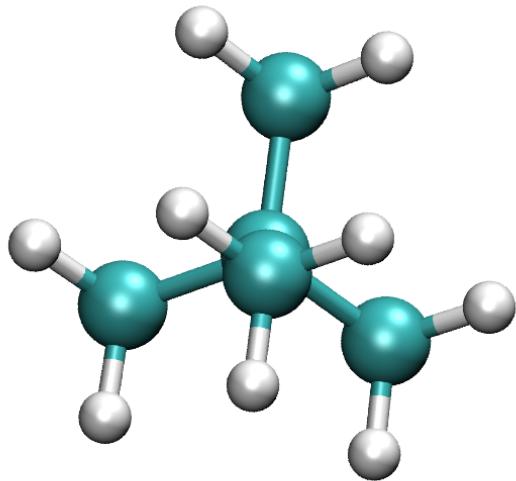
Equal



NeoConformation Número 528

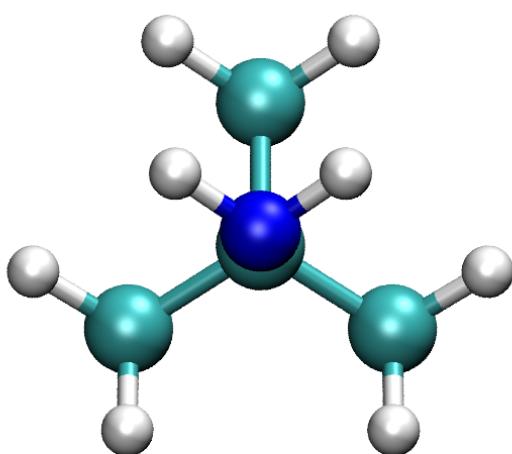
Molecule A

neopentane\_Symmetry\_out\_G09



Molecule B

tert-butylamine\_out\_G09

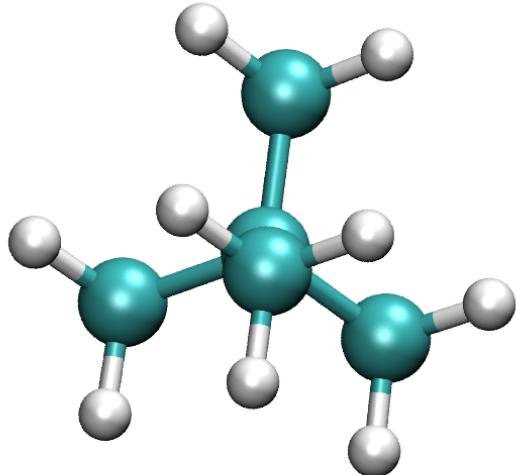


Different

NeoConformation Número 529

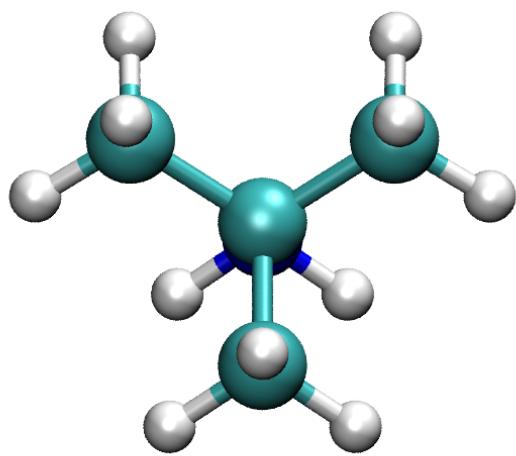
Molecule A

neopentane\_Symmetry\_out\_G09



Molecule B

tert-butylamine\_out\_G09\_inversion



Different

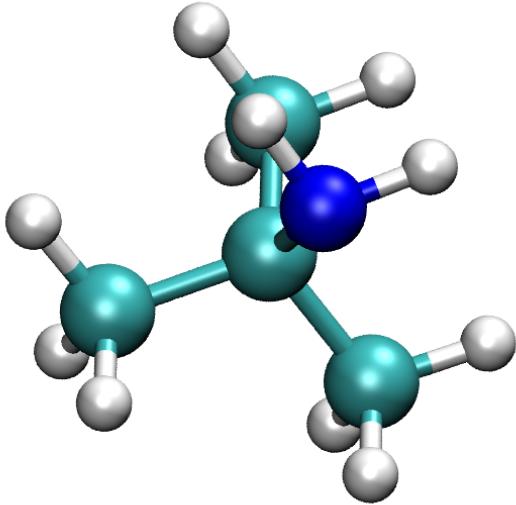
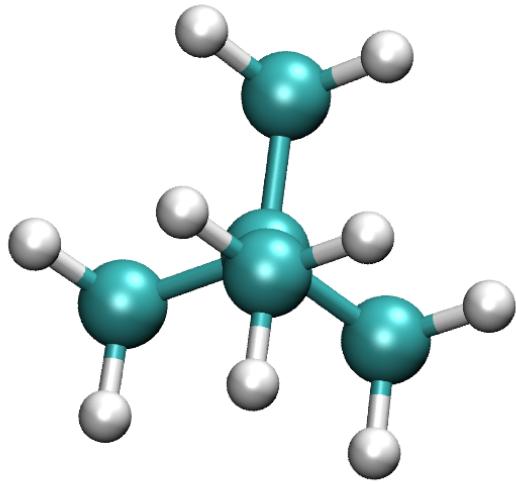
NeoConformation Número 530

Molecule A

neopentane\_Symmetry\_out\_G09

Molecule B

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15

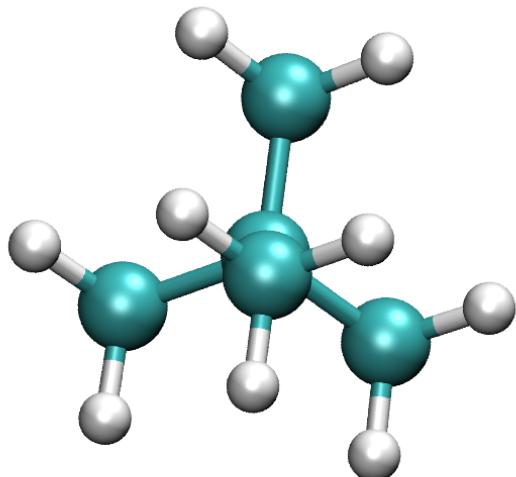


Different

NeoConformation Número 531

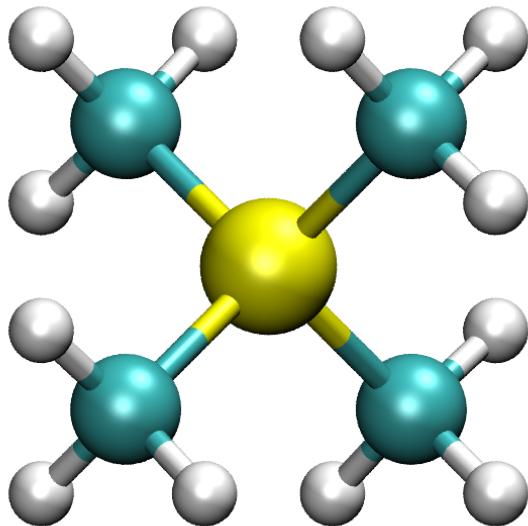
Molecule A

neopentane\_Symmetry\_out\_G09



Molecule B

tetramethylsilane\_out\_G09

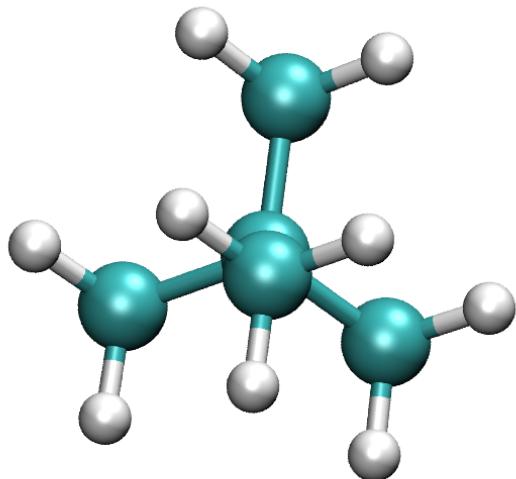


Different

NeoConformation Número 532

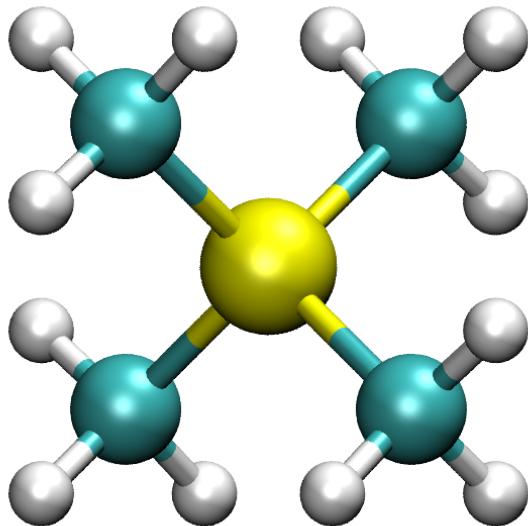
Molecule A

neopentane\_Symmetry\_out\_G09



Molecule B

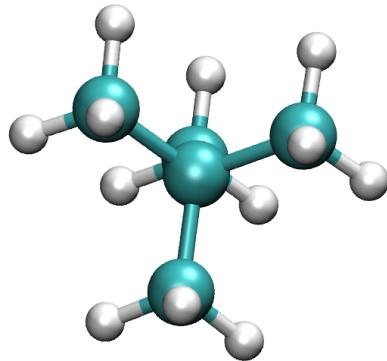
tetramethylsilane\_out\_G09\_inversion



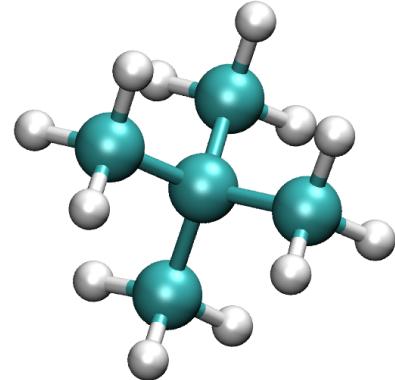
Different

NeoConformation Número 533

Molecule A  
neopentane\_Symmetry\_out\_G09\_inversion



Molecule B neopenta-  
ne\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Inertia Tensor - Molecule A			Inertia Tensor - Molecule B		
114.662	0.000161889	0.000173717	114.67	0.000461506	0.00322567
0.000161889	114.667	-0.000279052	0.000461506	114.665	-0.00251676
0.000173717	-0.000279052	114.672	0.00322567	-0.00251676	114.666

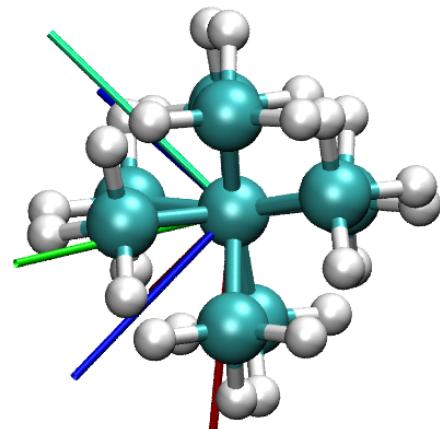
EingenVectors - Molecule A		
-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B		
0.324711	-0.637189	-0.698965
-0.422625	-0.758878	0.495472
0.846139	-0.134515	0.515708

EingenValues - Molecule A		
114.662	114.667	114.672

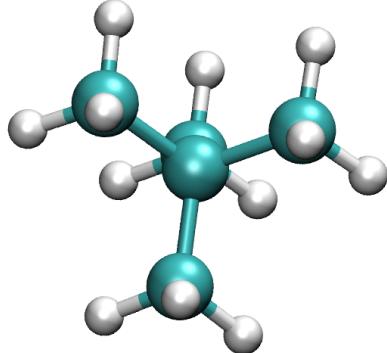
EingenValues - Molecule B		
114.662	114.667	114.672

Equal

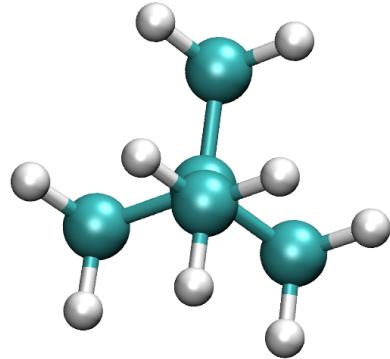


Molecule A

neopentane\_Symmetry\_out\_G09\_inversion



Molecule B neopentane\_out\_G09



Inertia Tensor - Molecule A

114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

Inertia Tensor - Molecule B

114.662	0.000172734	0.000184265
0.000172734	114.667	-0.000265353
0.000184265	-0.000265353	114.672

EingenVectors - Molecule A

-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B

-0.999133	0.0364989	0.020046
-0.0375297	-0.997851	-0.053713
0.0180425	-0.0544187	0.998355

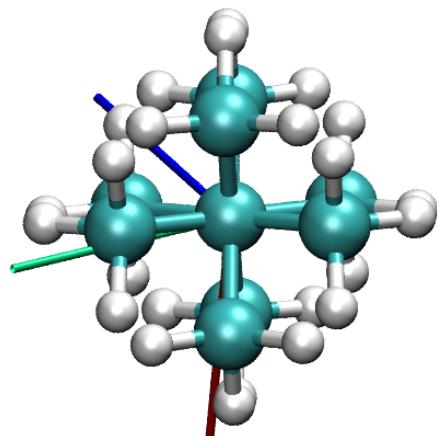
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

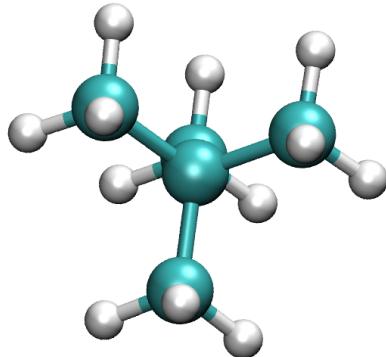
114.662	114.667	114.672
---------	---------	---------

Equal

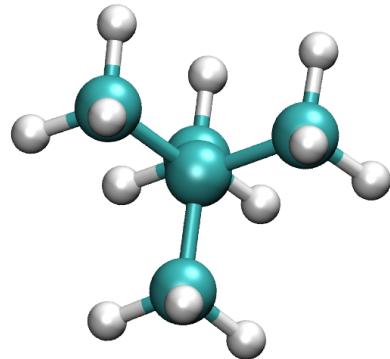


NeoConformation Número 535

Molecule A  
neopentane\_Symmetry\_out\_G09\_inversion



Molecule B neopentane\_out\_G09\_inversion



Inertia Tensor - Molecule A		
114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

Inertia Tensor - Molecule B		
114.662	0.000171373	0.000184362
0.000171373	114.667	-0.000257766
0.000184362	-0.000257766	114.672

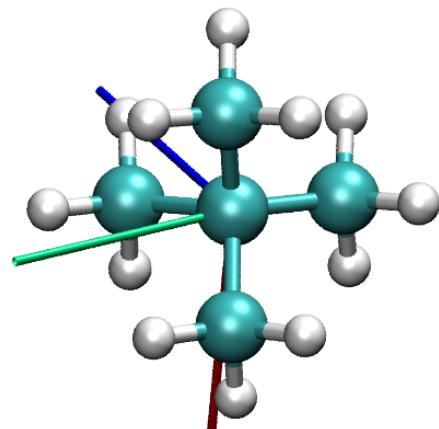
EingenVectors - Molecule A		
-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B		
-0.99917	0.035564	0.0198547
-0.0365606	-0.997961	-0.0523166
0.0179537	-0.0529991	0.998433

EingenValues - Molecule A		
114.662	114.667	114.672

EingenValues - Molecule B		
114.662	114.667	114.672

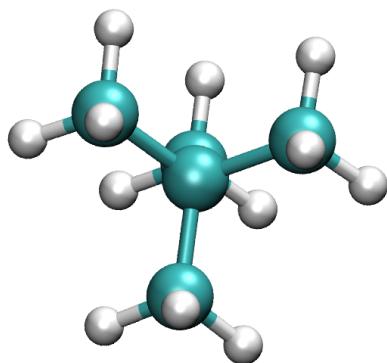
Equal



NeoConformation Número 536

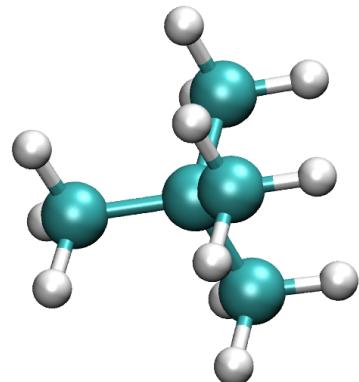
Molecule A

neopentane\_Symmetry\_out\_G09\_inversion



Molecule B

neopentane\_out\_G09\_rot\_x15-y15-z15



Inertia Tensor - Molecule A

114.662	0.000161889	0.000173717
0.000161889	114.667	-0.000279052
0.000173717	-0.000279052	114.672

Inertia Tensor - Molecule B

114.663	0.001484446	0.00262579
0.001484446	114.666	0.000207396
0.00262579	0.000207396	114.671

EingenVectors - Molecule A

-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

EingenVectors - Molecule B

0.919257	-0.288184	-0.268173
-0.236481	-0.948878	0.209061
0.314712	0.128763	0.940413

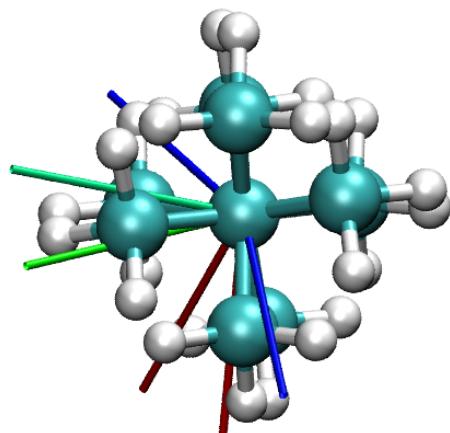
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

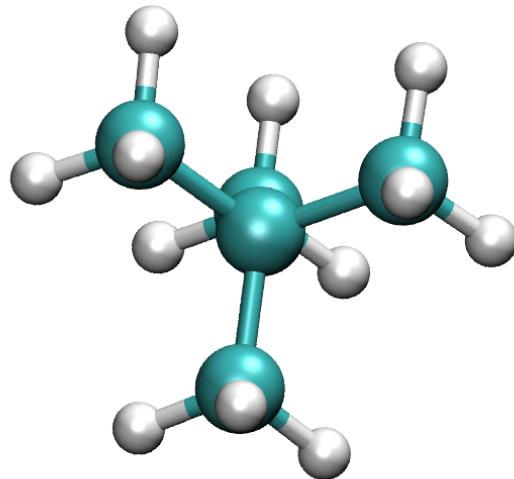
Equal



NeoConformation Número 537

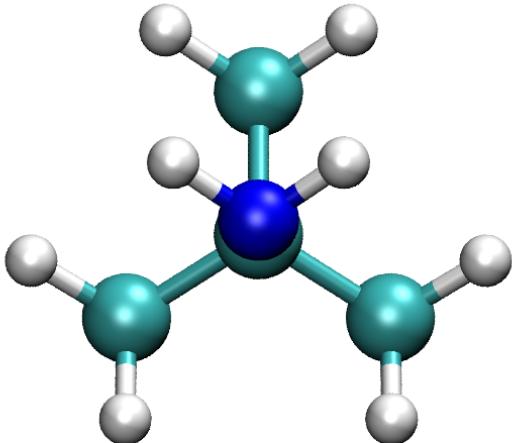
Molecule A

neopentane\_Symmetry\_out\_G09\_inversion



Molecule B

tert-butylamine\_out\_G09

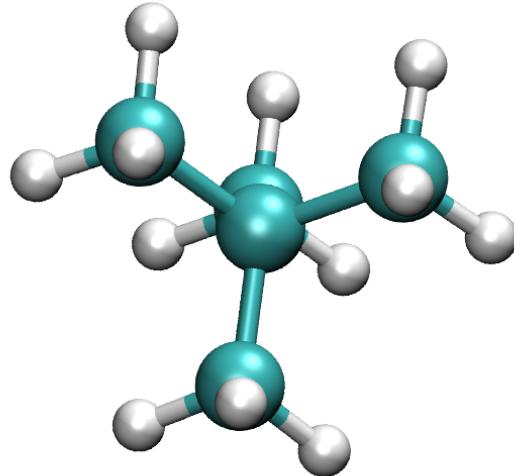


Different

NeoConformation Número 538

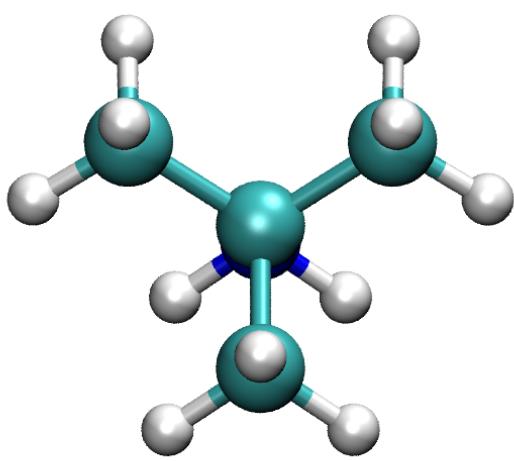
Molecule A

neopentane\_Symmetry\_out\_G09\_inversion



Molecule B

tert-butylamine\_out\_G09\_inversion

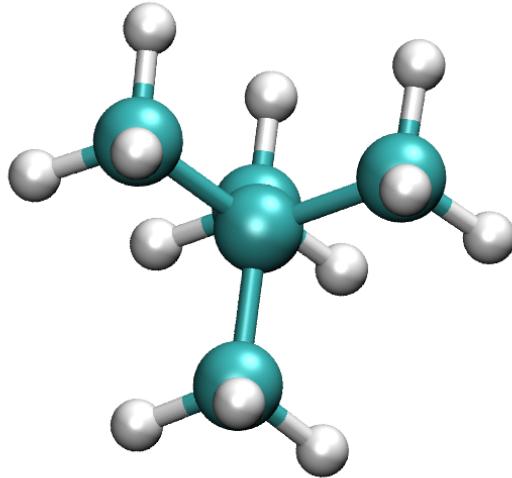


Different

NeoConformation Número 539

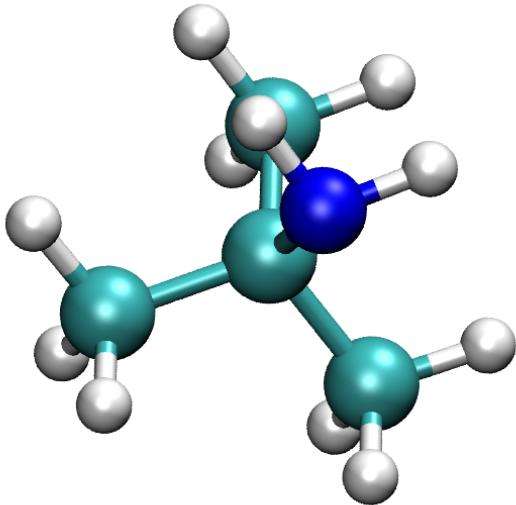
Molecule A

neopentane\_Symmetry\_out\_G09\_inversion



Molecule B

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15

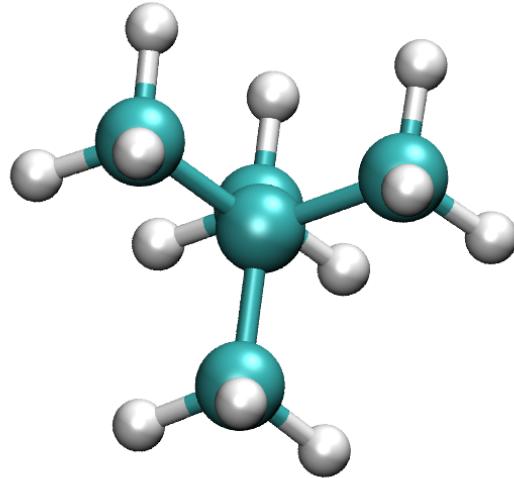


Different

NeoConformation Número 540

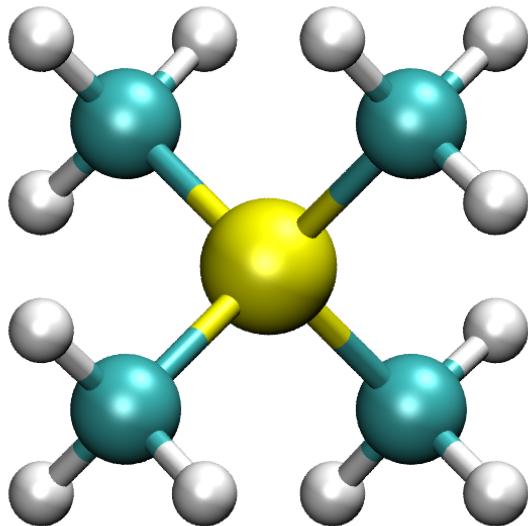
Molecule A

neopentane\_Symmetry\_out\_G09\_inversion



Molecule B

tetramethylsilane\_out\_G09

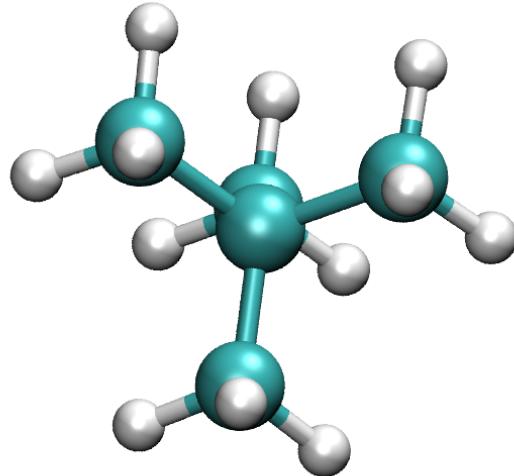


Different

NeoConformation Número 541

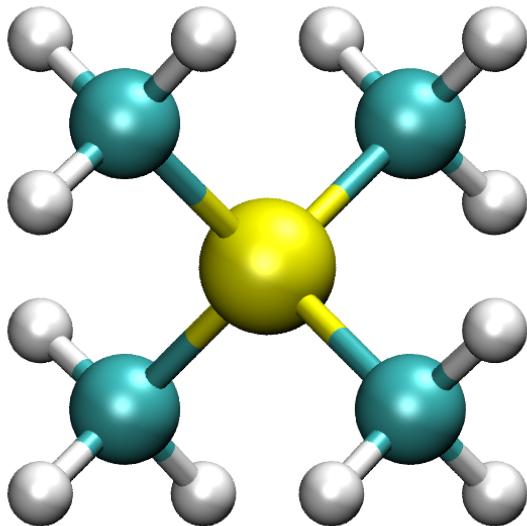
Molecule A

neopentane\_Symmetry\_out\_G09\_inversion



Molecule B

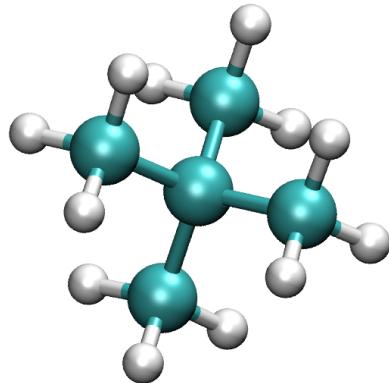
tetramethylsilane\_out\_G09\_inversion



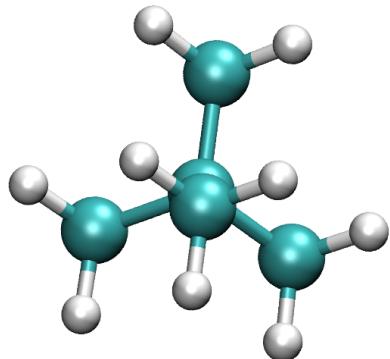
Different

NeoConformation Número 542

Molecule A neopenta-ne\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Molecule B neopentane\_out\_G09



Inertia Tensor - Molecule A

114.67	0.000461506	0.00322567
0.000461506	114.665	-0.00251676
0.00322567	-0.00251676	114.666

Inertia Tensor - Molecule B

114.662	0.000172734	0.000184265
0.000172734	114.667	-0.000265353
0.000184265	-0.000265353	114.672

EingenVectors - Molecule A

0.324711	-0.637189	-0.698965
-0.422625	-0.758878	0.495472
0.846139	-0.134515	0.515708

EingenVectors - Molecule B

-0.999133	0.0364989	0.020046
-0.0375297	-0.997851	-0.053713
0.0180425	-0.0544187	0.998355

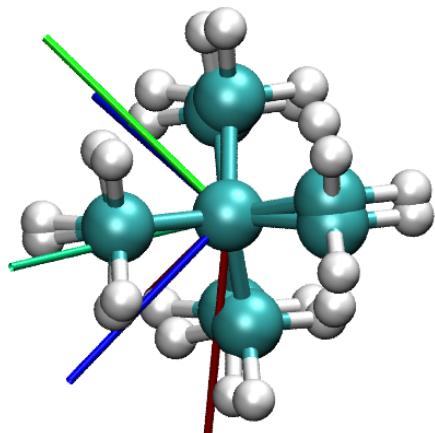
EingenValues - Molecule A

114.662	114.667	114.672
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EingenValues - Molecule B

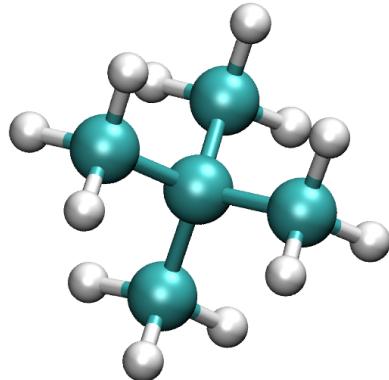
114.662	114.667	114.672
---------	---------	---------

Equal

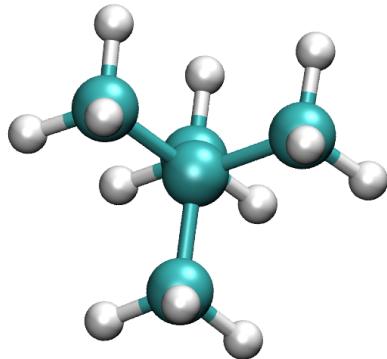


NeoConformation Número 543

Molecule A neopenta-ne\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Molecule B neopentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

114.67	0.000461506	0.00322567
0.000461506	114.665	-0.00251676
0.00322567	-0.00251676	114.666

Inertia Tensor - Molecule B

114.662	0.000171373	0.000184362
0.000171373	114.667	-0.000257766
0.000184362	-0.000257766	114.672

EingenVectors - Molecule A

0.324711	-0.637189	-0.698965
-0.422625	-0.758878	0.495472
0.846139	-0.134515	0.515708

EingenVectors - Molecule B

-0.99917	0.035564	0.0198547
-0.0365606	-0.997961	-0.0523166
0.0179537	-0.0529991	0.998433

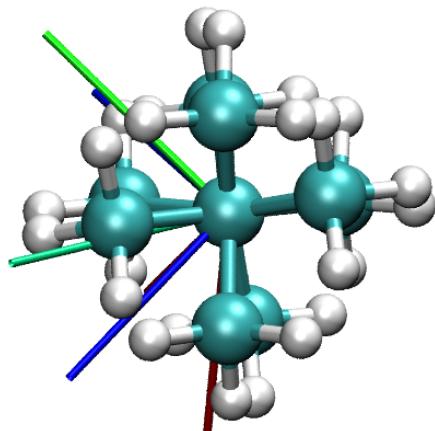
EingenValues - Molecule A

114.662	114.667	114.672
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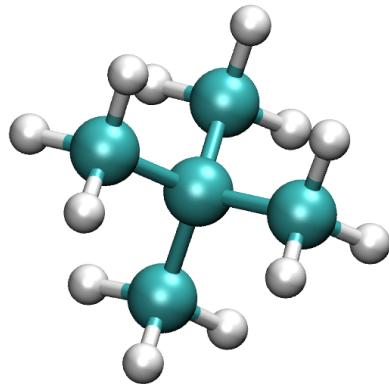
EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

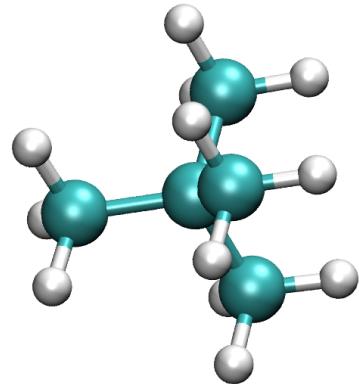
Equal



Molecule A neopenta-ne\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Molecule B neopentane\_out\_G09\_rot\_x15\_y15\_z15



Inertia Tensor - Molecule A

114.67	0.000461506	0.00322567
0.000461506	114.665	-0.00251676
0.00322567	-0.00251676	114.666

Inertia Tensor - Molecule B

114.663	0.001484446	0.00262579
0.001484446	114.666	0.000207396
0.00262579	0.000207396	114.671

EingenVectors - Molecule A

0.324711	-0.637189	-0.698965
-0.422625	-0.758878	0.495472
0.846139	-0.134515	0.515708

EingenVectors - Molecule B

0.919257	-0.288184	-0.268173
-0.236481	-0.948878	0.209061
0.314712	0.128763	0.940413

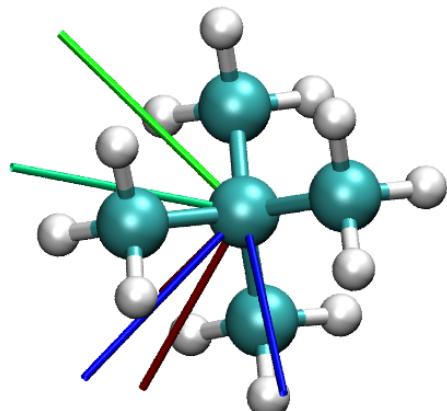
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

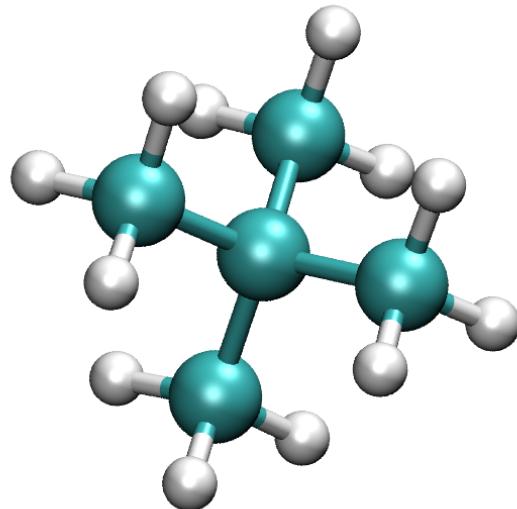
Equal



NeoConformation Número 545

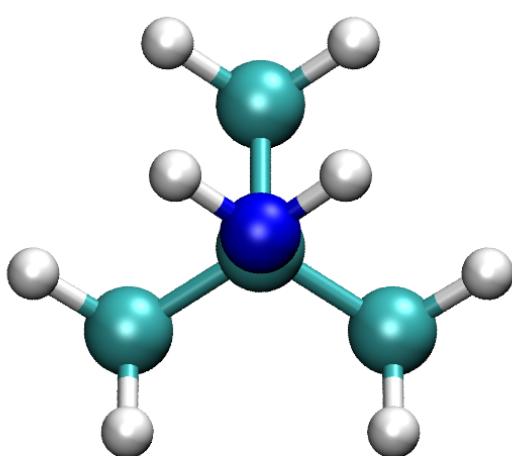
Molecule A

neopentane\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Molecule B

tert-butylamine\_out\_G09

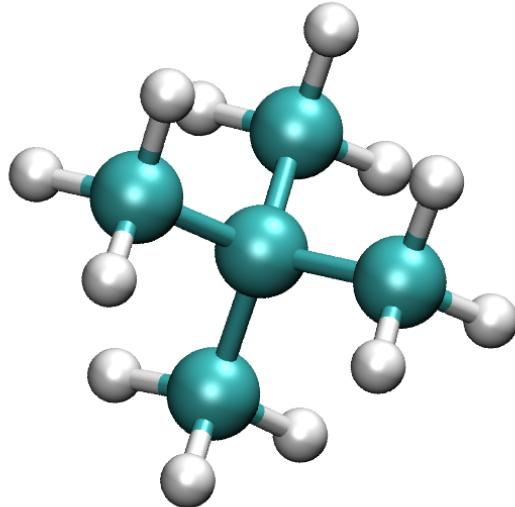


Different

NeoConformation Número 546

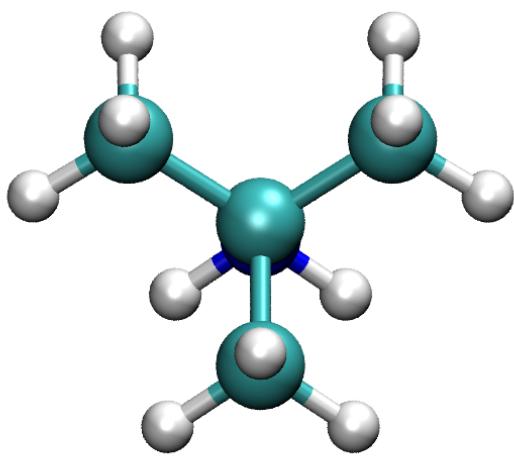
Molecule A

neopentane\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Molecule B

tert-butylamine\_out\_G09\_inversion

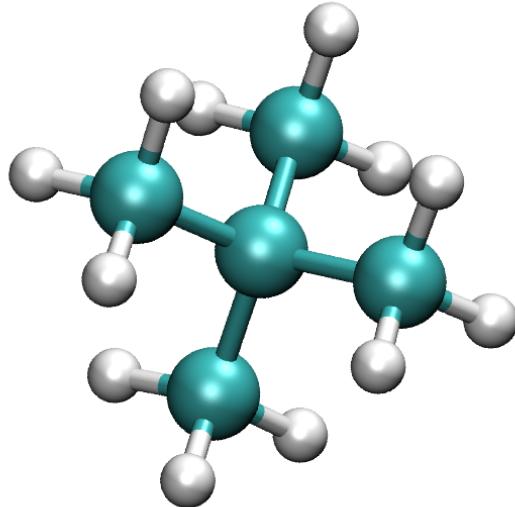


Different

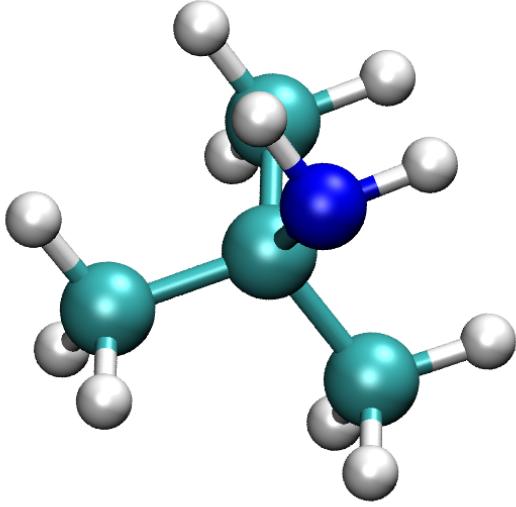
NeoConformation Número 547

Molecule A

neopentane\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Molecule B

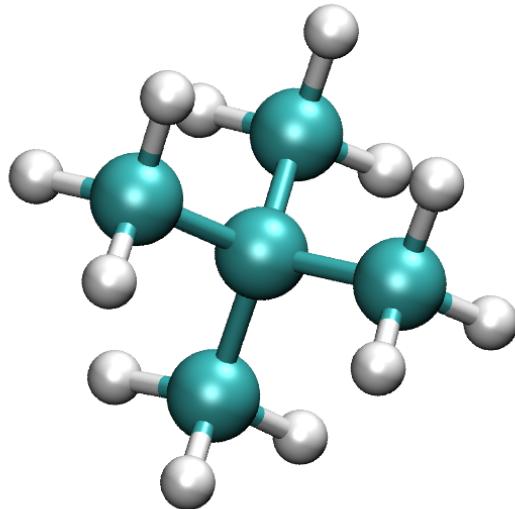


Different

NeoConformation Número 548

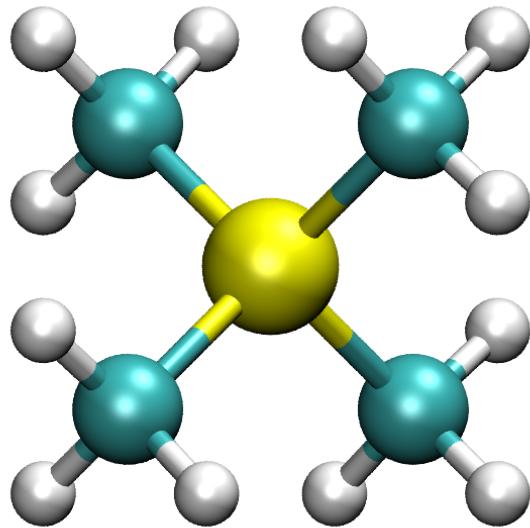
Molecule A

neopentane\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Molecule B

tetramethylsilane\_out\_G09

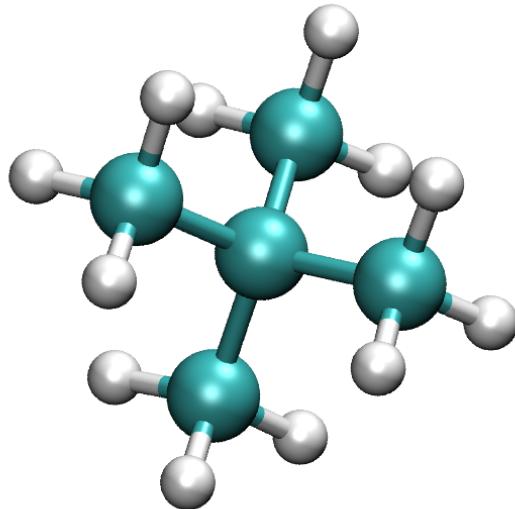


Different

NeoConformation Número 549

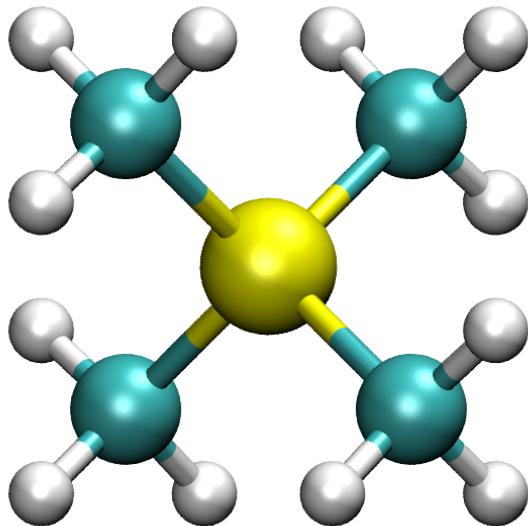
Molecule A

neopentane\_Symmetry\_out\_G09\_rot\_x45\_y45\_z60



Molecule B

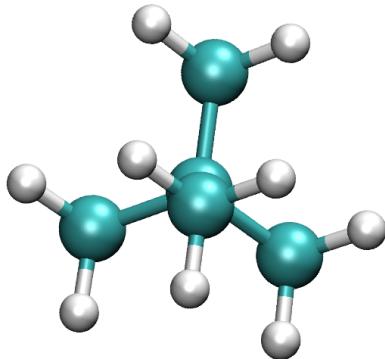
tetramethylsilane\_out\_G09\_inversion



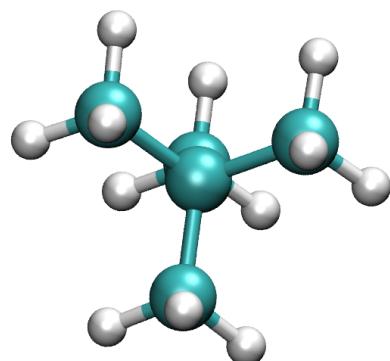
Different

NeoConformation Número 550

Molecule A neopentane\_out\_G09



Molecule B neopentane\_out\_G09\_inversion



Inertia Tensor - Molecule A

114.662	0.000172734	0.000184265
0.000172734	114.667	-0.000265353
0.000184265	-0.000265353	114.672

Inertia Tensor - Molecule B

114.662	0.000171373	0.000184362
0.000171373	114.667	-0.000257766
0.000184362	-0.000257766	114.672

EingenVectors - Molecule A

-0.999133	0.0364989	0.020046
-0.0375297	-0.997851	-0.053713
0.0180425	-0.0544187	0.998355

EingenVectors - Molecule B

-0.99917	0.035564	0.0198547
-0.0365606	-0.997961	-0.0523166
0.0179537	-0.0529991	0.998433

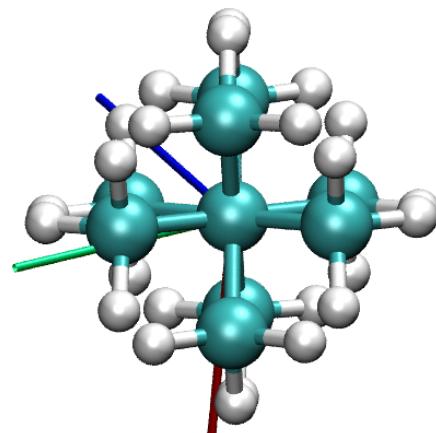
EingenValues - Molecule A

114.662	114.667	114.672
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EingenValues - Molecule B

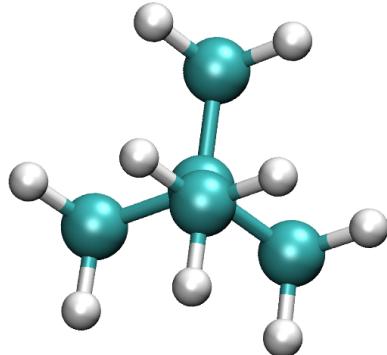
114.662	114.667	114.672
---------	---------	---------

Equal



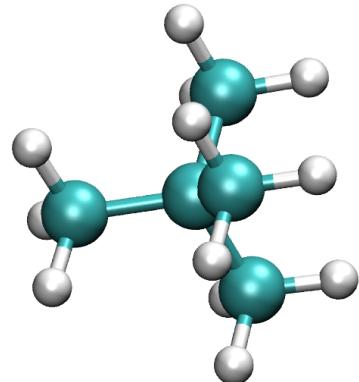
NeoConformation Número 551

Molecule A neopentane\_out\_G09



Molecule B

neopentane\_out\_G09\_rot\_x15-y15-z15



Inertia Tensor - Molecule A

114.662	0.000172734	0.000184265
0.000172734	114.667	-0.000265353
0.000184265	-0.000265353	114.672

Inertia Tensor - Molecule B

114.663	0.001484446	0.00262579
0.001484446	114.666	0.000207396
0.00262579	0.000207396	114.671

EingenVectors - Molecule A

-0.999133	0.0364989	0.020046
-0.0375297	-0.997851	-0.053713
0.0180425	-0.0544187	0.998355

EingenVectors - Molecule B

0.919257	-0.288184	-0.268173
-0.236481	-0.948878	0.209061
0.314712	0.128763	0.940413

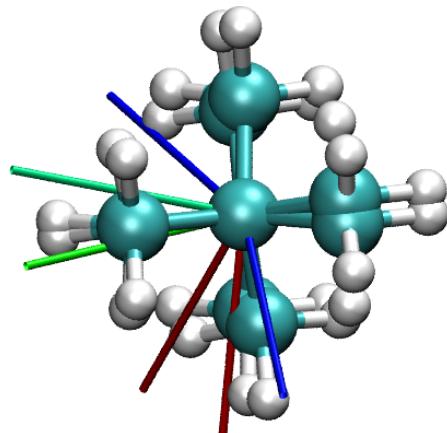
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

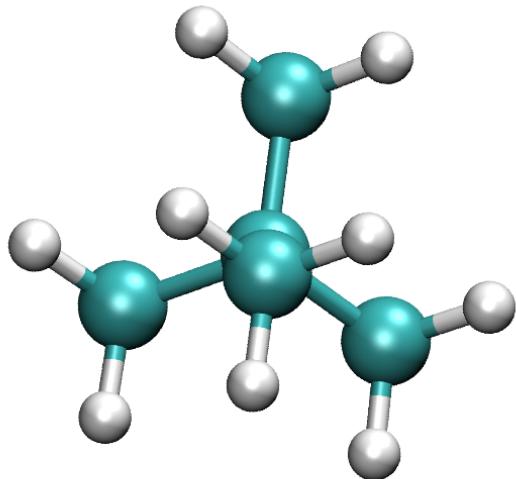
Equal



NeoConformation Número 552

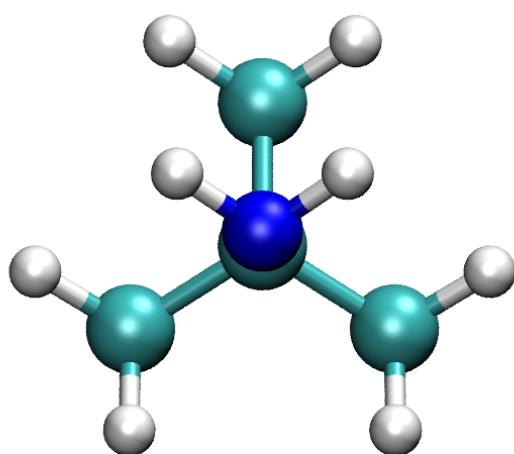
Molecule A

neopentane\_out\_G09



Molecule B

tert-butylamine\_out\_G09

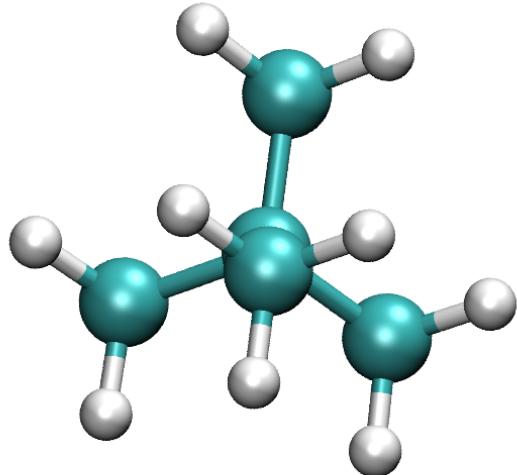


Different

NeoConformation Número 553

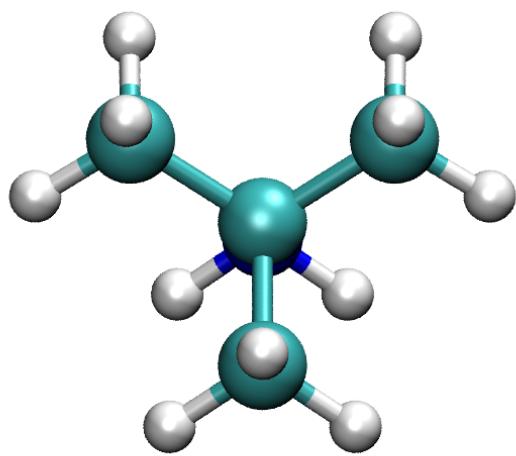
Molecule A

neopentane\_out\_G09



Molecule B

tert-butylamine\_out\_G09\_inversion

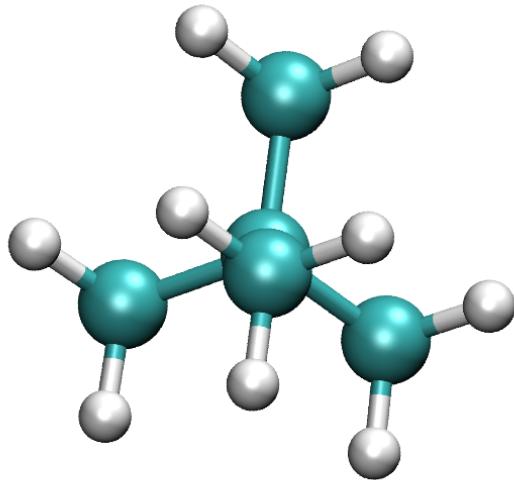


Different

NeoConformation Número 554

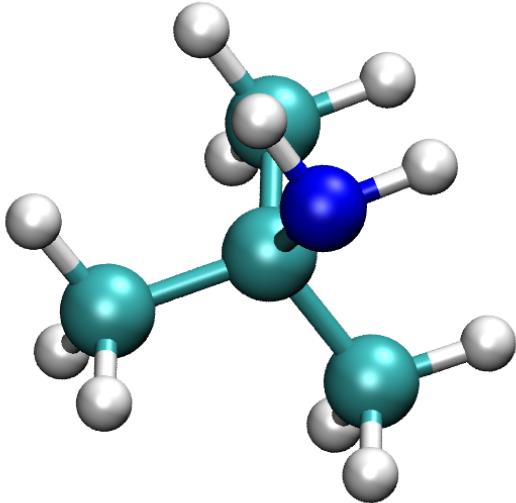
Molecule A

neopentane\_out\_G09



Molecule B

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15

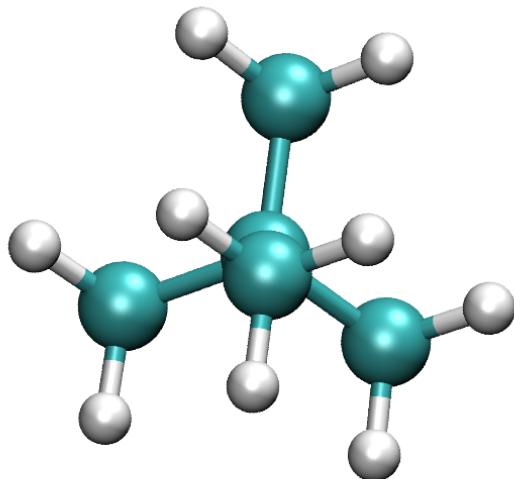


Different

NeoConformation Número 555

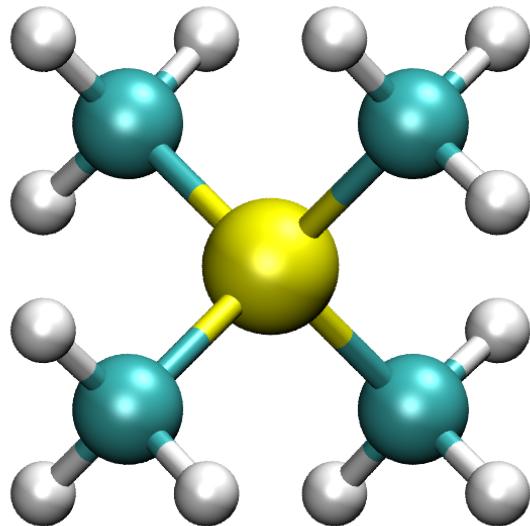
Molecule A

neopentane\_out\_G09



Molecule B

tetramethylsilane\_out\_G09

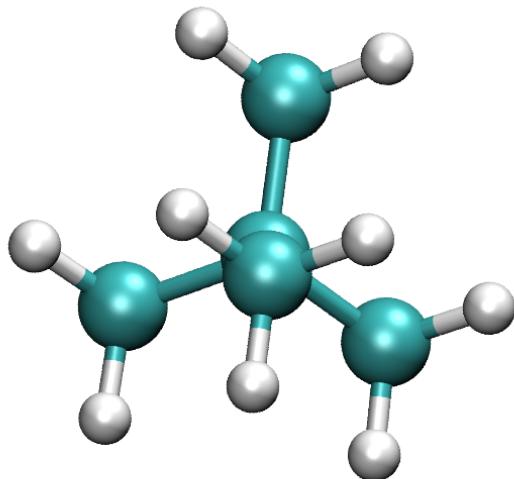


Different

NeoConformation Número 556

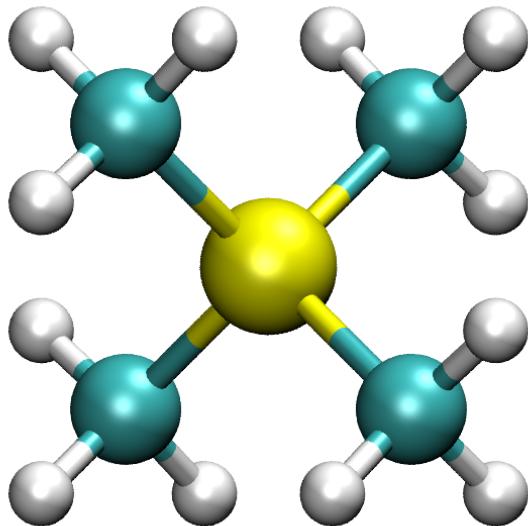
Molecule A

neopentane\_out\_G09



Molecule B

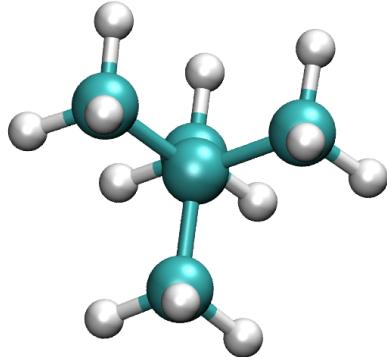
tetramethylsilane\_out\_G09\_inversion



Different

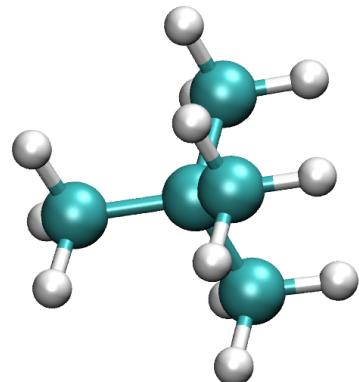
NeoConformation Número 557

Molecule A neopentane\_out\_G09\_inversion



Molecule B

neopentane\_out\_G09\_rot\_x15-y15-z15



Inertia Tensor - Molecule A

114.662	0.000171373	0.000184362
0.000171373	114.667	-0.000257766
0.000184362	-0.000257766	114.672

Inertia Tensor - Molecule B

114.663	0.00148446	0.00262579
0.00148446	114.666	0.000207396
0.00262579	0.000207396	114.671

EingenVectors - Molecule A

-0.99917	0.035564	0.0198547
-0.0365606	-0.997961	-0.0523166
0.0179537	-0.0529991	0.998433

EingenVectors - Molecule B

0.919257	-0.288184	-0.268173
-0.236481	-0.948878	0.209061
0.314712	0.128763	0.940413

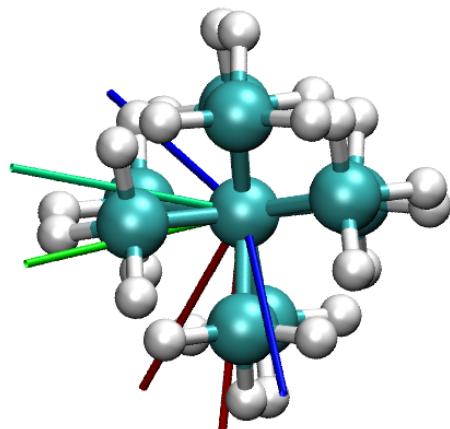
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

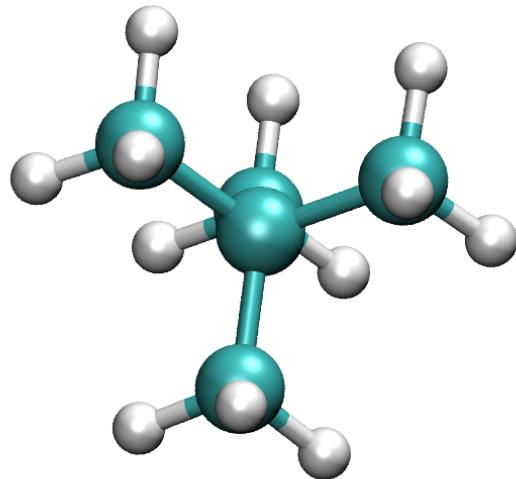
Equal



NeoConformation Número 558

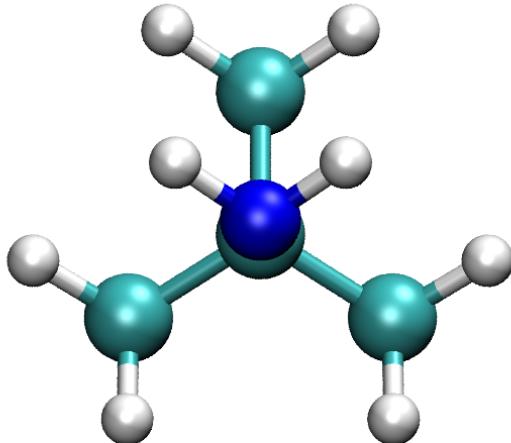
Molecule A

neopentane.out\_G09\_inversion



Molecule B

tert-butylamine.out\_G09

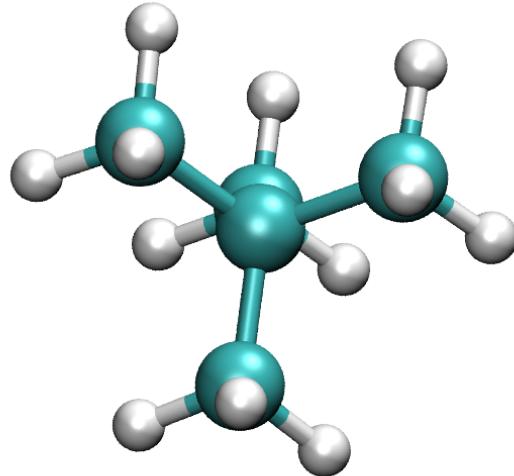


Different

NeoConformation Número 559

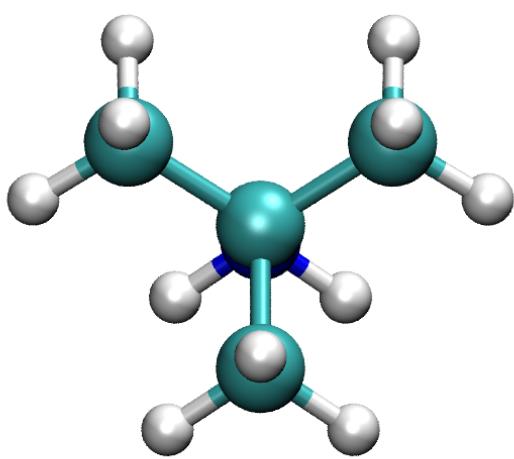
Molecule A

neopentane\_out\_G09\_inversion



Molecule B

tert-butylamine\_out\_G09\_inversion

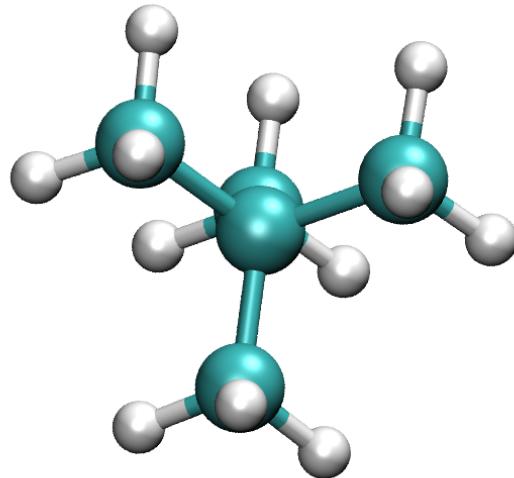


Different

NeoConformation Número 560

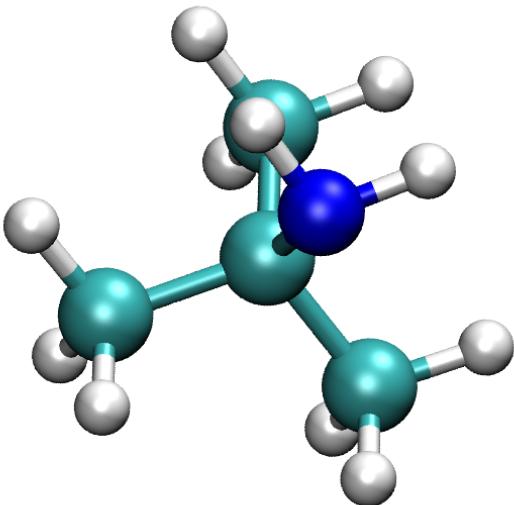
Molecule A

neopentane\_out\_G09\_inversion



Molecule B

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15

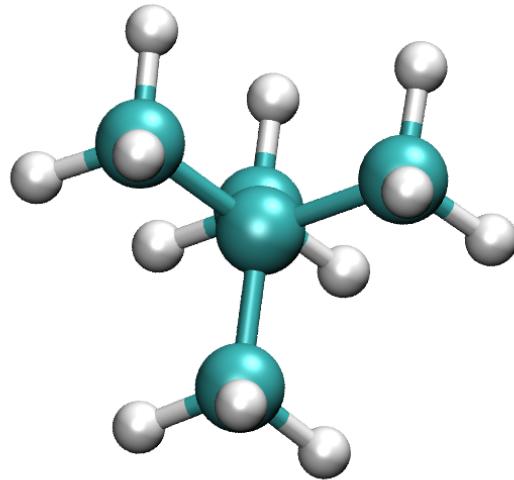


Different

NeoConformation Número 561

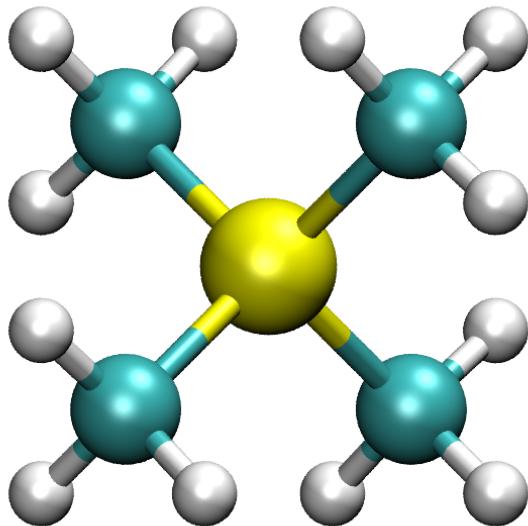
Molecule A

neopentane\_out\_G09\_inversion



Molecule B

tetramethylsilane\_out\_G09

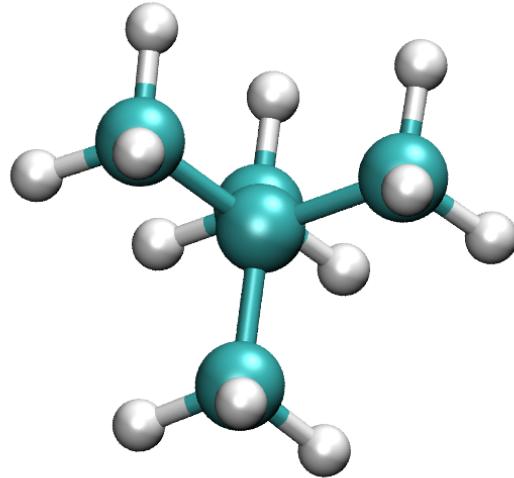


Different

NeoConformation Número 562

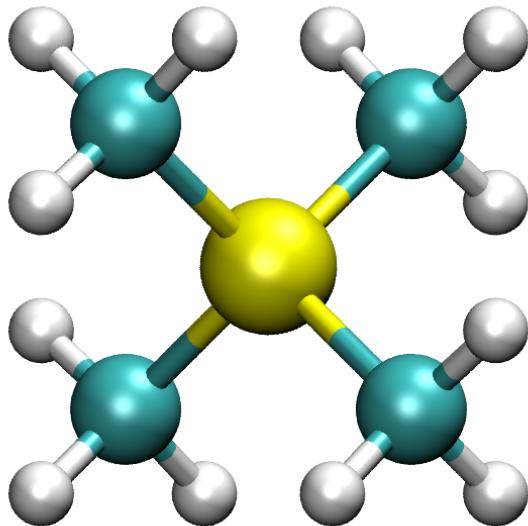
Molecule A

neopentane\_out\_G09\_inversion



Molecule B

tetramethylsilane\_out\_G09\_inversion

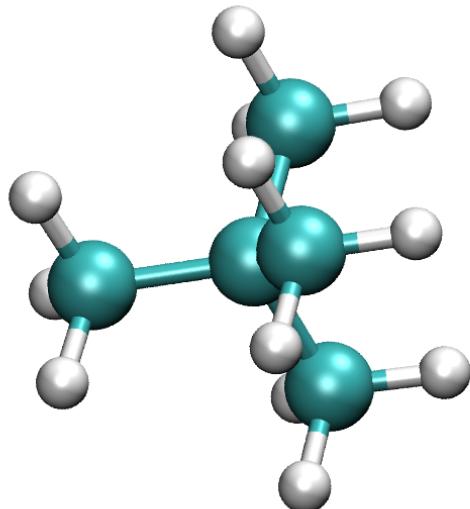


Different

NeoConformation Número 563

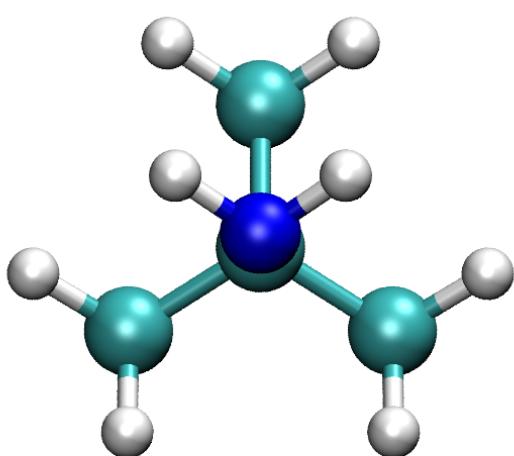
Molecule A

neopentane\_out\_G09\_rot\_x15-y15-z15



Molecule B

tert-butylamine\_out\_G09

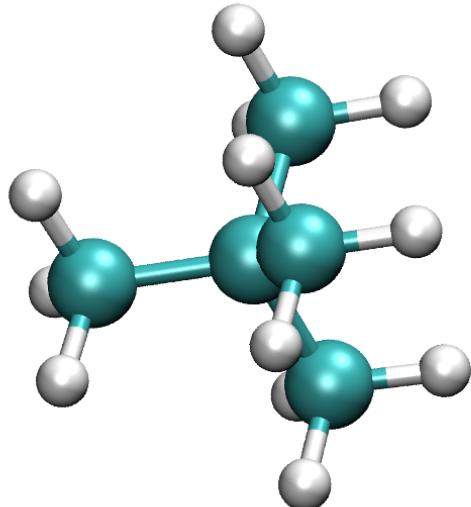


Different

NeoConformation Número 564

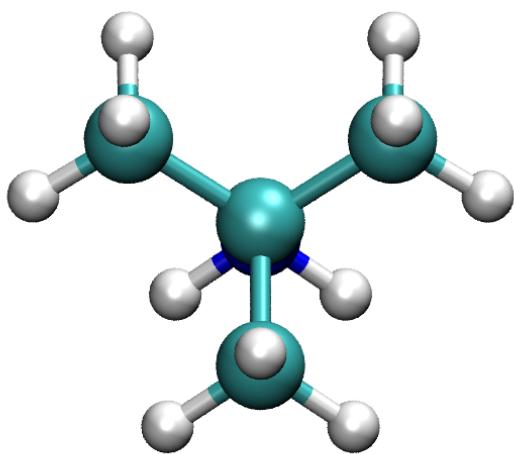
Molecule A

neopentane\_out\_G09\_rot\_x15-y15-z15



Molecule B

tert-butylamine\_out\_G09\_inversion

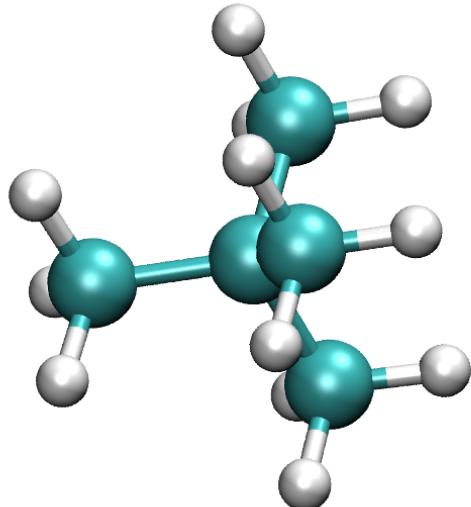


Different

NeoConformation Número 565

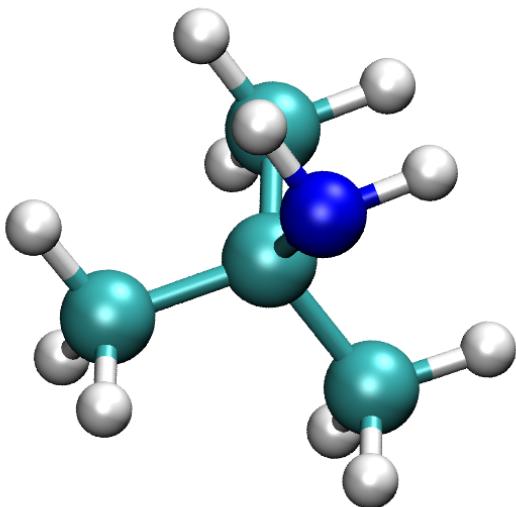
Molecule A

neopentane\_out\_G09\_rot\_x15-y15-z15



Molecule B

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15

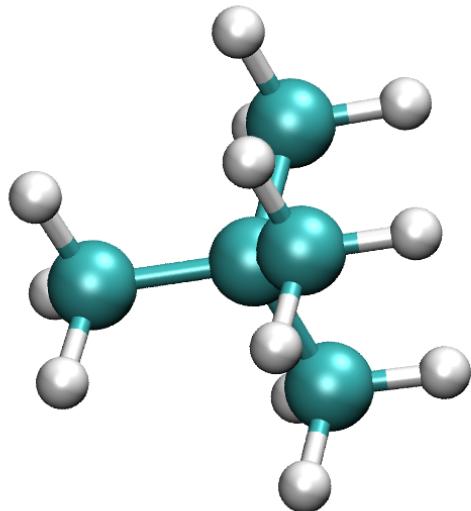


Different

NeoConformation Número 566

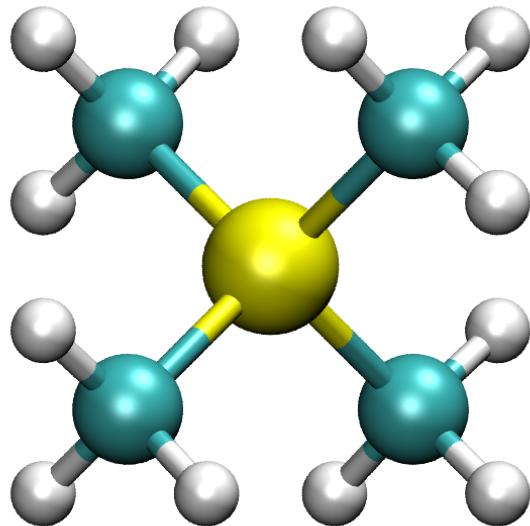
Molecule A

neopentane\_out\_G09\_rot\_x15-y15-z15



Molecule B

tetramethylsilane\_out\_G09

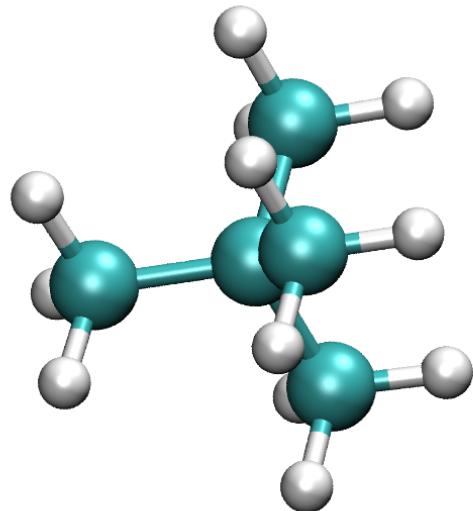


Different

NeoConformation Número 567

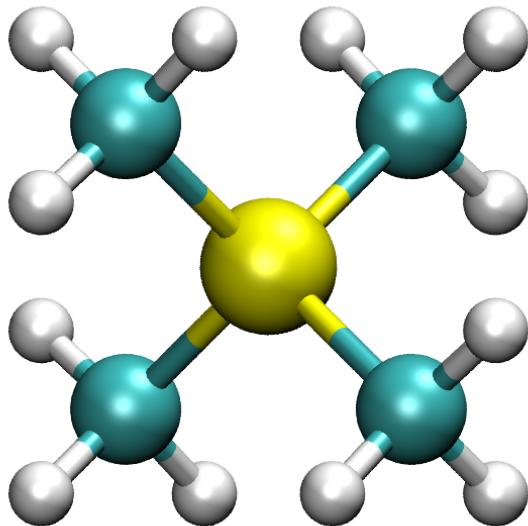
Molecule A

neopentane\_out\_G09\_rot\_x15-y15-z15



Molecule B

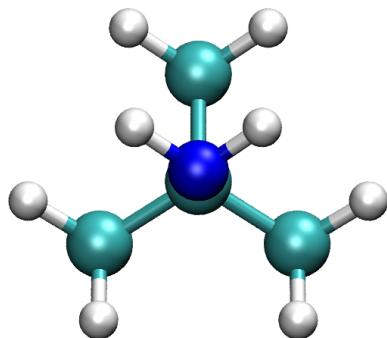
tetramethylsilane\_out\_G09\_inversion



Different

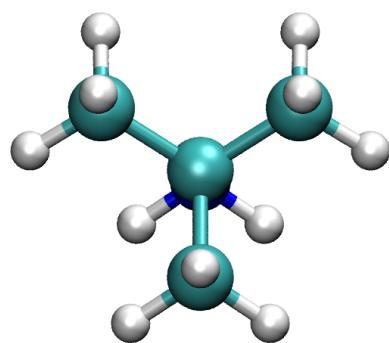
NeoConformation Número 568

Molecule A tert-butylamine\_out\_G09



Molecule B

tert-butylamine\_out\_G09\_inversion



Inertia Tensor - Molecule A

110.655	-1.46159e-05	4.47474e-05
-1.46159e-05	111.529	0.82631
4.47474e-05	0.82631	113.378

Inertia Tensor - Molecule B

110.655	-4.00493e-05	5.05193e-05
-4.00493e-05	111.529	0.826271
5.05193e-05	0.826271	113.378

EingenVectors - Molecule A

-1	-4.53031e-05	3.01901e-05
5.30915e-05	-0.934229	0.356674
1.2046e-05	0.356674	0.934229

EingenVectors - Molecule B

-1	-8.8937e-05	4.55534e-05
9.93354e-05	-0.934224	0.356687
1.08344e-05	0.356687	0.934224

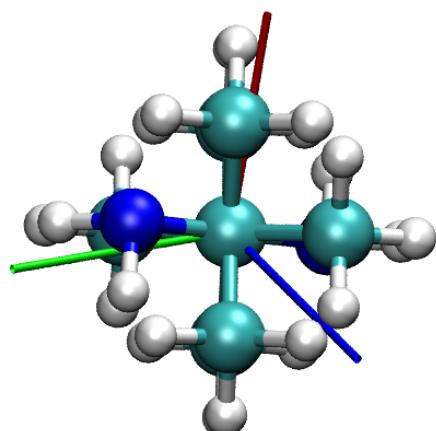
EingenValues - Molecule A

110.655	111.213	113.693
---------	---------	---------

EingenValues - Molecule B

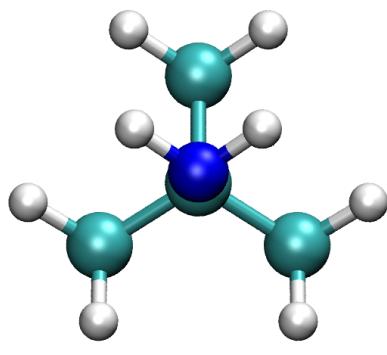
110.655	111.213	113.693
---------	---------	---------

Equal



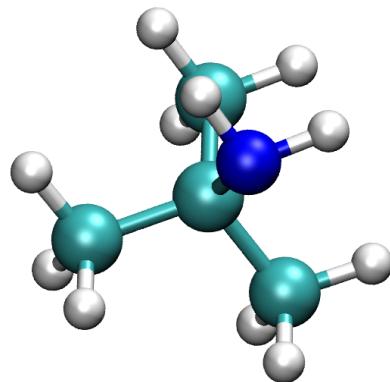
NeoConformation Número 569

Molecule A tert-butylamine\_out\_G09



Molecule B

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15



Inertia Tensor - Molecule A

110.655	-1.46159e-05	4.47474e-05
-1.46159e-05	111.529	0.82631
4.47474e-05	0.82631	113.378

Inertia Tensor - Molecule B

111.039	0.579971	0.822165
0.579971	111.829	0.957523
0.822165	0.957523	112.694

EingenVectors - Molecule A

-1	-4.53031e-05	3.01901e-05
5.30915e-05	-0.934229	0.356674
1.2046e-05	0.356674	0.934229

EingenVectors - Molecule B

-0.933012	0.249963	0.258859
-0.0630357	-0.821768	0.566325
0.354282	0.512071	0.782476

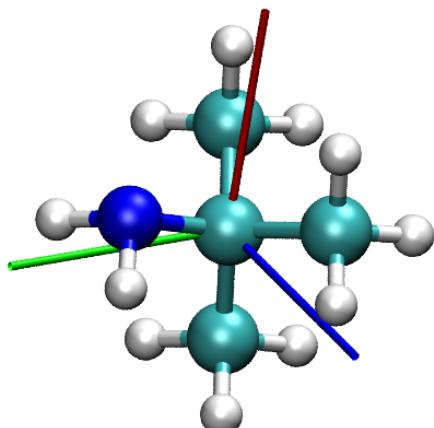
EingenValues - Molecule A

110.655	111.213	113.693
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EingenValues - Molecule B

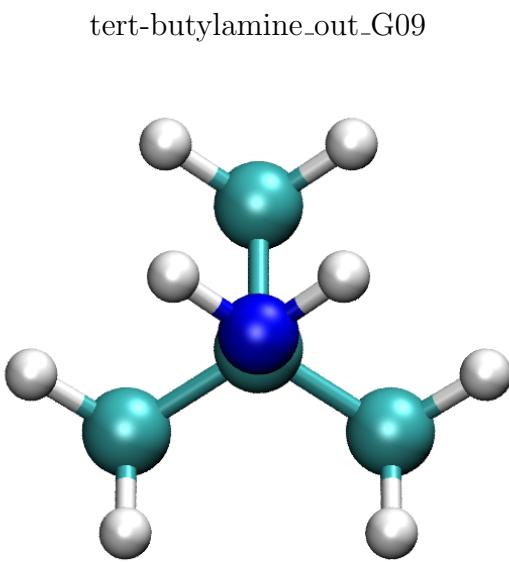
110.655	111.213	113.693
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Equal



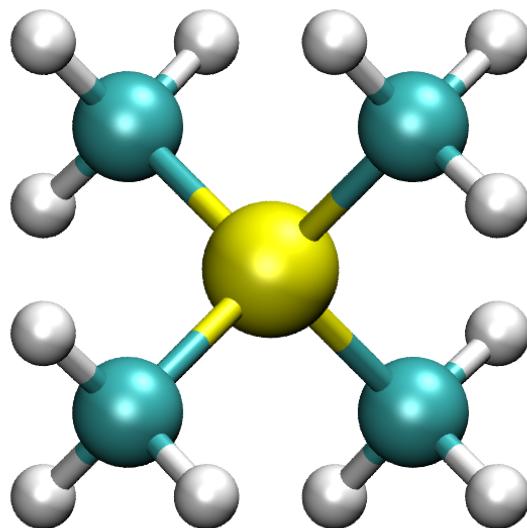
NeoConformation Número 570

Molecule A



Molecule B

tetramethylsilane\_out\_G09

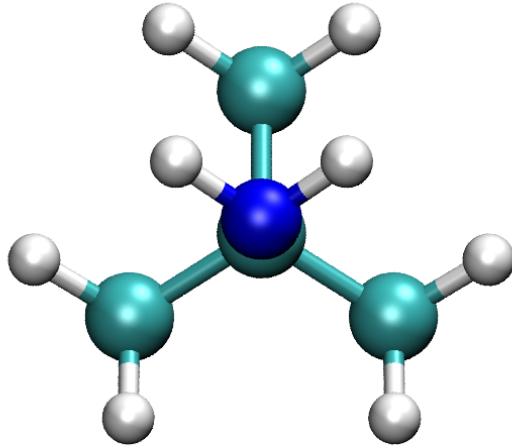


Different

NeoConformation Número 571

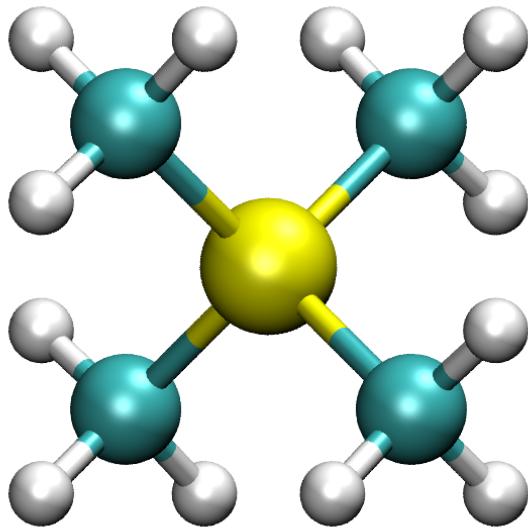
Molecule A

tert-butylamine\_out\_G09



Molecule B

tetramethylsilane\_out\_G09\_inversion

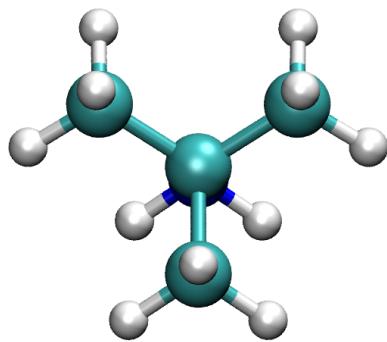


Different

NeoConformation Número 572

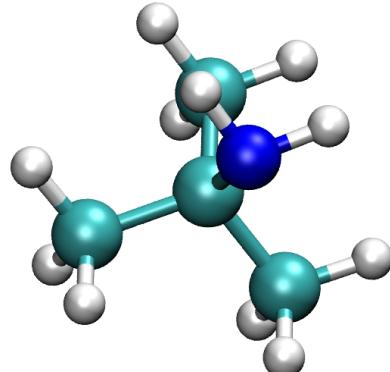
Molecule A

tert-butylamine\_out\_G09\_inversion



Molecule B

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15



Inertia Tensor - Molecule A

110.655	-4.00493e-05	5.05193e-05
-4.00493e-05	111.529	0.826271
5.05193e-05	0.826271	113.378

Inertia Tensor - Molecule B

111.039	0.579971	0.822165
0.579971	111.829	0.957523
0.822165	0.957523	112.694

EingenVectors - Molecule A

-1	-8.8937e-05	4.55534e-05
9.93354e-05	-0.934224	0.356687
1.08344e-05	0.356687	0.934224

EingenVectors - Molecule B

-0.933012	0.249963	0.258859
-0.0630357	-0.821768	0.566325
0.354282	0.512071	0.782476

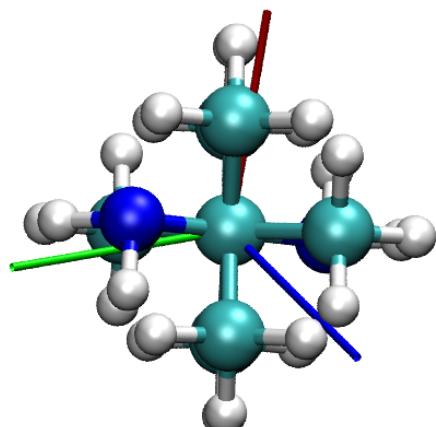
EingenValues - Molecule A

110.655	111.213	113.693
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EingenValues - Molecule B

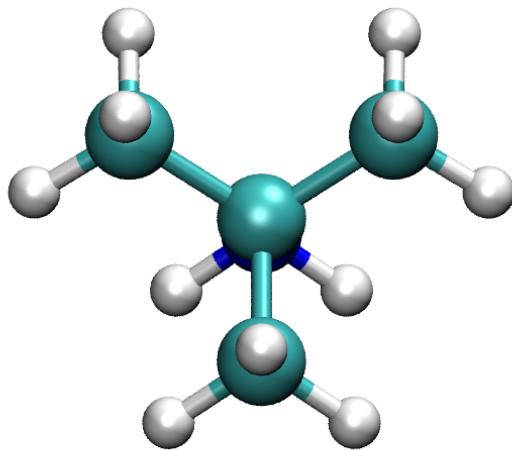
110.655	111.213	113.693
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Equal



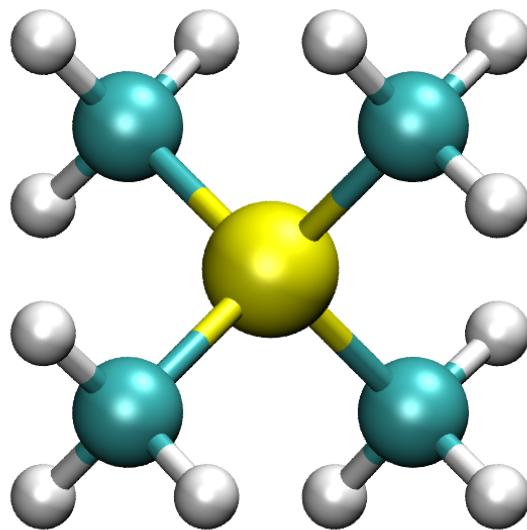
Molecule A

tert-butylamine\_out\_G09\_inversion



Molecule B

tetramethylsilane\_out\_G09

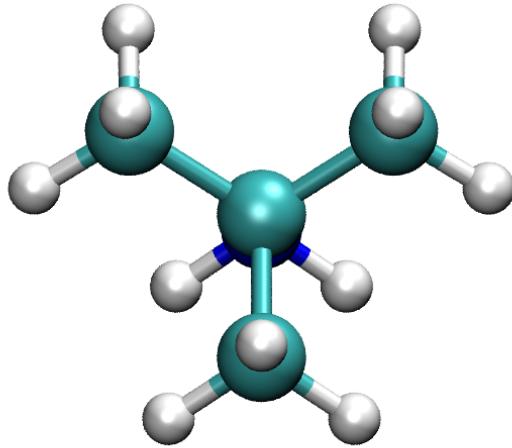


Different

NeoConformation Número 574

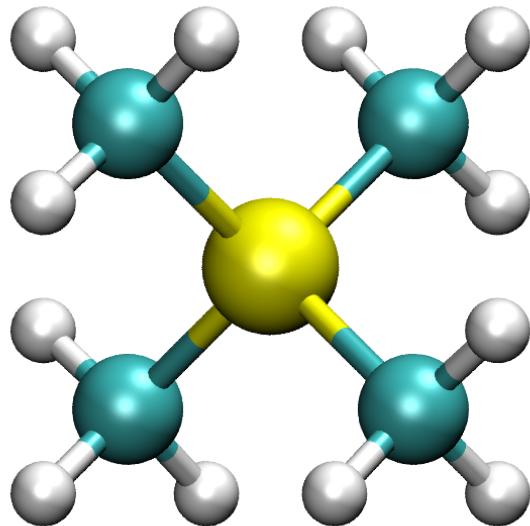
Molecule A

tert-butylamine\_out\_G09\_inversion



Molecule B

tetramethylsilane\_out\_G09\_inversion

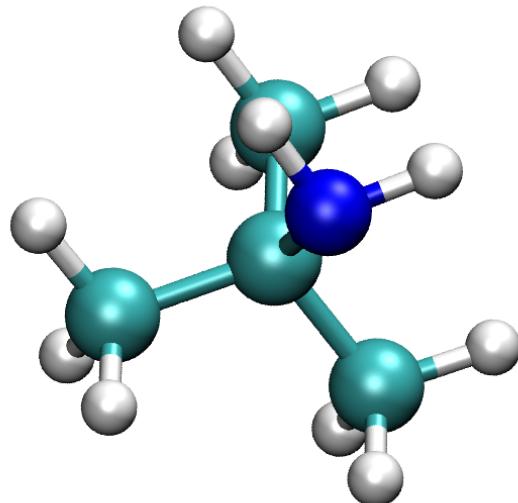


Different

NeoConformation Número 575

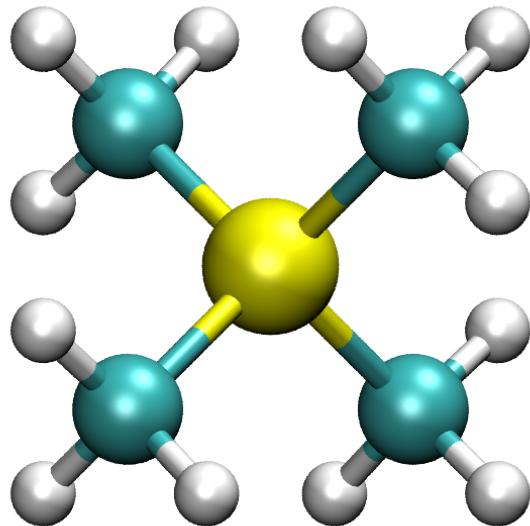
Molecule A

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15



Molecule B

tetramethylsilane\_out\_G09

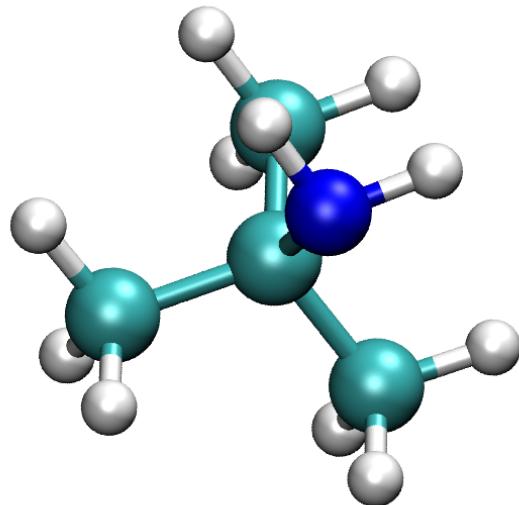


Different

NeoConformation Número 576

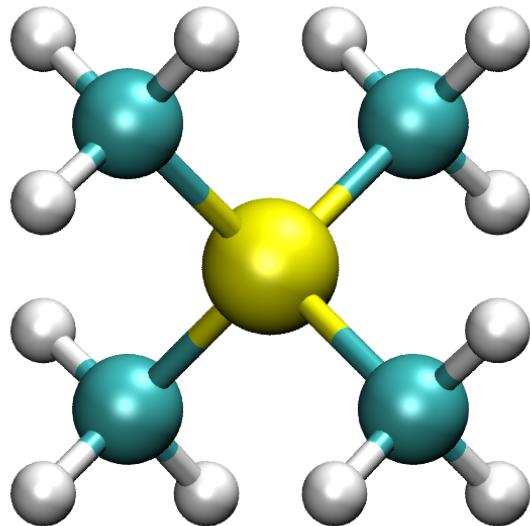
Molecule A

tert-butylamine\_out\_G09\_rot\_x15\_y15\_z15



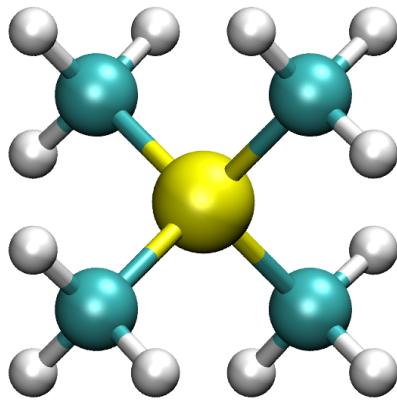
Molecule B

tetramethylsilane\_out\_G09\_inversion



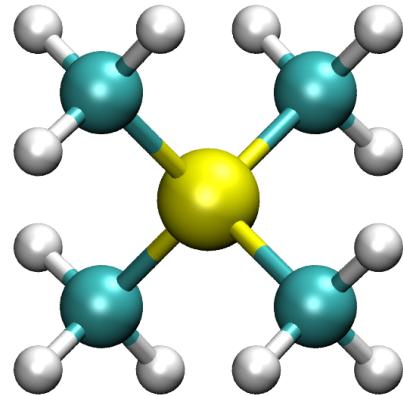
Different

Molecule A tetramethylsilane\_out\_G09



Molecule B

tetramethylsilane\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 166.054 & 0 & 0 \\ 0 & 166.054 & 0 \\ 0 & 0 & 166.054 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 166.053 & 0 & 0 \\ 0 & 166.053 & 0 \\ 0 & 0 & 166.053 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

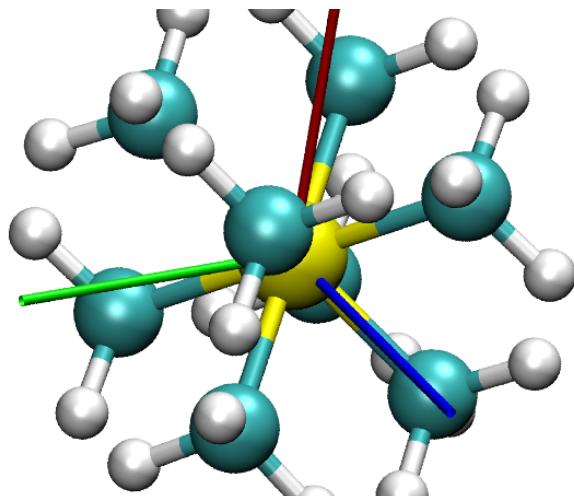
EingenValues - Molecule A

$$\begin{vmatrix} 166.054 & 166.054 & 166.054 \end{vmatrix}$$

EingenValues - Molecule B

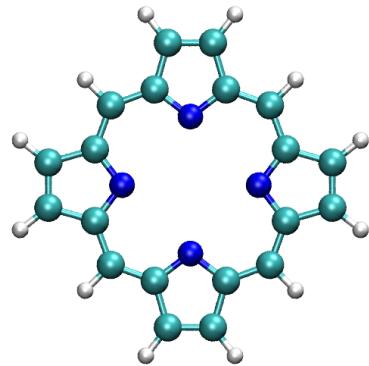
$$\begin{vmatrix} 166.053 & 166.053 & 166.053 \end{vmatrix}$$

Equal

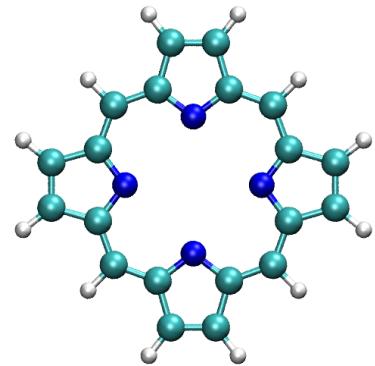


# RotationSameMolecule Número 578

Molecule A Porphin\_out\_G09



Molecule B Porphin\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 1914.06 & 0 & 0 \\ 0 & 1914.06 & 0 \\ 0 & 0 & 3828.12 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 1914.06 & 0 & 0 \\ 0 & 1914.06 & 0 \\ 0 & 0 & 3828.12 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

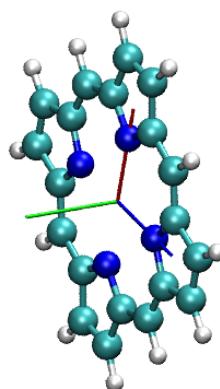
EingenValues - Molecule A

$$\begin{vmatrix} 1914.06 & 1914.06 & 3828.12 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 1914.06 & 1914.06 & 3828.12 \end{vmatrix}$$

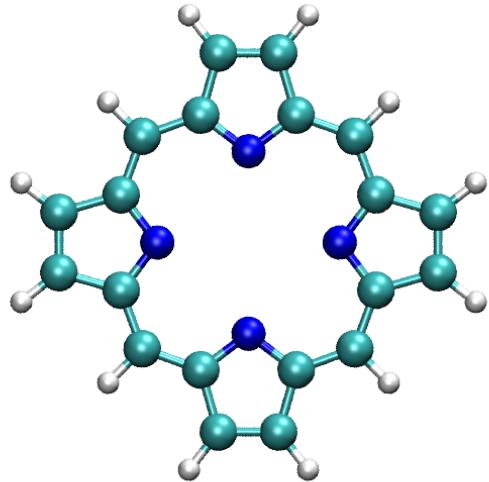
Equal



RotationSameMolecule Número 579

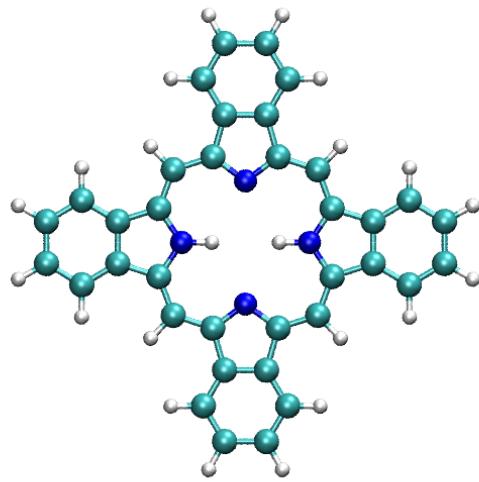
Molecule A

Porphin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_out\_G09

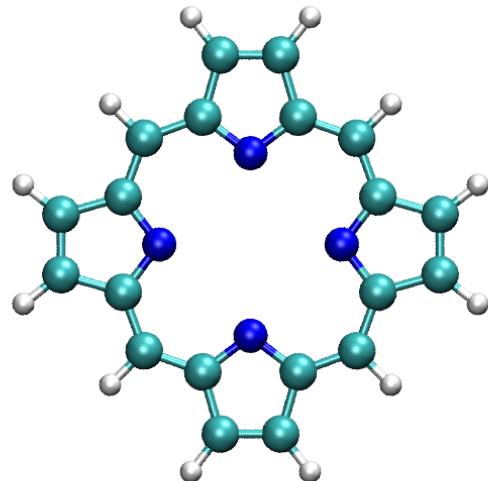


Different

RotationSameMolecule Número 580

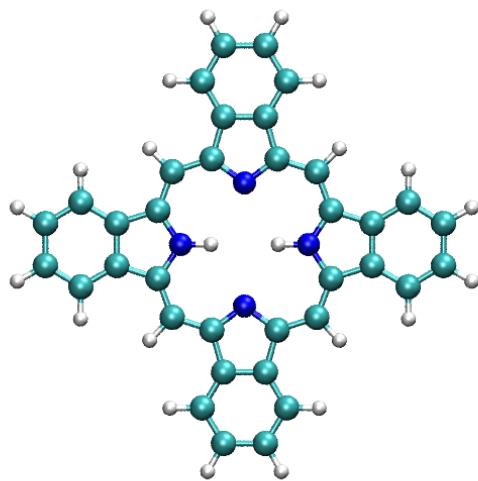
Molecule A

Porphin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_out\_G09\_inversion

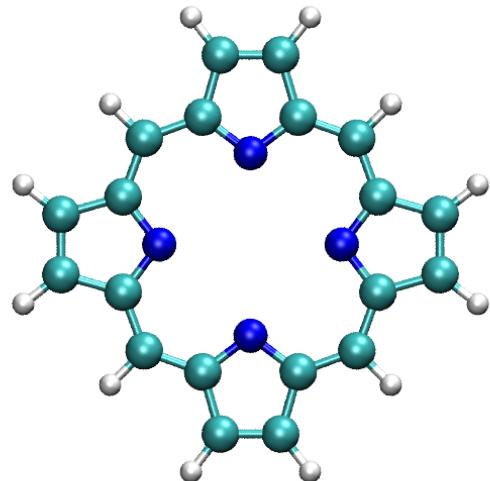


Different

RotationSameMolecule Número 581

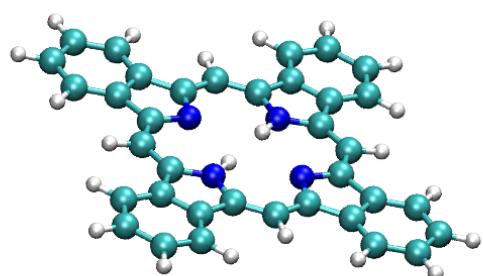
Molecule A

Porphin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_rotated02\_out\_G09

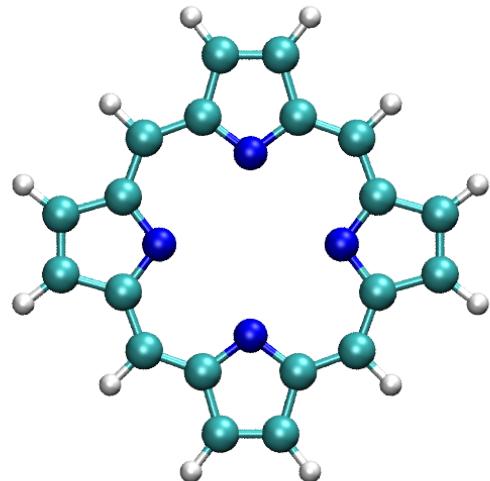


Different

RotationSameMolecule Número 582

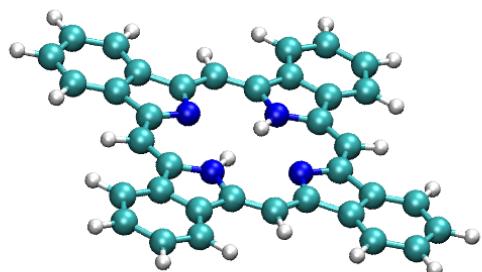
Molecule A

Porphin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_rotated02\_out\_G09\_inversion

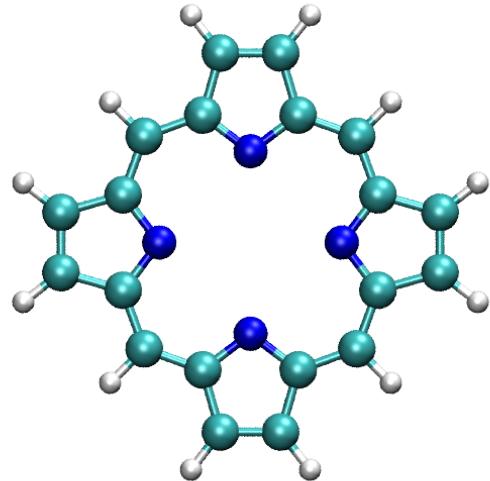


Different

RotationSameMolecule Número 583

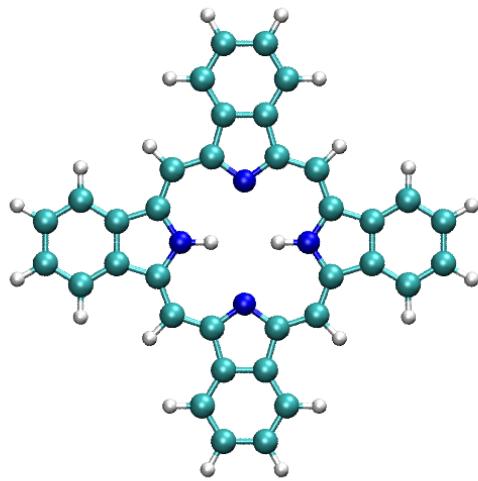
Molecule A

Porphin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_rotated\_out\_G09

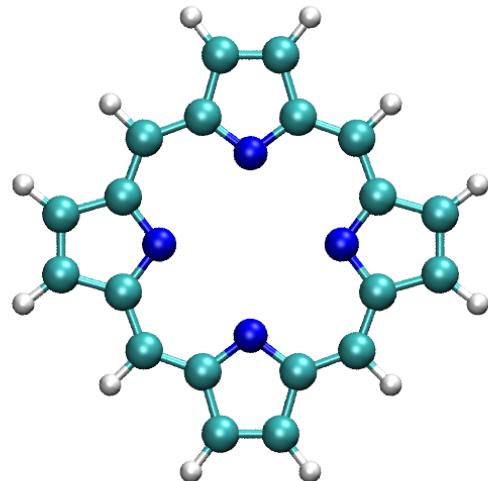


Different

RotationSameMolecule Número 584

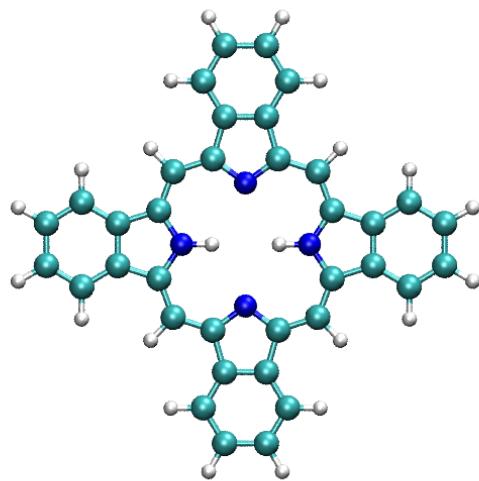
Molecule A

Porphin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_rotated\_out\_G09\_inversion

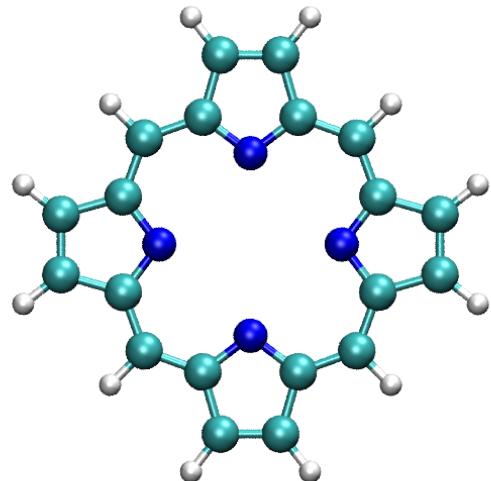


Different

RotationSameMolecule Número 585

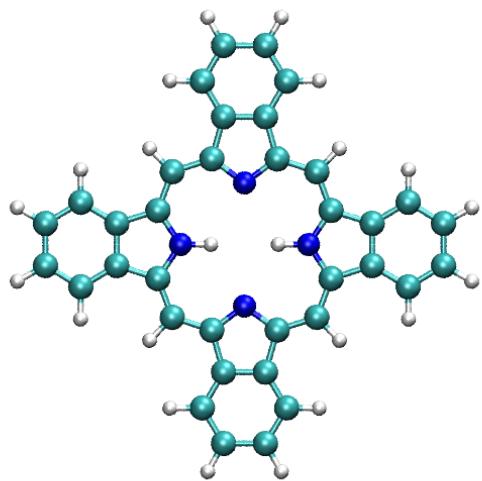
Molecule A

Porphin\_out\_G09\_inversion



Molecule B

Tetrabenzoporphyrin\_out\_G09

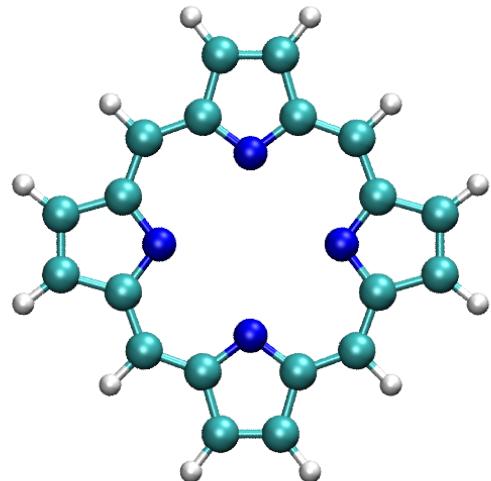


Different

RotationSameMolecule Número 586

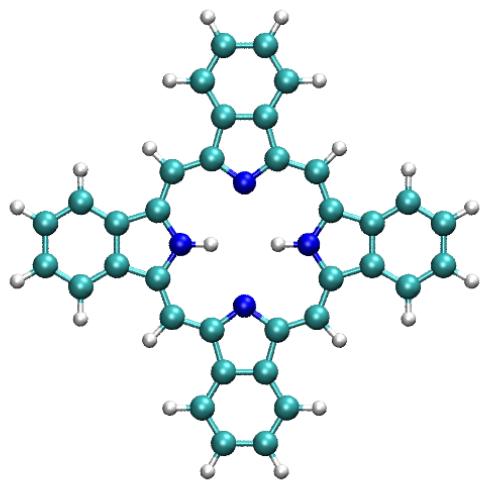
Molecule A

Porphin\_out\_G09\_inversion



Molecule B

Tetrabenzoporphyrin\_out\_G09\_inversion

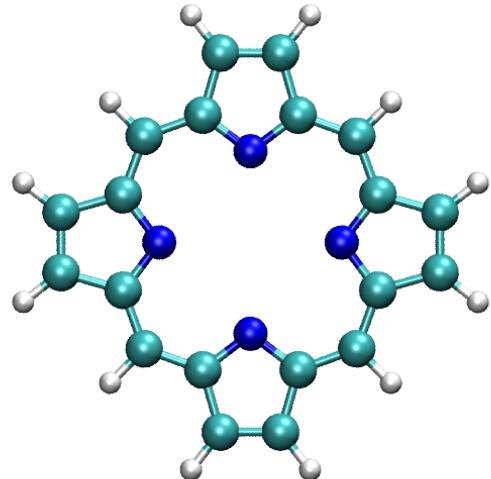


Different

RotationSameMolecule Número 587

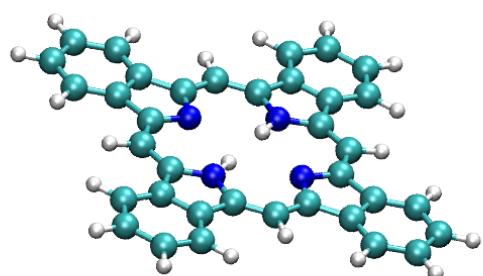
Molecule A

Porphin\_out\_G09\_inversion



Molecule B

Tetrabenzoporphyrin\_rotated02\_out\_G09

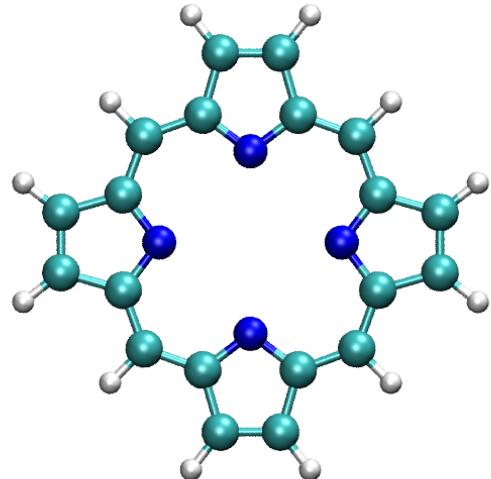


Different

RotationSameMolecule Número 588

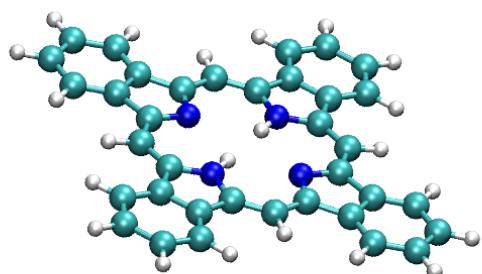
Molecule A

Porphin\_out\_G09\_inversion



Molecule B

Tetrabenzoporphyrin\_rotated02\_out\_G09\_inversion

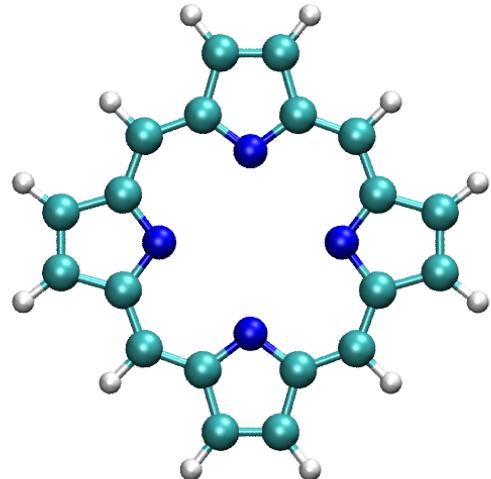


Different

RotationSameMolecule Número 589

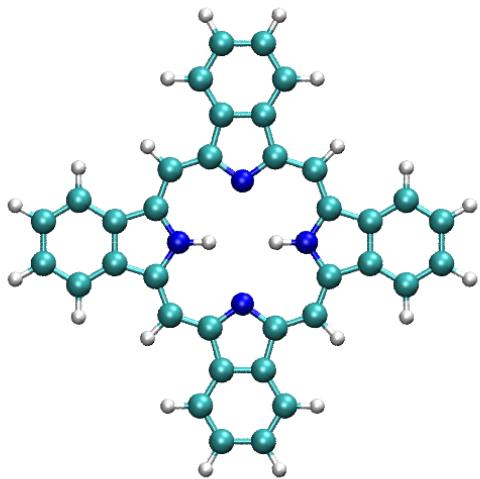
Molecule A

Porphin\_out\_G09\_inversion



Molecule B

Tetrabenzoporphyrin\_rotated\_out\_G09

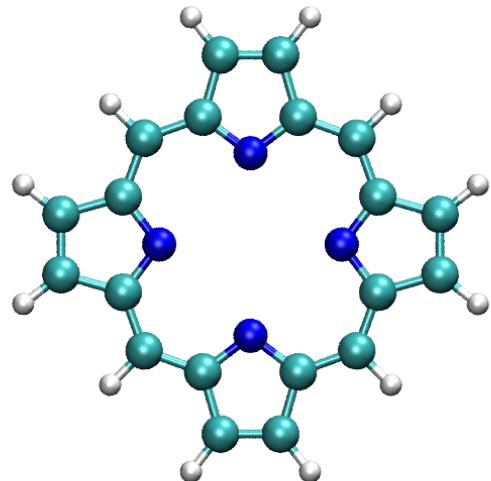


Different

RotationSameMolecule Número 590

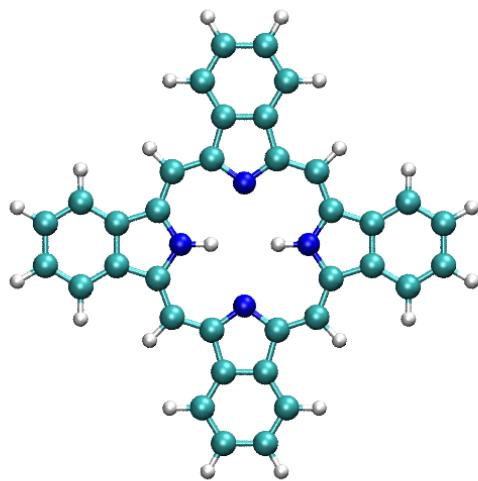
Molecule A

Porphin\_out\_G09\_inversion



Molecule B

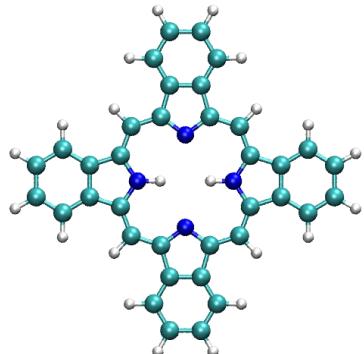
Tetrabenzoporphyrin\_rotated\_out\_G09\_inversion



Different

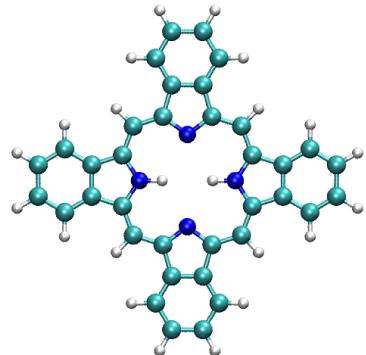
# RotationSameMolecule Número 591

Molecule A Tetrabenzoporphyrin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

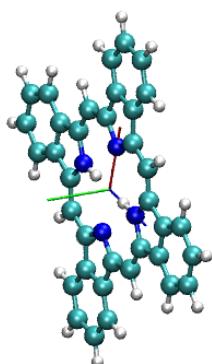
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

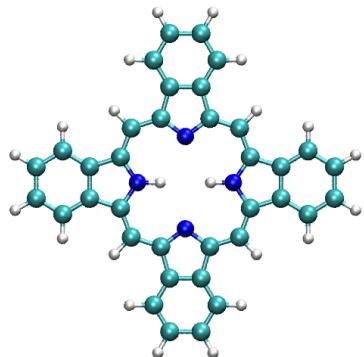
$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Equal



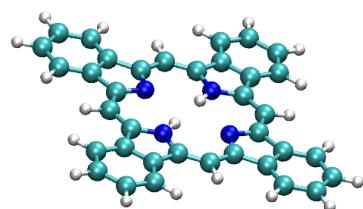
# RotationSameMolecule Número 592

Molecule A Tetrabenzoporphyrin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_rotated02.out\_G09



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 7791.57 & 2641.52 & -788.168 \\ 2641.52 & 9673.67 & -1103.82 \\ -788.168 & -1103.82 & 6265.27 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.771476 & 0.397136 & -0.497099 \\ 0.301236 & -0.460189 & -0.835154 \\ -0.56043 & -0.794046 & 0.235394 \end{vmatrix}$$

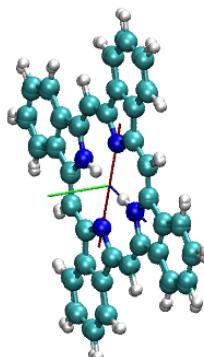
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

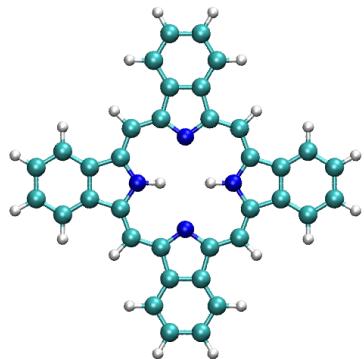
$$\begin{vmatrix} 5923.93 & 5941.33 & 11865.3 \end{vmatrix}$$

Enantiomers

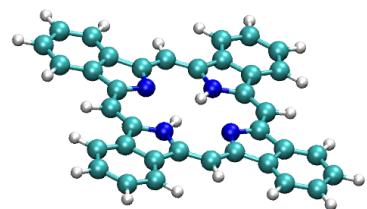


# RotationSameMolecule Número 593

Molecule A Tetrabenzoporphyrin\_out\_G09



Molecule B Tetrabenzoporphyrin\_rotated02\_out\_G09\_inversion



Inertia Tensor - Molecule A

11864.8	0	0
0	5941.95	0
0	0	5922.88

Inertia Tensor - Molecule B

7791.56	2641.52	-788.166
2641.52	9673.67	-1103.82
-788.166	-1103.82	6265.27

EingenVectors - Molecule A

0	0	1
0	1	0
1	0	0

EingenVectors - Molecule B

-0.771478	0.39714	-0.497093
0.30123	-0.460186	-0.835158
-0.56043	-0.794046	0.235393

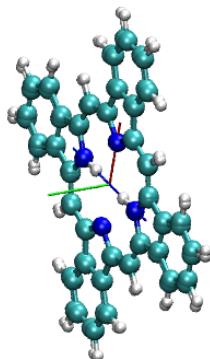
EingenValues - Molecule A

5922.88	5941.95	11864.8
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EingenValues - Molecule B

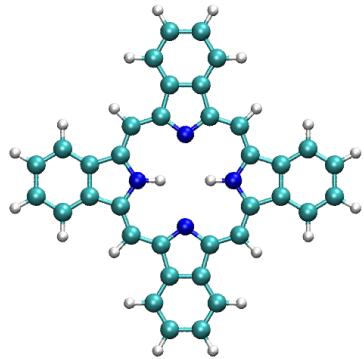
5923.93	5941.33	11865.3
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Enantiomers



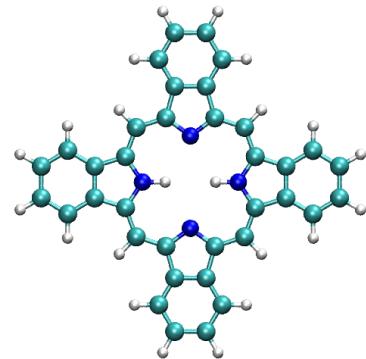
# RotationSameMolecule Número 594

Molecule A Tetrabenzoporphyrin\_out\_G09



Molecule B

Tetrabenzoporphyrin\_rotated\_out\_G09



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

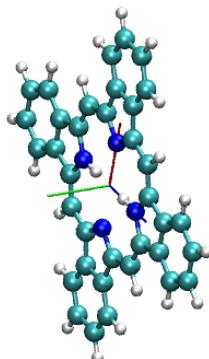
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

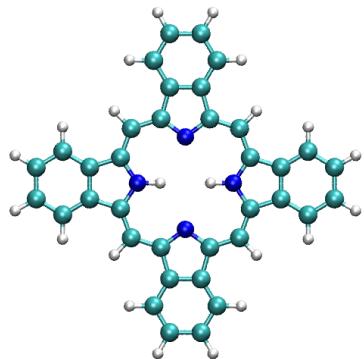
$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Equal

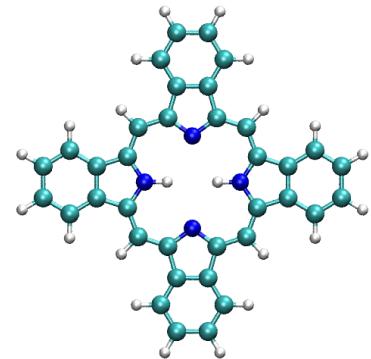


# RotationSameMolecule Número 595

Molecule A Tetrabenzoporphyrin\_out\_G09



Molecule B Tetrabenzoporphyrin\_rotated\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

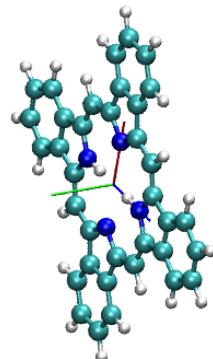
EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

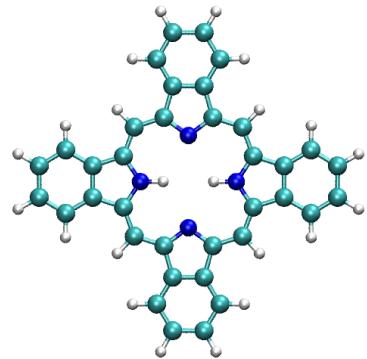
Equal



# RotationSameMolecule Número 596

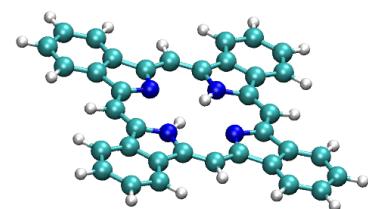
Molecule A

Tetrabenzoporphyrin.out.G09.inversion



Molecule B

Tetrabenzoporphyrin\_rotated02.out.G09



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 7791.57 & 2641.52 & -788.168 \\ 2641.52 & 9673.67 & -1103.82 \\ -788.168 & -1103.82 & 6265.27 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.771476 & 0.397136 & -0.497099 \\ 0.301236 & -0.460189 & -0.835154 \\ -0.56043 & -0.794046 & 0.235394 \end{vmatrix}$$

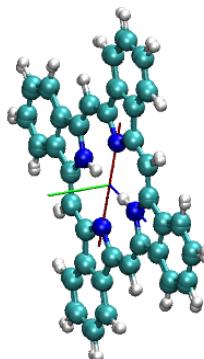
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

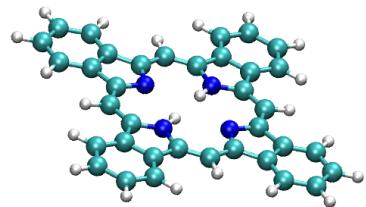
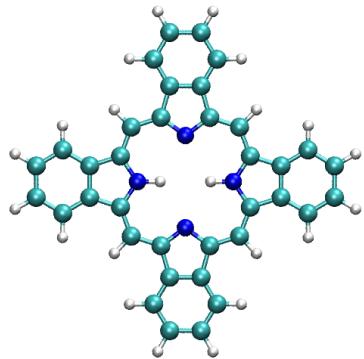
$$\begin{vmatrix} 5923.93 & 5941.33 & 11865.3 \end{vmatrix}$$

Enantiomers



Molecule A  
Tetrabenzoporphyrin\_out\_G09\_inversion

Molecule B Tetrabenzoporphyrin\_rotated02\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 7791.56 & 2641.52 & -788.166 \\ 2641.52 & 9673.67 & -1103.82 \\ -788.166 & -1103.82 & 6265.27 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.771478 & 0.39714 & -0.497093 \\ 0.30123 & -0.460186 & -0.835158 \\ -0.56043 & -0.794046 & 0.235393 \end{vmatrix}$$

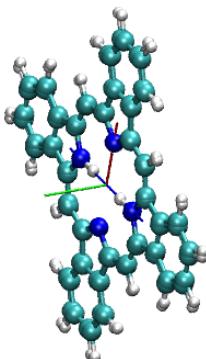
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

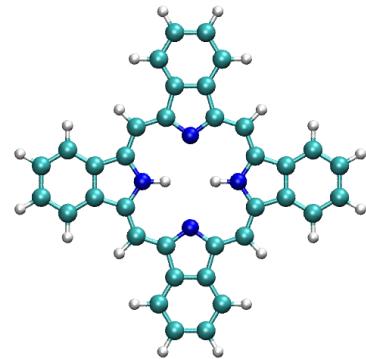
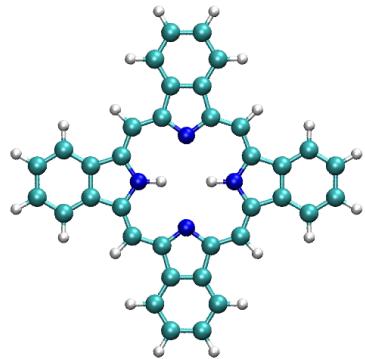
$$\begin{vmatrix} 5923.93 & 5941.33 & 11865.3 \end{vmatrix}$$

Enantiomers



# RotationSameMolecule Número 598

Molecule A    Molecule B  
 Tetrabenzoporphyrin\_out\_G09\_inversion      Tetrabenzoporphyrin\_rotated\_out\_G09



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

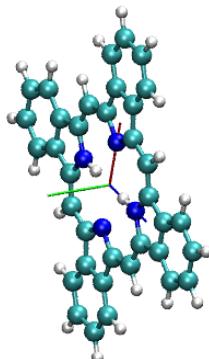
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

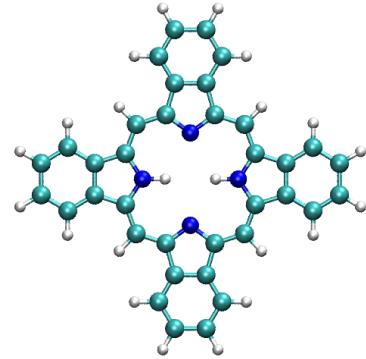
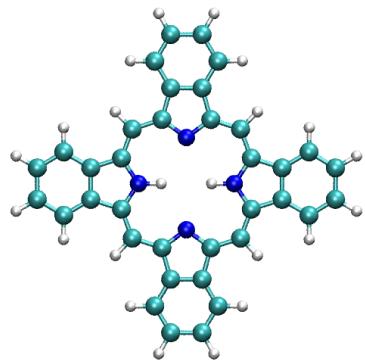
Equal



# RotationSameMolecule Número 599

Molecule A  
Tetrabenzoporphyrin\_out\_G09\_inversion

Molecule B Tetrabenzoporphyrin\_rotated\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

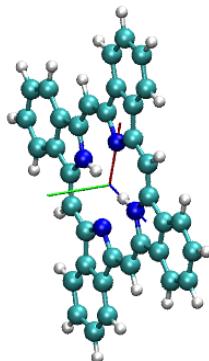
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

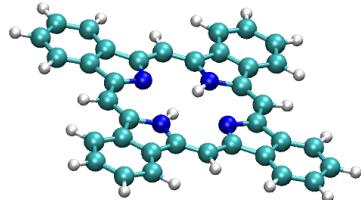
Equal



# RotationSameMolecule Número 600

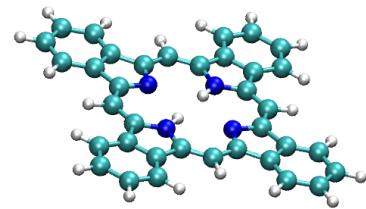
Molecule A

Tetrabenzoporphyrin\_rotated02\_out\_G09



Molecule B Tetrabenzoporphyrin

rin\_rotated02\_out\_G09\_inversion



Inertia Tensor - Molecule A

7791.57	2641.52	-788.168
2641.52	9673.67	-1103.82
-788.168	-1103.82	6265.27

Inertia Tensor - Molecule B

7791.56	2641.52	-788.166
2641.52	9673.67	-1103.82
-788.166	-1103.82	6265.27

EingenVectors - Molecule A

-0.771476	0.397136	-0.497099
0.301236	-0.460189	-0.835154
-0.56043	-0.794046	0.235394

EingenVectors - Molecule B

-0.771478	0.39714	-0.497093
0.30123	-0.460186	-0.835158
-0.56043	-0.794046	0.235393

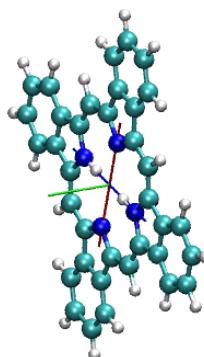
EingenValues - Molecule A

5923.93	5941.33	11865.3
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EingenValues - Molecule B

5923.93	5941.33	11865.3
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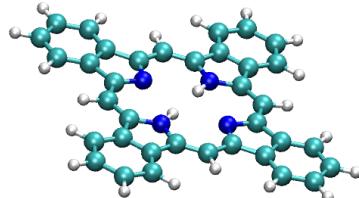
Equal



# RotationSameMolecule Número 601

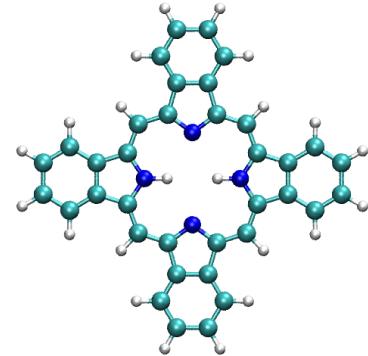
Molecule A

Tetrabenzoporphyrin\_rotated02\_out\_G09



Molecule B

Tetrabenzoporphyrin\_rotated.out\_G09



Inertia Tensor - Molecule A

7791.57	2641.52	-788.168
2641.52	9673.67	-1103.82
-788.168	-1103.82	6265.27

Inertia Tensor - Molecule B

11864.8	0	0
0	5941.95	0
0	0	5922.88

EigenVectors - Molecule A

-0.771476	0.397136	-0.497099
0.301236	-0.460189	-0.835154
-0.56043	-0.794046	0.235394

EigenVectors - Molecule B

0	0	1
0	1	0
1	0	0

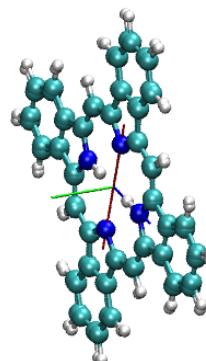
EigenValues - Molecule A

5923.93	5941.33	11865.3
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EigenValues - Molecule B

5922.88	5941.95	11864.8
---------	---------	---------

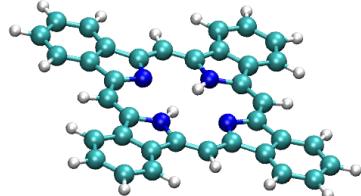
Enantiomers



# RotationSameMolecule Número 602

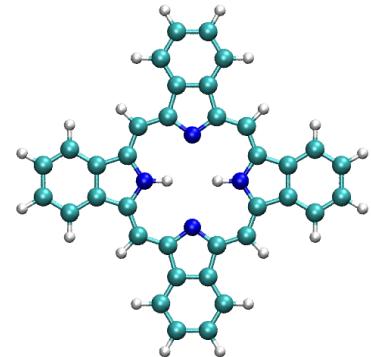
Molecule A

Tetrabenzoporphyrin\_rotated02\_out\_G09



Molecule B Tetrabenzoporphyrin

rin\_rotated\_out\_G09\_inversion



Inertia Tensor - Molecule A

7791.57	2641.52	-788.168
2641.52	9673.67	-1103.82
-788.168	-1103.82	6265.27

Inertia Tensor - Molecule B

11864.8	0	0
0	5941.95	0
0	0	5922.88

EingenVectors - Molecule A

-0.771476	0.397136	-0.497099
0.301236	-0.460189	-0.835154
-0.56043	-0.794046	0.235394

EingenVectors - Molecule B

0	0	1
0	1	0
1	0	0

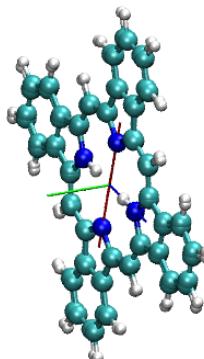
EingenValues - Molecule A

5923.93	5941.33	11865.3
---------	---------	---------

EingenValues - Molecule B

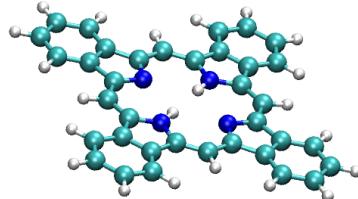
5922.88	5941.95	11864.8
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Enantiomers

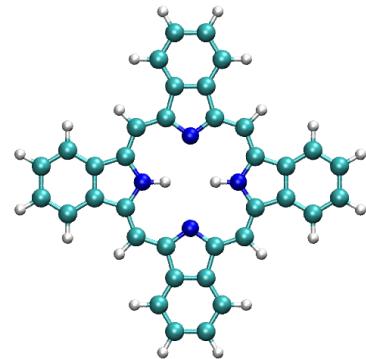


# RotationSameMolecule Número 603

Molecule A Tetrabenzoporphyrin\_rotated02.out.G09\_inversion



Molecule B  
Tetrabenzoporphyrin\_rotated.out.G09



Inertia Tensor - Molecule A

7791.56	2641.52	-788.166
2641.52	9673.67	-1103.82
-788.166	-1103.82	6265.27

Inertia Tensor - Molecule B

11864.8	0	0
0	5941.95	0
0	0	5922.88

EigenVectors - Molecule A

-0.771478	0.39714	-0.497093
0.30123	-0.460186	-0.835158
-0.56043	-0.794046	0.235393

EigenVectors - Molecule B

0	0	1
0	1	0
1	0	0

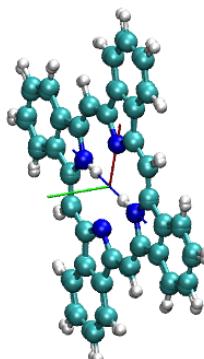
EigenValues - Molecule A

5923.93	5941.33	11865.3
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EigenValues - Molecule B

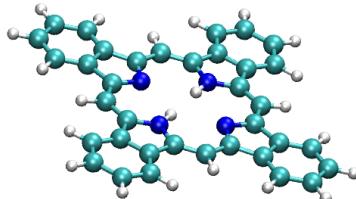
5922.88	5941.95	11864.8
---------	---------	---------

Enantiomers

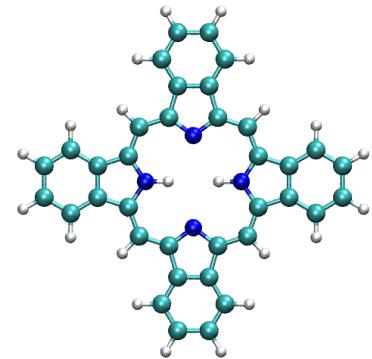


# RotationSameMolecule Número 604

Molecule A Tetrabenzoporphyrin\_rotated02.out\_G09\_inversion



Molecule B Tetrabenzoporphyrin\_rotated\_out\_G09\_inversion



Inertia Tensor - Molecule A

7791.56	2641.52	-788.166
2641.52	9673.67	-1103.82
-788.166	-1103.82	6265.27

Inertia Tensor - Molecule B

11864.8	0	0
0	5941.95	0
0	0	5922.88

EingenVectors - Molecule A

-0.771478	0.39714	-0.497093
0.30123	-0.460186	-0.835158
-0.56043	-0.794046	0.235393

EingenVectors - Molecule B

0	0	1
0	1	0
1	0	0

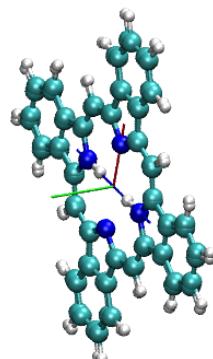
EingenValues - Molecule A

5923.93	5941.33	11865.3
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EingenValues - Molecule B

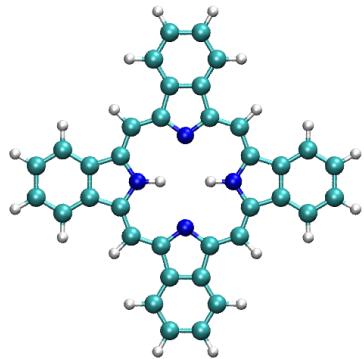
5922.88	5941.95	11864.8
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Enantiomers

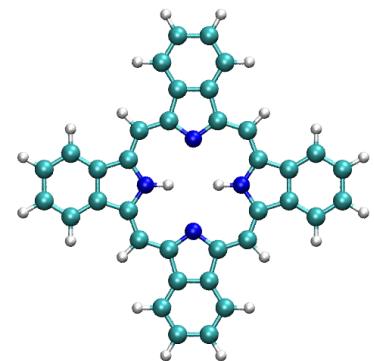


# RotationSameMolecule Número 605

Molecule A  
Tetrabenzoporphyrin\_rotated\_out\_G09



Molecule B Tetrabenzoporphyrin\_rotated\_out\_G09\_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

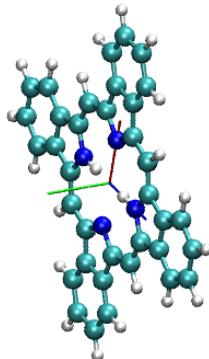
EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenValues - Molecule B

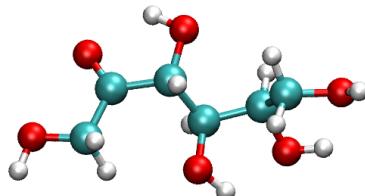
$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Equal

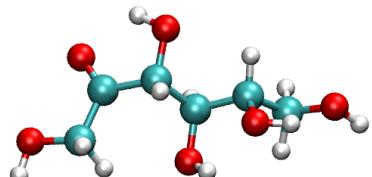


Sugars Número 606

Molecule A R-R-R-Fructuose\_out\_G09



Molecule B R-R-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

270.201	9.83383	1.05361
9.83383	1104.24	-0.466663
1.05361	-0.466663	1244.5

Inertia Tensor - Molecule B

258.009	6.71977	-10.1101
6.71977	1154.74	-1.24568
-10.1101	-1.24568	1276.63

EingenVectors - Molecule A

0.99993	-0.0117888	-0.00108684
-0.0117923	-0.999925	-0.00324079
0.00104856	-0.00325338	0.999994

EingenVectors - Molecule B

-0.999923	0.00747806	-0.00991386
0.00737058	0.999914	0.010833
-0.00999402	-0.0107591	0.999892

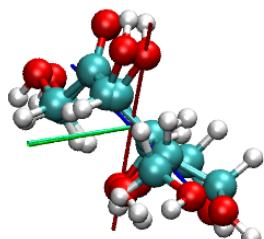
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

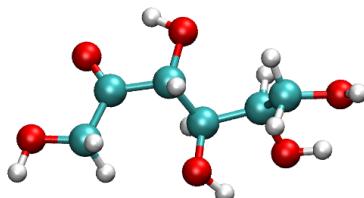
257.858	1154.77	1276.75
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Different

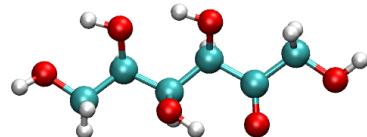


Sugars Número 607

Molecule A R-R-R-Fructuose\_out\_G09



Molecule B R-S-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

270.201	9.83383	1.05361
9.83383	1104.24	-0.466663
1.05361	-0.466663	1244.5

Inertia Tensor - Molecule B

203.246	14.6965	0.489268
14.6965	1215.65	-0.989769
0.489268	-0.989769	1332.21

EingenVectors - Molecule A

0.99993	-0.0117888	-0.00108684
-0.0117923	-0.999925	-0.00324079
0.00104856	-0.00325338	0.999994

EingenVectors - Molecule B

-0.999895	0.0145123	0.000445973
-0.0145155	-0.999859	-0.00844446
0.000323361	-0.00845004	0.999964

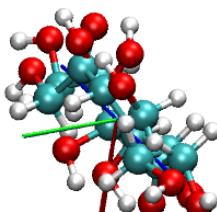
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

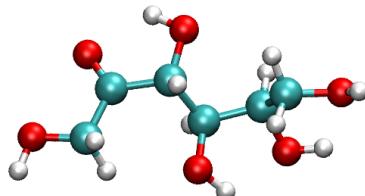
203.032	1215.85	1332.21
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Different

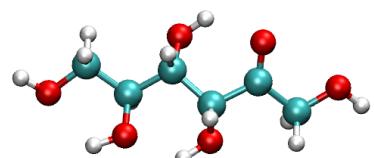


# Sugars Número 608

Molecule A R-R-R-Fructuose\_out\_G09



Molecule B R-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

270.201	9.83383	1.05361
9.83383	1104.24	-0.466663
1.05361	-0.466663	1244.5

Inertia Tensor - Molecule B

214.933	-13.9132	-6.26614
-13.9132	1186.84	0.567805
-6.26614	0.567805	1322.37

EingenVectors - Molecule A

0.99993	-0.0117888	-0.00108684
-0.0117923	-0.999925	-0.00324079
0.00104856	-0.00325338	0.999994

EingenVectors - Molecule B

0.999882	0.0143069	0.00564903
0.0142795	-0.999886	0.00485623
-0.00571786	0.00477499	0.999972

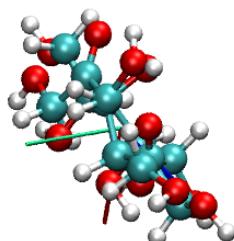
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

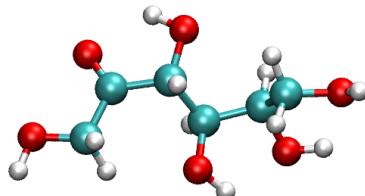
214.698	1187.04	1322.41
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Different

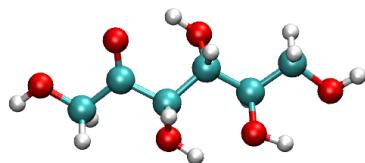


# Sugars Número 609

Molecule A R-R-R-Fructuose\_out\_G09



Molecule B S-R-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

270.201	9.83383	1.05361
9.83383	1104.24	-0.466663
1.05361	-0.466663	1244.5

Inertia Tensor - Molecule B

214.974	13.9189	6.25845
13.9189	1186.65	0.565787
6.25845	0.565787	1322.09

EingenVectors - Molecule A

0.99993	-0.0117888	-0.00108684
-0.0117923	-0.999925	-0.00324079
0.00104856	-0.00325338	0.999994

EingenVectors - Molecule B

-0.999882	0.0143163	0.00564373
0.014289	0.999886	-0.00484396
0.00571244	0.00476274	0.999972

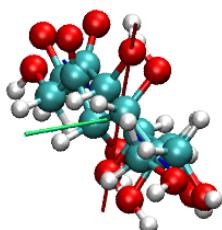
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

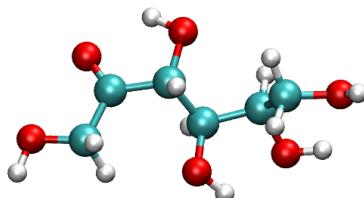
214.739	1186.84	1322.13
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Different

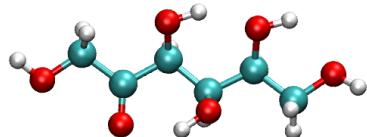


Sugars Número 610

Molecule A R-R-R-Fructuose\_out\_G09



Molecule B S-R-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

270.201	9.83383	1.05361
9.83383	1104.24	-0.466663
1.05361	-0.466663	1244.5

Inertia Tensor - Molecule B

203.262	-14.7021	-0.492665
-14.7021	1215.64	-0.989546
-0.492665	-0.989546	1332.23

EingenVectors - Molecule A

0.99993	-0.0117888	-0.00108684
-0.0117923	-0.999925	-0.00324079
0.00104856	-0.00325338	0.999994

EingenVectors - Molecule B

-0.999895	-0.0145182	-0.000448979
0.0145214	-0.999859	-0.00843991
-0.000326384	-0.00844554	0.999964

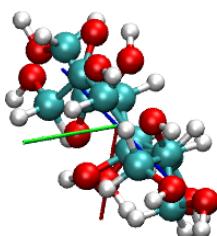
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

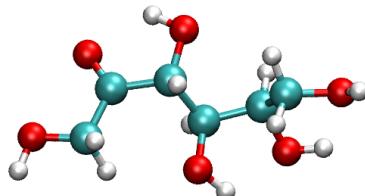
203.048	1215.85	1332.24
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Different

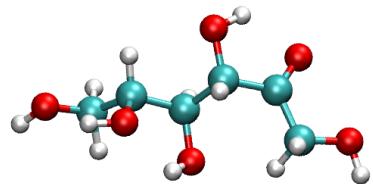


# Sugars Número 611

Molecule A R-R-R-Fructuose\_out\_G09



Molecule B S-S-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

270.201	9.83383	1.05361
9.83383	1104.24	-0.466663
1.05361	-0.466663	1244.5

Inertia Tensor - Molecule B

257.995	-6.7346	10.0985
-6.7346	1154.74	-1.24098
10.0985	-1.24098	1276.66

EingenVectors - Molecule A

0.99993	-0.0117888	-0.00108684
-0.0117923	-0.999925	-0.00324079
0.00104856	-0.00325338	0.999994

EingenVectors - Molecule B

0.999923	0.00749452	-0.00990206
0.00738758	-0.999914	-0.0107925
0.0099821	-0.0107185	0.999893

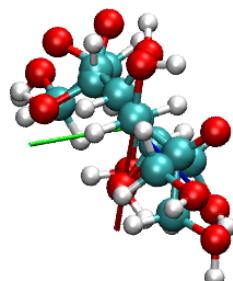
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

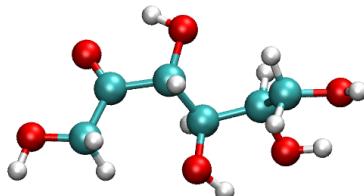
257.845	1154.78	1276.78
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Different

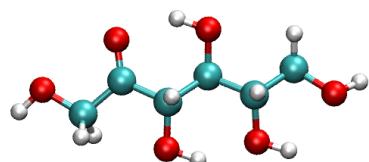


# Sugars Número 612

Molecule A R-R-R-Fructuose\_out\_G09



Molecule B S-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

270.201	9.83383	1.05361
9.83383	1104.24	-0.466663
1.05361	-0.466663	1244.5

Inertia Tensor - Molecule B

224.224	13.0406	-2.54457
13.0406	1180.14	-1.05607
-2.54457	-1.05607	1363.89

EingenVectors - Molecule A

0.99993	-0.0117888	-0.00108684
-0.0117923	-0.999925	-0.00324079
0.00104856	-0.00325338	0.999994

EingenVectors - Molecule B

-0.999905	0.0136356	-0.00221952
0.0136222	0.99989	0.00594071
-0.00230028	-0.00590991	0.99998

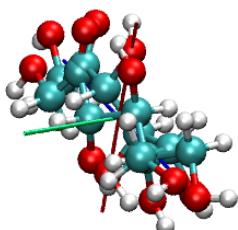
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

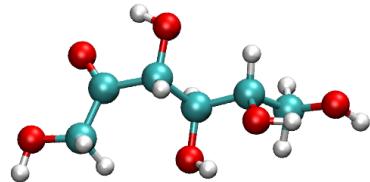
224.041	1180.31	1363.9
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Different

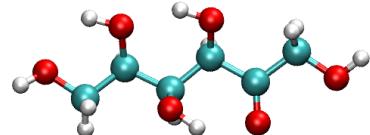


Sugars Número 613

Molecule A R-R-S-Fructuose\_out\_G09



Molecule B R-S-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

258.009	6.71977	-10.1101
6.71977	1154.74	-1.24568
-10.1101	-1.24568	1276.63

Inertia Tensor - Molecule B

203.246	14.6965	0.489268
14.6965	1215.65	-0.989769
0.489268	-0.989769	1332.21

EingenVectors - Molecule A

-0.999923	0.00747806	-0.00991386
0.00737058	0.999914	0.010833
-0.00999402	-0.0107591	0.999892

EingenVectors - Molecule B

-0.999895	0.0145123	0.000445973
-0.0145155	-0.999859	-0.00844446
0.000323361	-0.00845004	0.999964

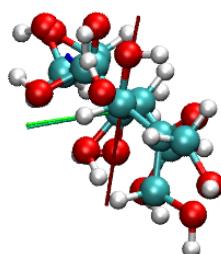
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

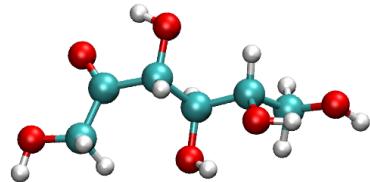
203.032	1215.85	1332.21
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Different

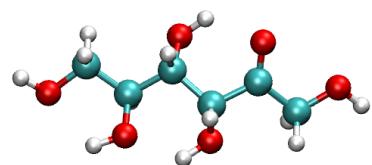


# Sugars Número 614

Molecule A R-R-S-Fructuose\_out\_G09



Molecule B R-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

258.009	6.71977	-10.1101
6.71977	1154.74	-1.24568
-10.1101	-1.24568	1276.63

Inertia Tensor - Molecule B

214.933	-13.9132	-6.26614
-13.9132	1186.84	0.567805
-6.26614	0.567805	1322.37

EingenVectors - Molecule A

-0.999923	0.00747806	-0.00991386
0.00737058	0.999914	0.010833
-0.00999402	-0.0107591	0.999892

EingenVectors - Molecule B

0.999882	0.0143069	0.00564903
0.0142795	-0.999886	0.00485623
-0.00571786	0.00477499	0.999972

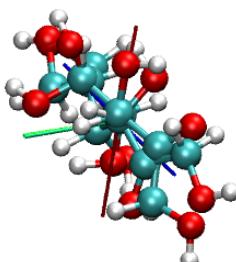
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

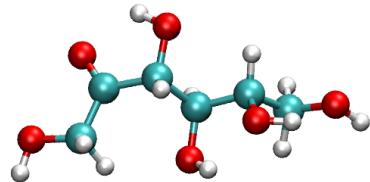
214.698	1187.04	1322.41
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Different

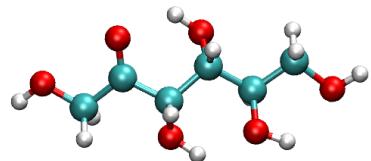


Sugars Número 615

Molecule A R-R-S-Fructuose\_out\_G09



Molecule B S-R-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

258.009	6.71977	-10.1101
6.71977	1154.74	-1.24568
-10.1101	-1.24568	1276.63

Inertia Tensor - Molecule B

214.974	13.9189	6.25845
13.9189	1186.65	0.565787
6.25845	0.565787	1322.09

EingenVectors - Molecule A

-0.999923	0.00747806	-0.00991386
0.00737058	0.999914	0.010833
-0.00999402	-0.0107591	0.999892

EingenVectors - Molecule B

-0.999882	0.0143163	0.00564373
0.014289	0.999886	-0.00484396
0.00571244	0.00476274	0.999972

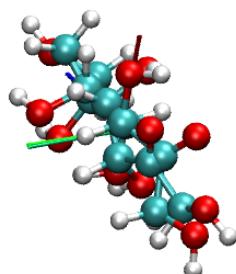
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

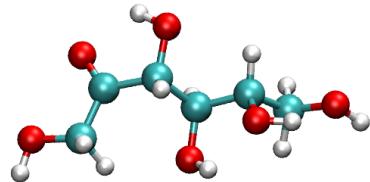
214.739	1186.84	1322.13
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Different

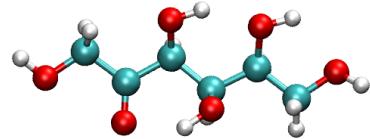


Sugars Número 616

Molecule A R-R-S-Fructuose\_out\_G09



Molecule B S-R-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

258.009	6.71977	-10.1101
6.71977	1154.74	-1.24568
-10.1101	-1.24568	1276.63

Inertia Tensor - Molecule B

203.262	-14.7021	-0.492665
-14.7021	1215.64	-0.989546
-0.492665	-0.989546	1332.23

EingenVectors - Molecule A

-0.999923	0.00747806	-0.00991386
0.00737058	0.999914	0.010833
-0.00999402	-0.0107591	0.999892

EingenVectors - Molecule B

-0.999895	-0.0145182	-0.000448979
0.0145214	-0.999859	-0.00843991
-0.000326384	-0.00844554	0.999964

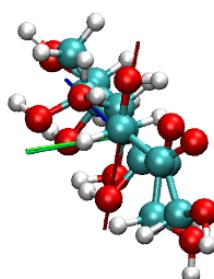
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

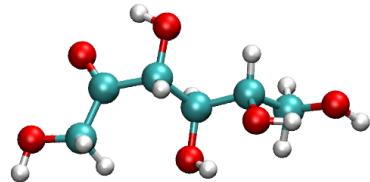
203.048	1215.85	1332.24
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Different

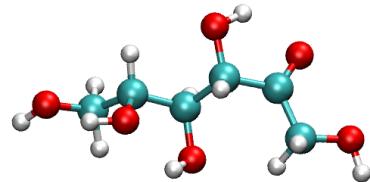


Sugars Número 617

Molecule A R-R-S-Fructuose\_out\_G09



Molecule B S-S-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

258.009	6.71977	-10.1101
6.71977	1154.74	-1.24568
-10.1101	-1.24568	1276.63

Inertia Tensor - Molecule B

257.995	-6.7346	10.0985
-6.7346	1154.74	-1.24098
10.0985	-1.24098	1276.66

EingenVectors - Molecule A

-0.999923	0.00747806	-0.00991386
0.00737058	0.999914	0.010833
-0.00999402	-0.0107591	0.999892

EingenVectors - Molecule B

0.999923	0.00749452	-0.00990206
0.00738758	-0.999914	-0.0107925
0.0099821	-0.0107185	0.999893

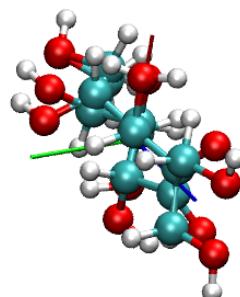
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

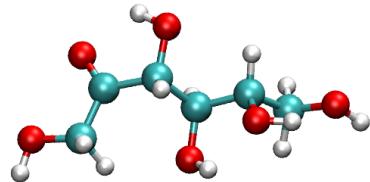
257.845	1154.78	1276.78
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Enantiomers

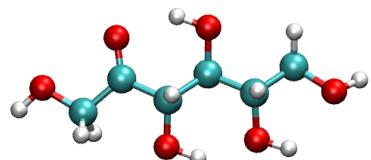


# Sugars Número 618

Molecule A R-R-S-Fructuose\_out\_G09



Molecule B S-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

258.009	6.71977	-10.1101
6.71977	1154.74	-1.24568
-10.1101	-1.24568	1276.63

Inertia Tensor - Molecule B

224.224	13.0406	-2.54457
13.0406	1180.14	-1.05607
-2.54457	-1.05607	1363.89

EingenVectors - Molecule A

-0.999923	0.00747806	-0.00991386
0.00737058	0.999914	0.010833
-0.00999402	-0.0107591	0.999892

EingenVectors - Molecule B

-0.999905	0.0136356	-0.00221952
0.0136222	0.99989	0.00594071
-0.00230028	-0.00590991	0.99998

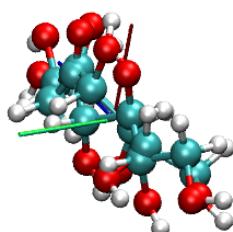
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

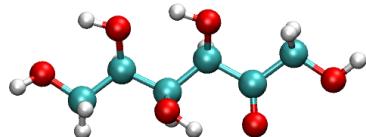
224.041	1180.31	1363.9
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Different

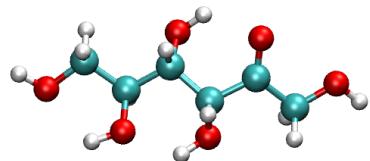


# Sugars Número 619

Molecule A R-S-R-Fructuose\_out\_G09



Molecule B R-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

203.246	14.6965	0.489268
14.6965	1215.65	-0.989769
0.489268	-0.989769	1332.21

Inertia Tensor - Molecule B

214.933	-13.9132	-6.26614
-13.9132	1186.84	0.567805
-6.26614	0.567805	1322.37

EingenVectors - Molecule A

-0.999895	0.0145123	0.000445973
-0.0145155	-0.999859	-0.00844446
0.000323361	-0.00845004	0.999964

EingenVectors - Molecule B

0.999882	0.0143069	0.00564903
0.0142795	-0.999886	0.00485623
-0.00571786	0.00477499	0.999972

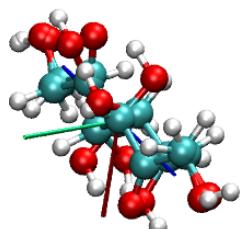
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

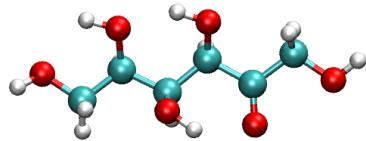
214.698	1187.04	1322.41
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Different

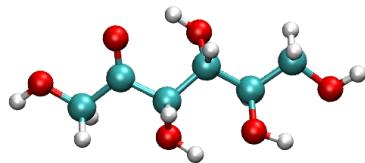


Sugars Número 620

Molecule A R-S-R-Fructuose\_out\_G09



Molecule B S-R-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

203.246	14.6965	0.489268
14.6965	1215.65	-0.989769
0.489268	-0.989769	1332.21

Inertia Tensor - Molecule B

214.974	13.9189	6.25845
13.9189	1186.65	0.565787
6.25845	0.565787	1322.09

EingenVectors - Molecule A

-0.999895	0.0145123	0.000445973
-0.0145155	-0.999859	-0.00844446
0.000323361	-0.00845004	0.999964

EingenVectors - Molecule B

-0.999882	0.0143163	0.00564373
0.014289	0.999886	-0.00484396
0.00571244	0.00476274	0.999972

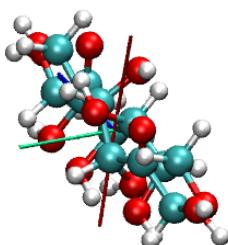
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

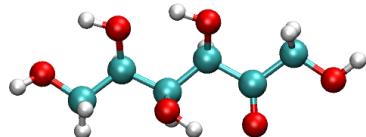
214.739	1186.84	1322.13
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Different

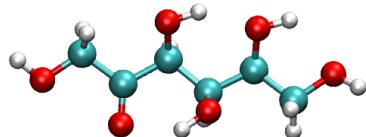


# Sugars Número 621

Molecule A R-S-R-Fructuose\_out\_G09



Molecule B S-R-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

203.246	14.6965	0.489268
14.6965	1215.65	-0.989769
0.489268	-0.989769	1332.21

Inertia Tensor - Molecule B

203.262	-14.7021	-0.492665
-14.7021	1215.64	-0.989546
-0.492665	-0.989546	1332.23

EingenVectors - Molecule A

-0.999895	0.0145123	0.000445973
-0.0145155	-0.999859	-0.00844446
0.000323361	-0.00845004	0.999964

EingenVectors - Molecule B

-0.999895	-0.0145182	-0.000448979
0.0145214	-0.999859	-0.00843991
-0.000326384	-0.00844554	0.999964

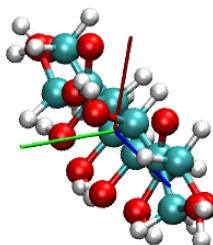
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

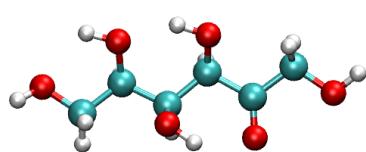
203.048	1215.85	1332.24
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Enantiomers

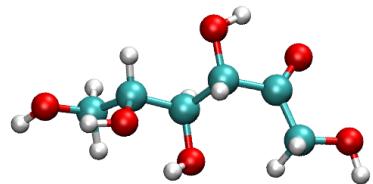


Sugars Número 622

Molecule A R-S-R-Fructuose\_out\_G09



Molecule B S-S-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

203.246	14.6965	0.489268
14.6965	1215.65	-0.989769
0.489268	-0.989769	1332.21

Inertia Tensor - Molecule B

257.995	-6.7346	10.0985
-6.7346	1154.74	-1.24098
10.0985	-1.24098	1276.66

EingenVectors - Molecule A

-0.999895	0.0145123	0.000445973
-0.0145155	-0.999859	-0.00844446
0.000323361	-0.00845004	0.999964

EingenVectors - Molecule B

0.999923	0.00749452	-0.00990206
0.00738758	-0.999914	-0.0107925
0.0099821	-0.0107185	0.999893

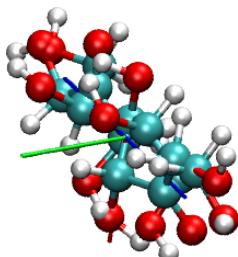
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

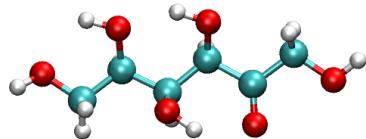
257.845	1154.78	1276.78
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Different

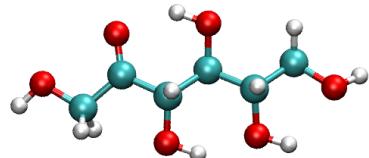


# Sugars Número 623

Molecule A R-S-R-Fructuose\_out\_G09



Molecule B S-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

203.246	14.6965	0.489268
14.6965	1215.65	-0.989769
0.489268	-0.989769	1332.21

Inertia Tensor - Molecule B

224.224	13.0406	-2.54457
13.0406	1180.14	-1.05607
-2.54457	-1.05607	1363.89

EingenVectors - Molecule A

-0.999895	0.0145123	0.000445973
-0.0145155	-0.999859	-0.00844446
0.000323361	-0.00845004	0.999964

EingenVectors - Molecule B

-0.999905	0.0136356	-0.00221952
0.0136222	0.99989	0.00594071
-0.00230028	-0.00590991	0.99998

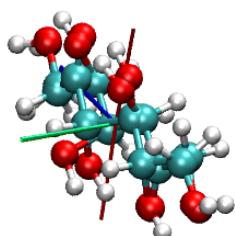
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

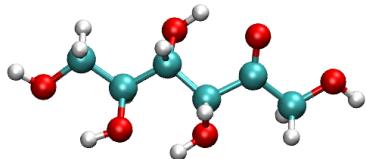
224.041	1180.31	1363.9
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Different



# Sugars Número 624

Molecule A R-S-S-Fructuose\_out\_G09



Molecule B S-R-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

214.933	-13.9132	-6.26614
-13.9132	1186.84	0.567805
-6.26614	0.567805	1322.37

Inertia Tensor - Molecule B

214.974	13.9189	6.25845
13.9189	1186.65	0.565787
6.25845	0.565787	1322.09

EingenVectors - Molecule A

0.999882	0.0143069	0.00564903
0.0142795	-0.999886	0.00485623
-0.00571786	0.00477499	0.999972

EingenVectors - Molecule B

-0.999882	0.0143163	0.00564373
0.014289	0.999886	-0.00484396
0.00571244	0.00476274	0.999972

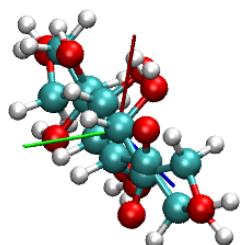
EingenValues - Molecule A

214.698	1187.04	1322.41
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EingenValues - Molecule B

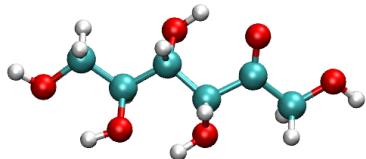
214.739	1186.84	1322.13
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Enantiomers

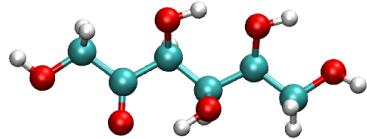


# Sugars Número 625

Molecule A R-S-S-Fructuose\_out\_G09



Molecule B S-R-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

214.933	-13.9132	-6.26614
-13.9132	1186.84	0.567805
-6.26614	0.567805	1322.37

Inertia Tensor - Molecule B

203.262	-14.7021	-0.492665
-14.7021	1215.64	-0.989546
-0.492665	-0.989546	1332.23

EingenVectors - Molecule A

0.999882	0.0143069	0.00564903
0.0142795	-0.999886	0.00485623
-0.00571786	0.00477499	0.999972

EingenVectors - Molecule B

-0.999895	-0.0145182	-0.000448979
0.0145214	-0.999859	-0.00843991
-0.000326384	-0.00844554	0.999964

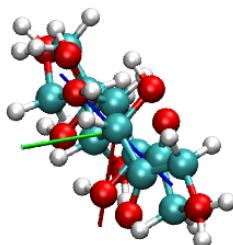
EingenValues - Molecule A

214.698	1187.04	1322.41
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EingenValues - Molecule B

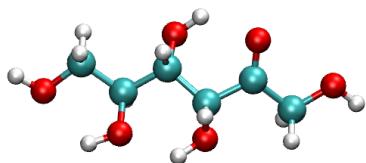
203.048	1215.85	1332.24
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Different

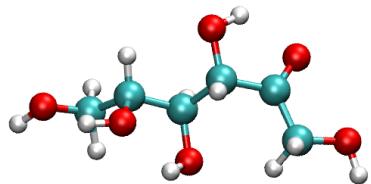


# Sugars Número 626

Molecule A R-S-S-Fructuose\_out\_G09



Molecule B S-S-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

214.933	-13.9132	-6.26614
-13.9132	1186.84	0.567805
-6.26614	0.567805	1322.37

Inertia Tensor - Molecule B

257.995	-6.7346	10.0985
-6.7346	1154.74	-1.24098
10.0985	-1.24098	1276.66

EingenVectors - Molecule A

0.999882	0.0143069	0.00564903
0.0142795	-0.999886	0.00485623
-0.00571786	0.00477499	0.999972

EingenVectors - Molecule B

0.999923	0.00749452	-0.00990206
0.00738758	-0.999914	-0.0107925
0.0099821	-0.0107185	0.999893

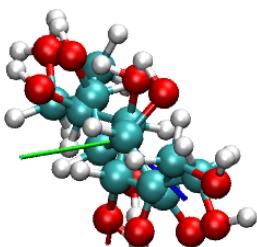
EingenValues - Molecule A

214.698	1187.04	1322.41
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EingenValues - Molecule B

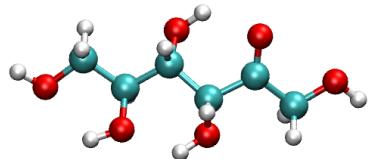
257.845	1154.78	1276.78
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Different

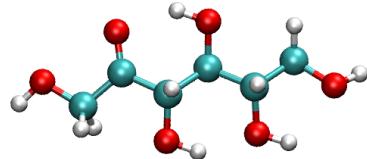


Sugars Número 627

Molecule A R-S-S-Fructuose\_out\_G09



Molecule B S-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

214.933	-13.9132	-6.26614
-13.9132	1186.84	0.567805
-6.26614	0.567805	1322.37

Inertia Tensor - Molecule B

224.224	13.0406	-2.54457
13.0406	1180.14	-1.05607
-2.54457	-1.05607	1363.89

EingenVectors - Molecule A

0.999882	0.0143069	0.00564903
0.0142795	-0.999886	0.00485623
-0.00571786	0.00477499	0.999972

EingenVectors - Molecule B

-0.999905	0.0136356	-0.00221952
0.0136222	0.99989	0.00594071
-0.00230028	-0.00590991	0.99998

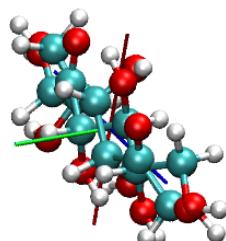
EingenValues - Molecule A

214.698	1187.04	1322.41
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EingenValues - Molecule B

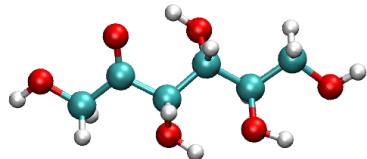
224.041	1180.31	1363.9
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Different

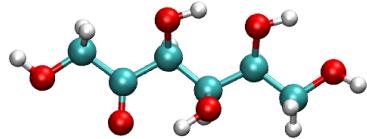


Sugars Número 628

Molecule A S-R-R-Fructuose\_out\_G09



Molecule B S-R-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

214.974	13.9189	6.25845
13.9189	1186.65	0.565787
6.25845	0.565787	1322.09

Inertia Tensor - Molecule B

203.262	-14.7021	-0.492665
-14.7021	1215.64	-0.989546
-0.492665	-0.989546	1332.23

EingenVectors - Molecule A

-0.999882	0.0143163	0.00564373
0.014289	0.999886	-0.00484396
0.00571244	0.00476274	0.999972

EingenVectors - Molecule B

-0.999895	-0.0145182	-0.000448979
0.0145214	-0.999859	-0.00843991
-0.000326384	-0.00844554	0.999964

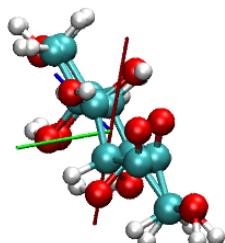
EingenValues - Molecule A

214.739	1186.84	1322.13
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EingenValues - Molecule B

203.048	1215.85	1332.24
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Different

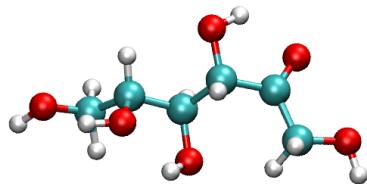


Sugars Número 629

Molecule A S-R-R-Fructuose\_out\_G09



Molecule B S-S-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

214.974	13.9189	6.25845
13.9189	1186.65	0.565787
6.25845	0.565787	1322.09

Inertia Tensor - Molecule B

257.995	-6.7346	10.0985
-6.7346	1154.74	-1.24098
10.0985	-1.24098	1276.66

EingenVectors - Molecule A

-0.999882	0.0143163	0.00564373
0.014289	0.999886	-0.00484396
0.00571244	0.00476274	0.999972

EingenVectors - Molecule B

0.999923	0.00749452	-0.00990206
0.00738758	-0.999914	-0.0107925
0.0099821	-0.0107185	0.999893

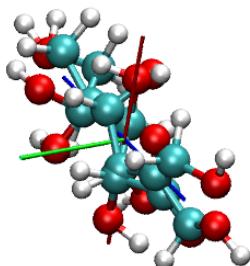
EingenValues - Molecule A

214.739	1186.84	1322.13
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EingenValues - Molecule B

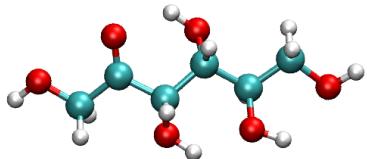
257.845	1154.78	1276.78
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Different

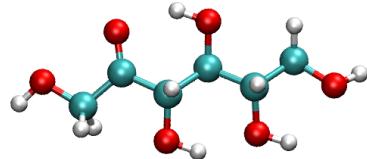


# Sugars Número 630

Molecule A S-R-R-Fructuose\_out\_G09



Molecule B S-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

214.974	13.9189	6.25845
13.9189	1186.65	0.565787
6.25845	0.565787	1322.09

Inertia Tensor - Molecule B

224.224	13.0406	-2.54457
13.0406	1180.14	-1.05607
-2.54457	-1.05607	1363.89

EingenVectors - Molecule A

-0.999882	0.0143163	0.00564373
0.014289	0.999886	-0.00484396
0.00571244	0.00476274	0.999972

EingenVectors - Molecule B

-0.999905	0.0136356	-0.00221952
0.0136222	0.99989	0.00594071
-0.00230028	-0.00590991	0.99998

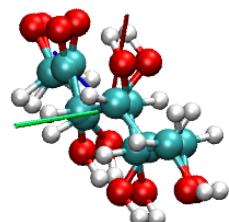
EingenValues - Molecule A

214.739	1186.84	1322.13
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EingenValues - Molecule B

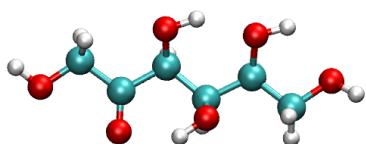
224.041	1180.31	1363.9
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Different

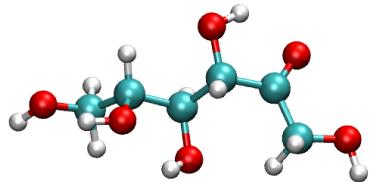


Sugars Número 631

Molecule A S-R-S-Fructuose\_out\_G09



Molecule B S-S-R-Fructuose\_out\_G09



Inertia Tensor - Molecule A

203.262	-14.7021	-0.492665
-14.7021	1215.64	-0.989546
-0.492665	-0.989546	1332.23

Inertia Tensor - Molecule B

257.995	-6.7346	10.0985
-6.7346	1154.74	-1.24098
10.0985	-1.24098	1276.66

EingenVectors - Molecule A

-0.999895	-0.0145182	-0.000448979
0.0145214	-0.999859	-0.00843991
-0.000326384	-0.00844554	0.999964

EingenVectors - Molecule B

0.999923	0.00749452	-0.00990206
0.00738758	-0.999914	-0.0107925
0.0099821	-0.0107185	0.999893

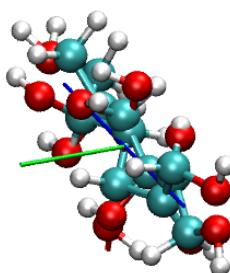
EingenValues - Molecule A

203.048	1215.85	1332.24
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EingenValues - Molecule B

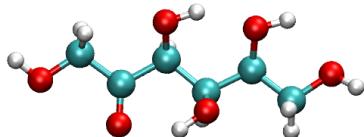
257.845	1154.78	1276.78
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Different

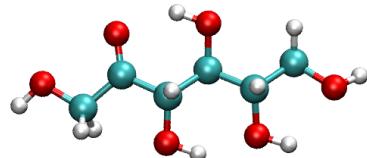


# Sugars Número 632

Molecule A S-R-S-Fructuose\_out\_G09



Molecule B S-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

203.262	-14.7021	-0.492665
-14.7021	1215.64	-0.989546
-0.492665	-0.989546	1332.23

Inertia Tensor - Molecule B

224.224	13.0406	-2.54457
13.0406	1180.14	-1.05607
-2.54457	-1.05607	1363.89

EingenVectors - Molecule A

-0.999895	-0.0145182	-0.000448979
0.0145214	-0.999859	-0.00843991
-0.000326384	-0.00844554	0.999964

EingenVectors - Molecule B

-0.999905	0.0136356	-0.00221952
0.0136222	0.99989	0.00594071
-0.00230028	-0.00590991	0.99998

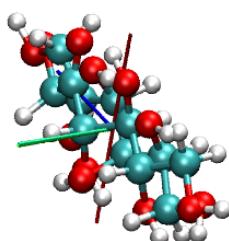
EingenValues - Molecule A

203.048	1215.85	1332.24
---------	---------	---------

EingenValues - Molecule B

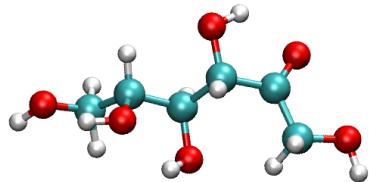
224.041	1180.31	1363.9
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Different

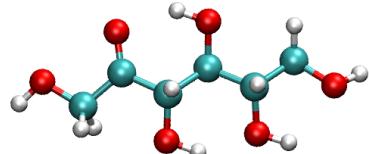


# Sugars Número 633

Molecule A S-S-R-Fructuose\_out\_G09



Molecule B S-S-S-Fructuose\_out\_G09



Inertia Tensor - Molecule A

257.995	-6.7346	10.0985
-6.7346	1154.74	-1.24098
10.0985	-1.24098	1276.66

Inertia Tensor - Molecule B

224.224	13.0406	-2.54457
13.0406	1180.14	-1.05607
-2.54457	-1.05607	1363.89

EingenVectors - Molecule A

0.999923	0.00749452	-0.00990206
0.00738758	-0.999914	-0.0107925
0.0099821	-0.0107185	0.999893

EingenVectors - Molecule B

-0.999905	0.0136356	-0.00221952
0.0136222	0.99989	0.00594071
-0.00230028	-0.00590991	0.99998

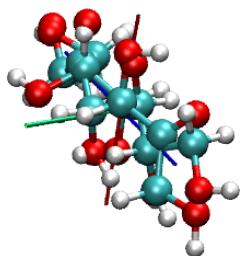
EingenValues - Molecule A

257.845	1154.78	1276.78
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EingenValues - Molecule B

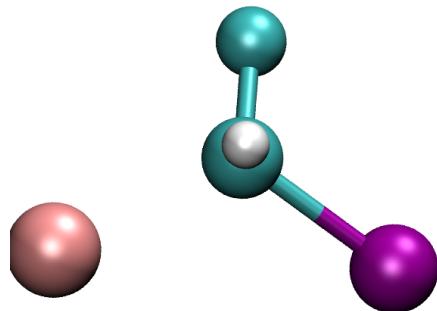
224.041	1180.31	1363.9
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Different



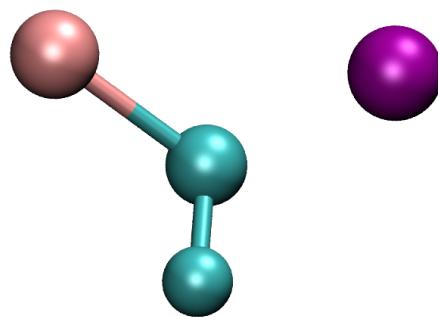
# SymmetricEnantiomers Número 634

Molecule A r-enan\_out\_G09



Molecule B

r-enan\_out\_G09\_inversion\_output



Inertia Tensor - Molecule A

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

Inertia Tensor - Molecule B

103.745	1.51041	1.05457
1.51041	629.841	1.67376
1.05457	1.67376	722.187

EingenVectors - Molecule A

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

EingenVectors - Molecule B

-0.999994	0.00286553	0.00169742
-0.00283425	-0.999831	0.018149
0.00174914	0.0181441	0.999834

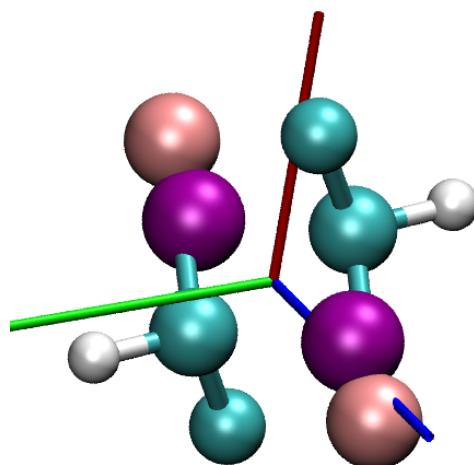
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

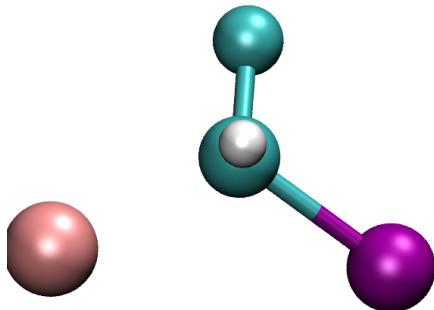
103.739	629.815	722.22
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Enantiomers

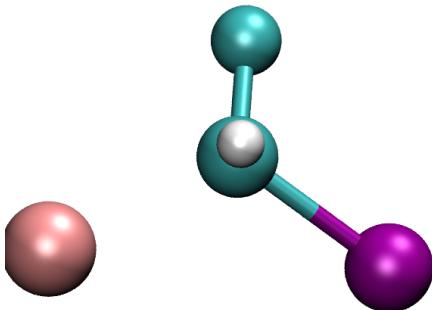


SymmetricEnantiomers Número 635

Molecule A r-enan\_out\_G09



Molecule B r-enan\_rotated\_out\_G09



Inertia Tensor - Molecule A

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

Inertia Tensor - Molecule B

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

EingenVectors - Molecule A

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

EingenVectors - Molecule B

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

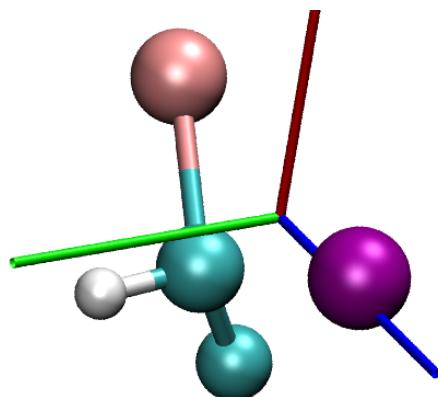
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

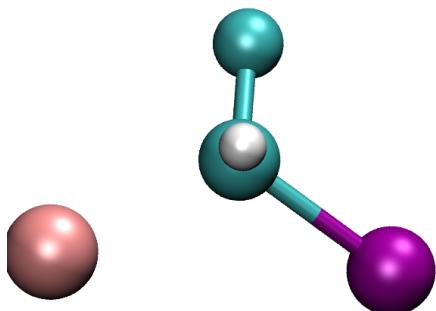
103.739	629.816	722.221
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Equal

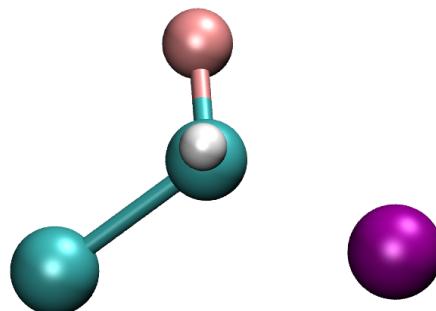


# SymmetricEnantiomers Número 636

Molecule A r-enan\_out\_G09



Molecule B s-enan\_out\_G09



Inertia Tensor - Molecule A

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

Inertia Tensor - Molecule B

103.707	-1.51142	-1.05403
-1.51142	630.103	1.67204
-1.05403	1.67204	722.42

EingenVectors - Molecule A

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

EingenVectors - Molecule B

-0.999994	-0.00286582	-0.00169581
0.0028346	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

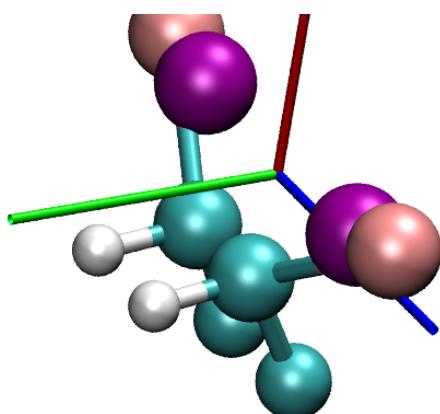
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

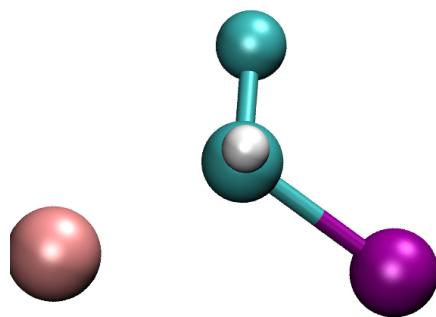
103.701	630.077	722.452
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Enantiomers



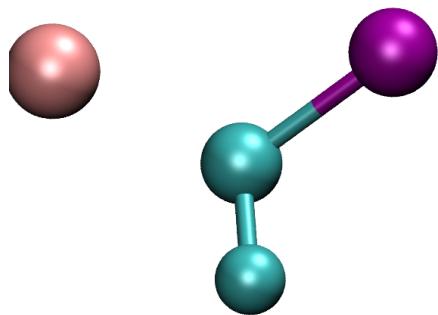
SymmetricEnantiomers Número 637

Molecule A r-enan\_out\_G09



Molecule B

s-enan\_out\_G09\_inversion\_output



Inertia Tensor - Molecule A

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

Inertia Tensor - Molecule B

103.707	-1.51147	-1.05403
-1.51147	630.105	1.67201
-1.05403	1.67201	722.422

EingenVectors - Molecule A

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

EingenVectors - Molecule B

-0.999994	-0.0028659	-0.0016958
0.00283468	-0.999832	0.0181359
-0.00174749	0.018131	0.999834

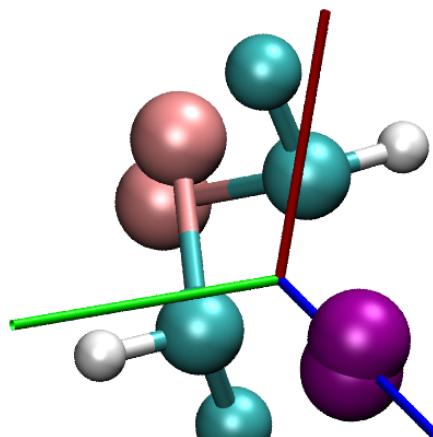
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

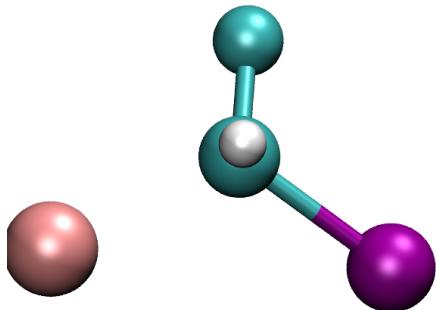
103.7	630.079	722.455
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Equal

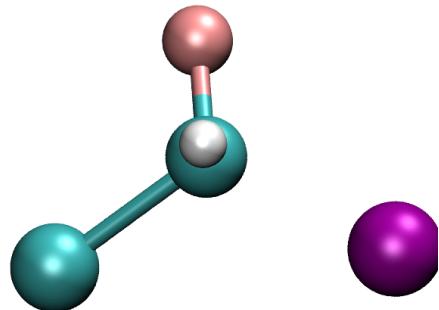


# SymmetricEnantiomers Número 638

Molecule A r-enan\_out\_G09



Molecule B s-enan\_rotated\_out\_G09



Inertia Tensor - Molecule A

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

Inertia Tensor - Molecule B

103.707	-1.51138	-1.05403
-1.51138	630.103	1.67204
-1.05403	1.67204	722.42

EingenVectors - Molecule A

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

EingenVectors - Molecule B

-0.999994	-0.00286575	-0.00169582
0.00283453	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

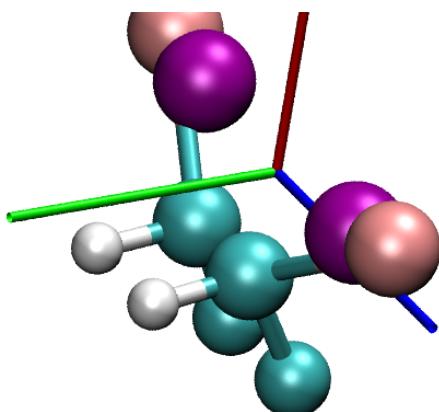
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

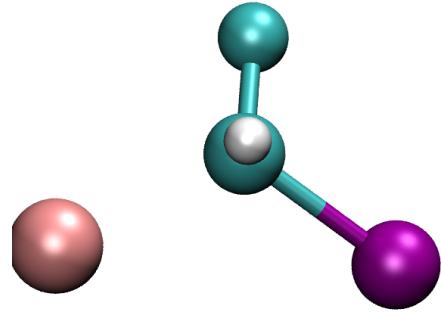
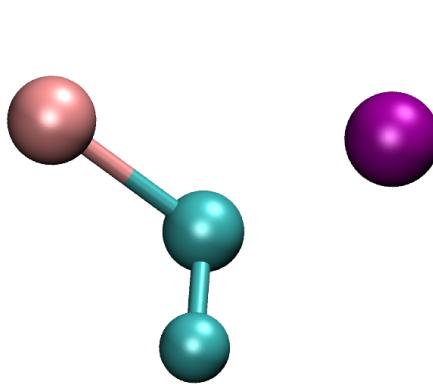
103.701	630.077	722.452
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Enantiomers



SymmetricEnantiomers Número 639

Molecule A Molecule B r-enan\_rotated\_out\_G09  
r-enan\_out\_G09\_inversion\_output



Inertia Tensor - Molecule A

103.745	1.51041	1.05457
1.51041	629.841	1.67376
1.05457	1.67376	722.187

Inertia Tensor - Molecule B

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

EingenVectors - Molecule A

-0.999994	0.00286553	0.00169742
-0.00283425	-0.999831	0.018149
0.00174914	0.0181441	0.999834

EingenVectors - Molecule B

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

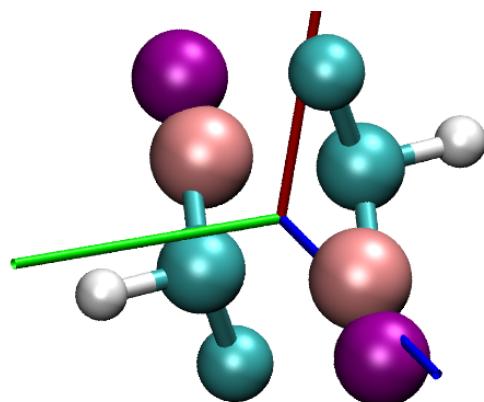
EingenValues - Molecule A

103.739	629.815	722.22
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EingenValues - Molecule B

103.739	629.816	722.221
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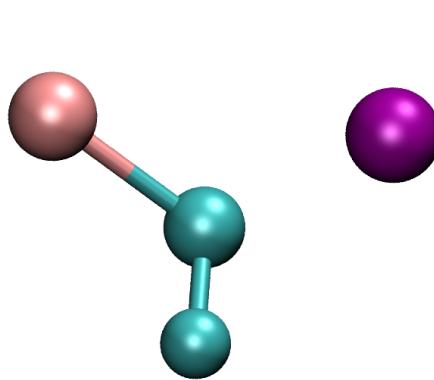
Enantiomers



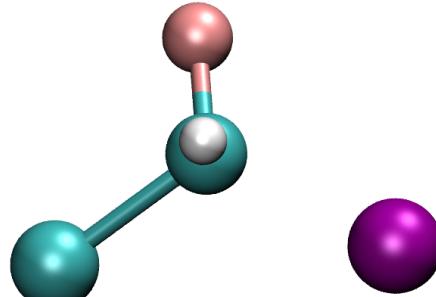
SymmetricEnantiomers Número 640

Molecule A

r-enan\_out\_G09\_inversion\_output



Molecule B s-enan\_out\_G09



Inertia Tensor - Molecule A

103.745	1.51041	1.05457
1.51041	629.841	1.67376
1.05457	1.67376	722.187

Inertia Tensor - Molecule B

103.707	-1.51142	-1.05403
-1.51142	630.103	1.67204
-1.05403	1.67204	722.42

EingenVectors - Molecule A

-0.999994	0.00286553	0.00169742
-0.00283425	-0.999831	0.018149
0.00174914	0.0181441	0.999834

EingenVectors - Molecule B

-0.999994	-0.00286582	-0.00169581
0.0028346	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

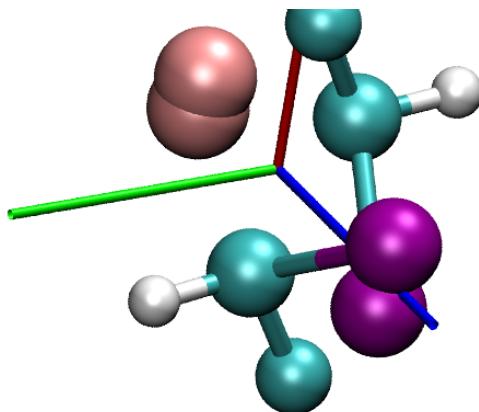
EingenValues - Molecule A

103.739	629.815	722.22
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EingenValues - Molecule B

103.701	630.077	722.452
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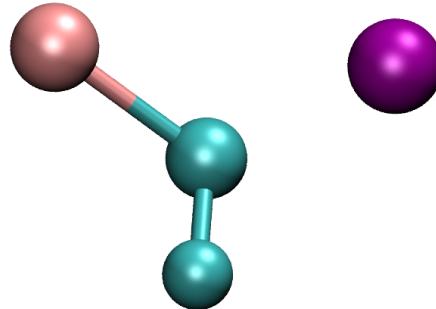
Equal



SymmetricEnantiomers Número 641

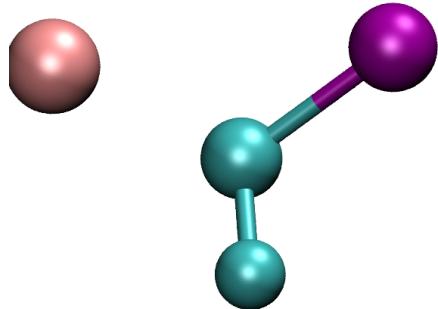
Molecule A

r-enan\_out\_G09\_inversion\_output



Molecule B

s-enan\_out\_G09\_inversion\_output



Inertia Tensor - Molecule A

103.745	1.51041	1.05457
1.51041	629.841	1.67376
1.05457	1.67376	722.187

Inertia Tensor - Molecule B

103.707	-1.51147	-1.05403
-1.51147	630.105	1.67201
-1.05403	1.67201	722.422

EingenVectors - Molecule A

-0.999994	0.00286553	0.00169742
-0.00283425	-0.999831	0.018149
0.00174914	0.0181441	0.999834

EingenVectors - Molecule B

-0.999994	-0.0028659	-0.0016958
0.00283468	-0.999832	0.0181359
-0.00174749	0.018131	0.999834

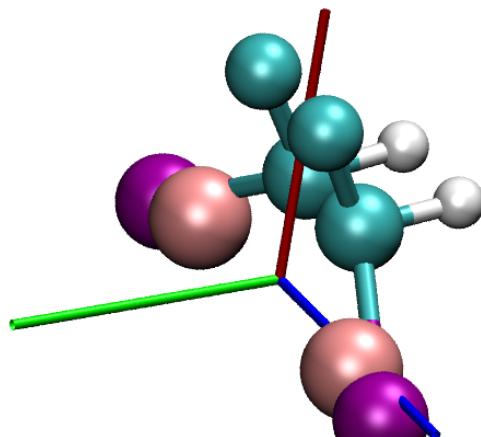
EingenValues - Molecule A

103.739	629.815	722.22
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EingenValues - Molecule B

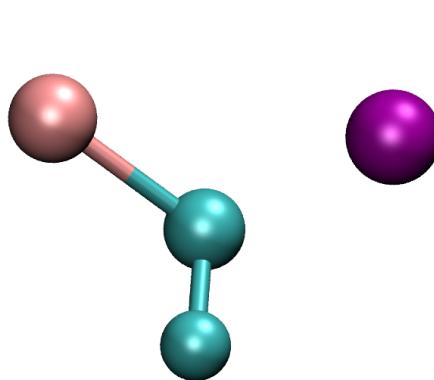
103.7	630.079	722.455
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Enantiomers

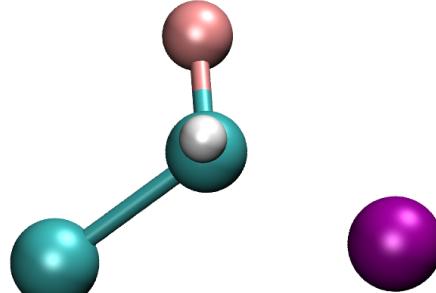


SymmetricEnantiomers Número 642

Molecule A  
r-enan\_out\_G09\_inversion\_output



Molecule B s-enan\_rotated\_out\_G09



Inertia Tensor - Molecule A

103.745	1.51041	1.05457
1.51041	629.841	1.67376
1.05457	1.67376	722.187

Inertia Tensor - Molecule B

103.707	-1.51138	-1.05403
-1.51138	630.103	1.67204
-1.05403	1.67204	722.42

EingenVectors - Molecule A

-0.999994	0.00286553	0.00169742
-0.00283425	-0.999831	0.018149
0.00174914	0.0181441	0.999834

EingenVectors - Molecule B

-0.999994	-0.00286575	-0.00169582
0.00283453	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

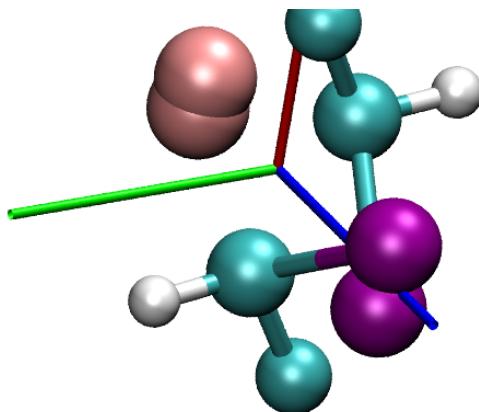
EingenValues - Molecule A

103.739	629.815	722.22
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EingenValues - Molecule B

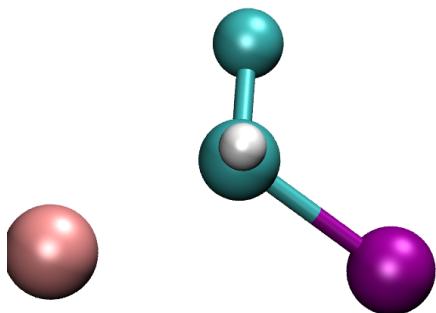
103.701	630.077	722.452
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Equal

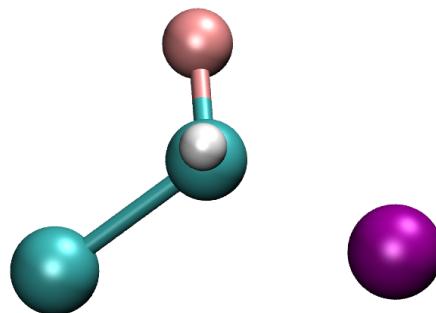


SymmetricEnantiomers Número 643

Molecule A r-enan\_rotated\_out\_G09



Molecule B s-enan\_out\_G09



Inertia Tensor - Molecule A

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

Inertia Tensor - Molecule B

103.707	-1.51142	-1.05403
-1.51142	630.103	1.67204
-1.05403	1.67204	722.42

EingenVectors - Molecule A

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

EingenVectors - Molecule B

-0.999994	-0.00286582	-0.00169581
0.0028346	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

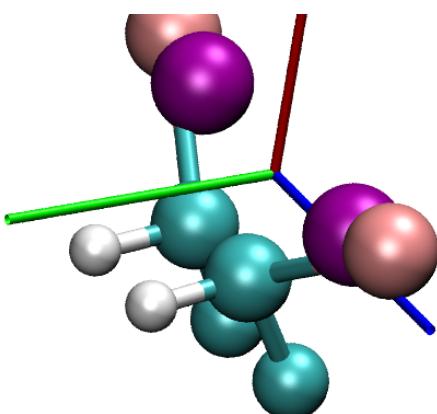
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

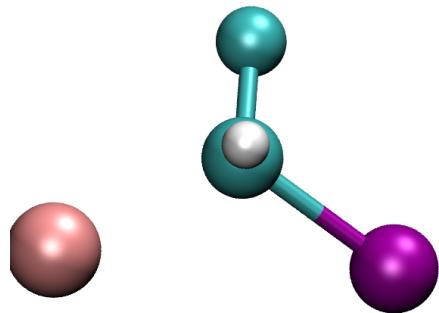
103.701	630.077	722.452
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Enantiomers



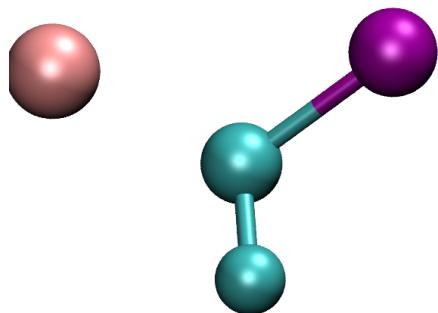
SymmetricEnantiomers Número 644

Molecule A r-enan\_rotated\_out\_G09



Molecule B

s-enan\_out\_G09\_inversion\_output



Inertia Tensor - Molecule A

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

Inertia Tensor - Molecule B

103.707	-1.51147	-1.05403
-1.51147	630.105	1.67201
-1.05403	1.67201	722.422

EingenVectors - Molecule A

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

EingenVectors - Molecule B

-0.999994	-0.0028659	-0.0016958
0.00283468	-0.999832	0.0181359
-0.00174749	0.018131	0.999834

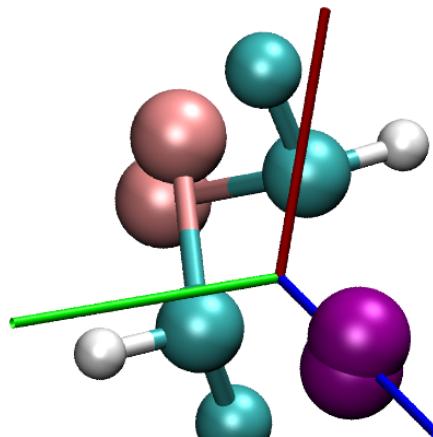
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

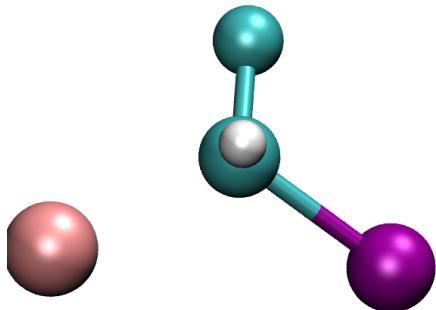
103.7	630.079	722.455
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Equal

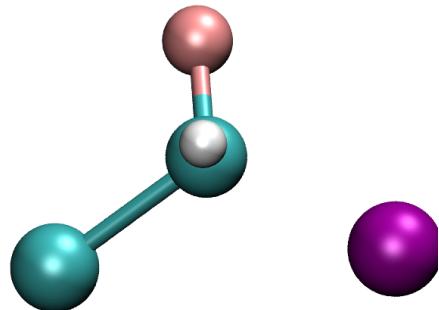


SymmetricEnantiomers Número 645

Molecule A r-enan\_rotated\_out\_G09



Molecule B s-enan\_rotated\_out\_G09



Inertia Tensor - Molecule A

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

Inertia Tensor - Molecule B

103.707	-1.51138	-1.05403
-1.51138	630.103	1.67204
-1.05403	1.67204	722.42

EingenVectors - Molecule A

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

EingenVectors - Molecule B

-0.999994	-0.00286575	-0.00169582
0.00283453	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

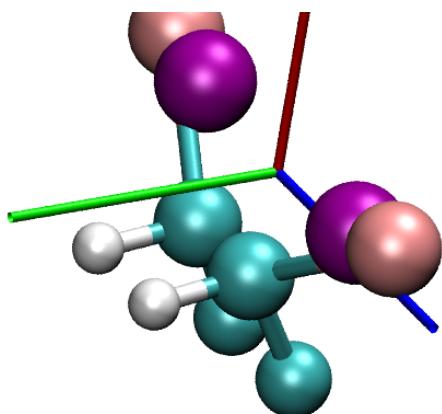
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

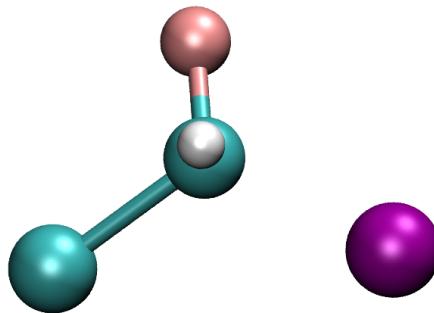
103.701	630.077	722.452
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Enantiomers



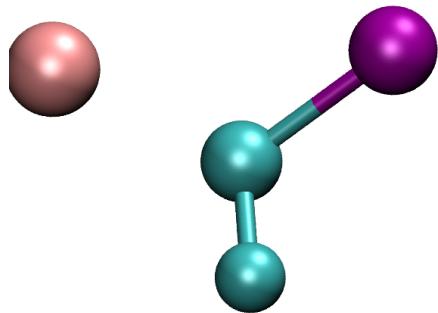
SymmetricEnantiomers Número 646

Molecule A s-enan\_out\_G09



Molecule B

s-enan\_out\_G09\_inversion\_output



Inertia Tensor - Molecule A

103.707	-1.51142	-1.05403
-1.51142	630.103	1.67204
-1.05403	1.67204	722.42

Inertia Tensor - Molecule B

103.707	-1.51147	-1.05403
-1.51147	630.105	1.67201
-1.05403	1.67201	722.422

EingenVectors - Molecule A

-0.999994	-0.00286582	-0.00169581
0.0028346	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

EingenVectors - Molecule B

-0.999994	-0.0028659	-0.0016958
0.00283468	-0.999832	0.0181359
-0.00174749	0.018131	0.999834

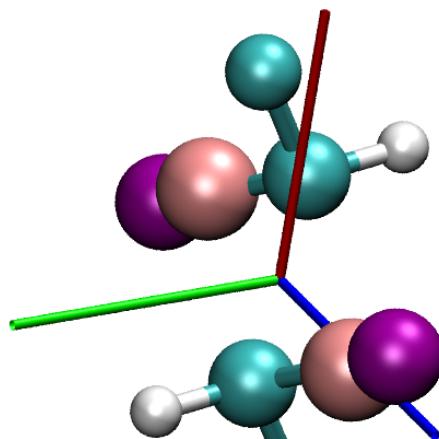
EingenValues - Molecule A

103.701	630.077	722.452
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EingenValues - Molecule B

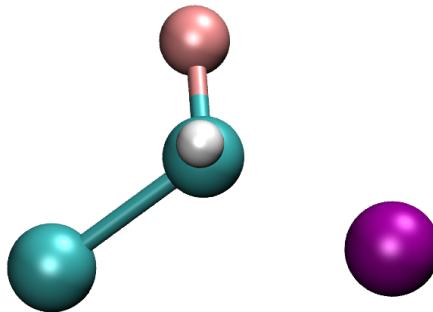
103.7	630.079	722.455
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Enantiomers

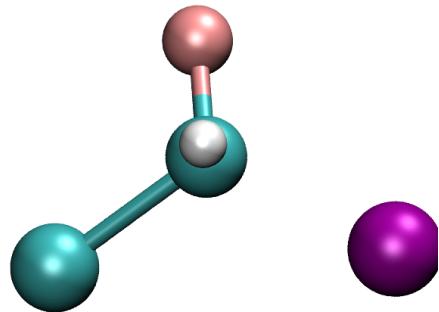


SymmetricEnantiomers Número 647

Molecule A s-enan\_out\_G09



Molecule B s-enan\_rotated\_out\_G09



Inertia Tensor - Molecule A

103.707	-1.51142	-1.05403
-1.51142	630.103	1.67204
-1.05403	1.67204	722.42

Inertia Tensor - Molecule B

103.707	-1.51138	-1.05403
-1.51138	630.103	1.67204
-1.05403	1.67204	722.42

EingenVectors - Molecule A

-0.999994	-0.00286582	-0.00169581
0.0028346	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

EingenVectors - Molecule B

-0.999994	-0.00286575	-0.00169582
0.00283453	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

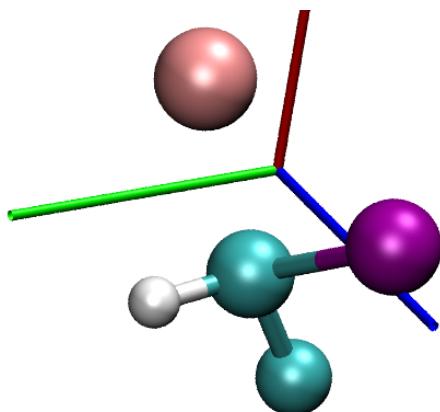
EingenValues - Molecule A

103.701	630.077	722.452
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EingenValues - Molecule B

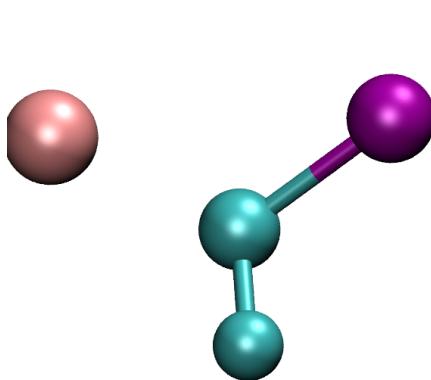
103.701	630.077	722.452
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Equal

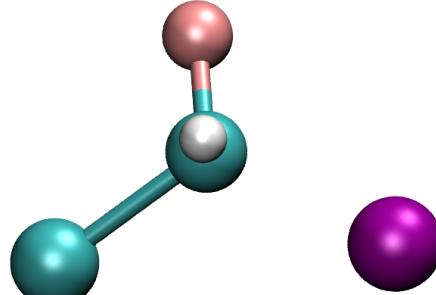


SymmetricEnantiomers Número 648

Molecule A  
s-enan\_out\_G09\_inversion\_output



Molecule B s-enan\_rotated\_out\_G09



Inertia Tensor - Molecule A

103.707	-1.51147	-1.05403
-1.51147	630.105	1.67201
-1.05403	1.67201	722.422

Inertia Tensor - Molecule B

103.707	-1.51138	-1.05403
-1.51138	630.103	1.67204
-1.05403	1.67204	722.42

EingenVectors - Molecule A

-0.999994	-0.0028659	-0.0016958
0.00283468	-0.999832	0.0181359
-0.00174749	0.018131	0.999834

EingenVectors - Molecule B

-0.999994	-0.00286575	-0.00169582
0.00283453	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

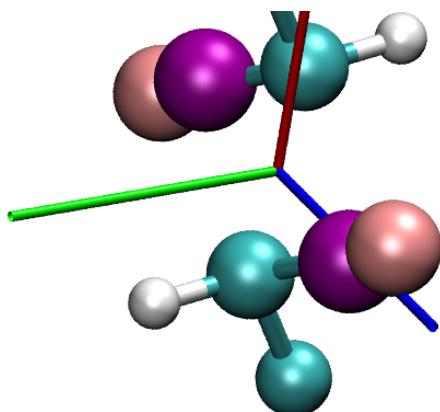
EingenValues - Molecule A

103.7	630.079	722.455
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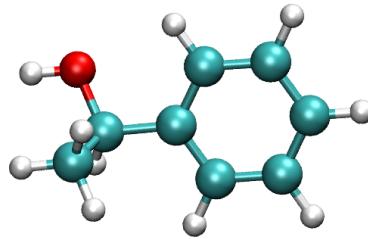
EingenValues - Molecule B

103.701	630.077	722.452
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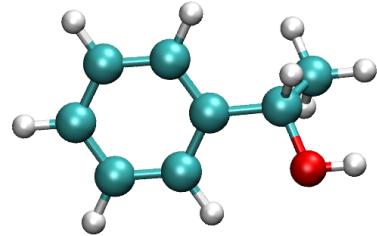
Enantiomers



Molecule A test-R\_out\_G09



Molecule B test-R\_out\_G09\_inversion



Inertia Tensor - Molecule A

146.29	5.10986	-3.31731
5.10986	442.839	1.31633
-3.31731	1.31633	530.688

Inertia Tensor - Molecule B

146.29	5.10969	-3.31735
5.10969	442.839	1.31631
-3.31735	1.31631	530.688

EingenVectors - Molecule A

0.999813	-0.0172596	0.00868475
-0.017383	-0.999746	0.0143352
-0.00843513	0.0144835	0.99986

EingenVectors - Molecule B

0.999813	-0.017259	0.00868483
-0.0173824	-0.999746	0.014335
-0.00843522	0.0144833	0.99986

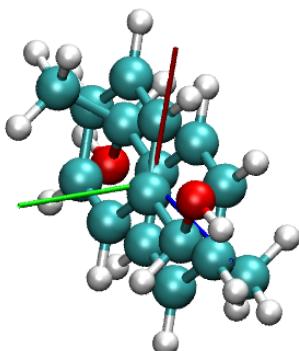
EingenValues - Molecule A

146.173	442.909	530.735
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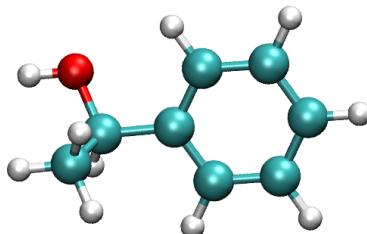
EingenValues - Molecule B

146.173	442.909	530.735
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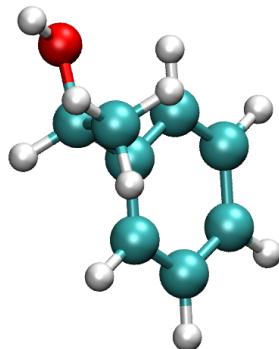
Enantiomers



Molecule A test-R\_out\_G09



Molecule B test-R\_out\_G09\_rot-45-45-45



Inertia Tensor - Molecule A

146.29	5.10986	-3.31731
5.10986	442.839	1.31633
-3.31731	1.31633	530.688

Inertia Tensor - Molecule B

430.951	89.0849	141.239
89.0849	367.04	-98.5816
141.239	-98.5816	321.828

EingenVectors - Molecule A

0.999813	-0.0172596	0.00868475
-0.017383	-0.999746	0.0143352
-0.00843513	0.0144835	0.99986

EingenVectors - Molecule B

0.504792	-0.513366	-0.694003
0.142865	0.842546	-0.519332
-0.851337	-0.163006	-0.498652

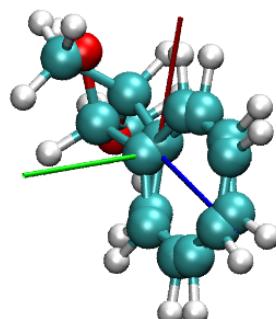
EingenValues - Molecule A

146.173	442.909	530.735
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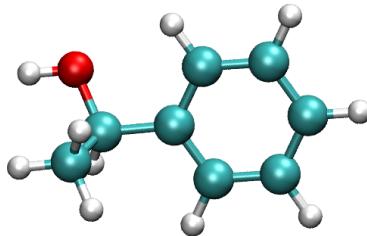
EingenValues - Molecule B

146.173	442.909	530.735
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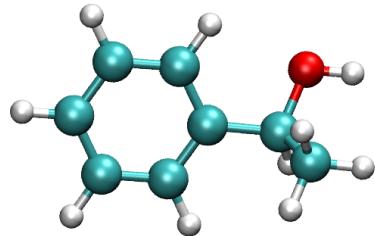
Equal



Molecule A test-R\_out\_G09



Molecule B test-S\_out\_G09



Inertia Tensor - Molecule A

146.29	5.10986	-3.31731
5.10986	442.839	1.31633
-3.31731	1.31633	530.688

Inertia Tensor - Molecule B

146.29	-5.10986	3.31731
-5.10986	442.839	1.31633
3.31731	1.31633	530.688

EingenVectors - Molecule A

0.999813	-0.0172596	0.00868475
-0.017383	-0.999746	0.0143352
-0.00843513	0.0144835	0.99986

EingenVectors - Molecule B

-0.999813	-0.0172596	0.00868475
-0.017383	0.999746	-0.0143352
0.00843513	0.0144835	0.99986

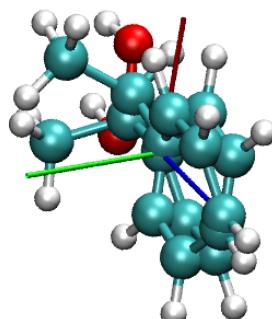
EingenValues - Molecule A

146.173	442.909	530.735
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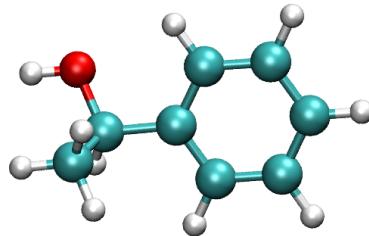
EingenValues - Molecule B

146.173	442.909	530.735
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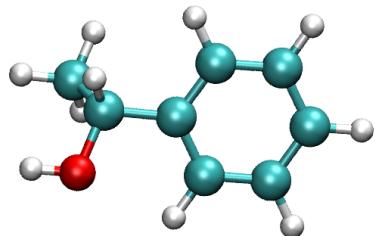
Enantiomers



Molecule A test-R\_out\_G09



Molecule B test-S\_out\_G09\_inversion



Inertia Tensor - Molecule A

146.29	5.10986	-3.31731
5.10986	442.839	1.31633
-3.31731	1.31633	530.688

Inertia Tensor - Molecule B

146.29	-5.10969	3.31735
-5.10969	442.839	1.31631
3.31735	1.31631	530.688

EingenVectors - Molecule A

0.999813	-0.0172596	0.00868475
-0.017383	-0.999746	0.0143352
-0.00843513	0.0144835	0.99986

EingenVectors - Molecule B

-0.999813	-0.017259	0.00868483
-0.0173824	0.999746	-0.014335
0.00843522	0.0144833	0.99986

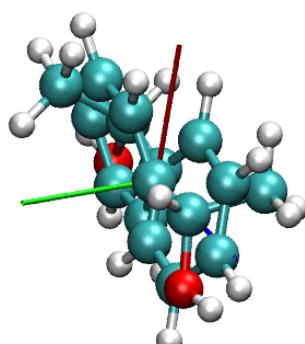
EingenValues - Molecule A

146.173	442.909	530.735
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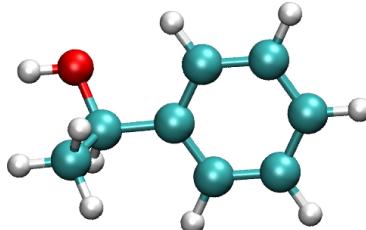
EingenValues - Molecule B

146.173	442.909	530.735
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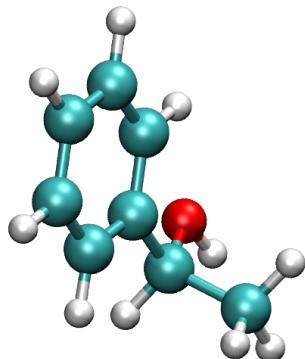
Equal



Molecule A test-R\_out\_G09



Molecule B test-S\_out\_G09\_rot-45-45-45



Inertia Tensor - Molecule A

146.29	5.10986	-3.31731
5.10986	442.839	1.31633
-3.31731	1.31633	530.688

Inertia Tensor - Molecule B

435.116	83.1261	142.506
83.1261	374.791	-97.314
142.506	-97.314	309.91

EingenVectors - Molecule A

0.999813	-0.0172596	0.00868475
-0.017383	-0.999746	0.0143352
-0.00843513	0.0144835	0.99986

EingenVectors - Molecule B

0.495022	-0.486446	-0.719947
0.125483	0.859929	-0.494748
-0.859771	-0.15457	-0.486725

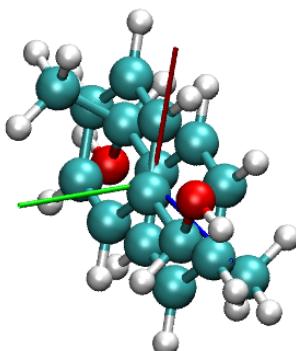
EingenValues - Molecule A

146.173	442.909	530.735
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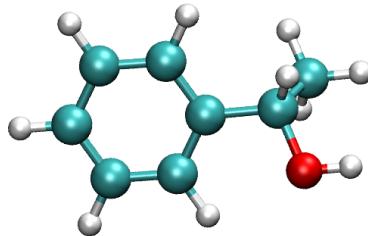
EingenValues - Molecule B

146.173	442.909	530.735
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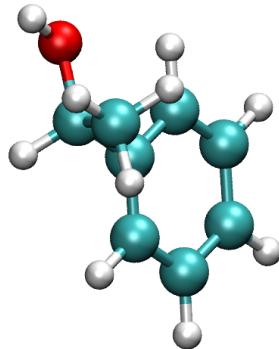
Enantiomers



Molecule A test-R\_out\_G09\_inversion



Molecule B test-R\_out\_G09\_rot-45-45-45



Inertia Tensor - Molecule A

146.29	5.10969	-3.31735
5.10969	442.839	1.31631
-3.31735	1.31631	530.688

Inertia Tensor - Molecule B

430.951	89.0849	141.239
89.0849	367.04	-98.5816
141.239	-98.5816	321.828

EingenVectors - Molecule A

0.999813	-0.017259	0.00868483
-0.0173824	-0.999746	0.014335
-0.00843522	0.0144833	0.99986

EingenVectors - Molecule B

0.504792	-0.513366	-0.694003
0.142865	0.842546	-0.519332
-0.851337	-0.163006	-0.498652

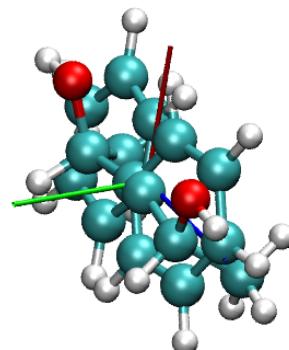
EingenValues - Molecule A

146.173	442.909	530.735
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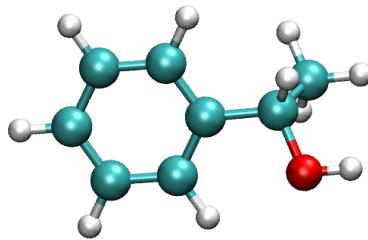
EingenValues - Molecule B

146.173	442.909	530.735
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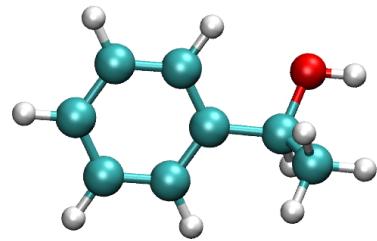
Enantiomers



Molecule A test-R\_out\_G09\_inversion



Molecule B test-S\_out\_G09



Inertia Tensor - Molecule A

146.29	5.10969	-3.31735
5.10969	442.839	1.31631
-3.31735	1.31631	530.688

Inertia Tensor - Molecule B

146.29	-5.10986	3.31731
-5.10986	442.839	1.31633
3.31731	1.31633	530.688

EingenVectors - Molecule A

0.999813	-0.017259	0.00868483
-0.0173824	-0.999746	0.014335
-0.00843522	0.0144833	0.99986

EingenVectors - Molecule B

-0.999813	-0.0172596	0.00868475
-0.017383	0.999746	-0.0143352
0.00843513	0.0144835	0.99986

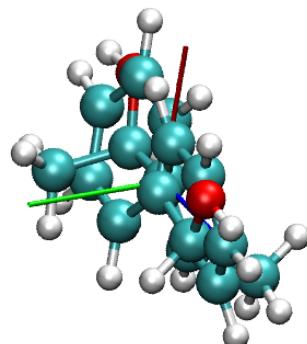
EingenValues - Molecule A

146.173	442.909	530.735
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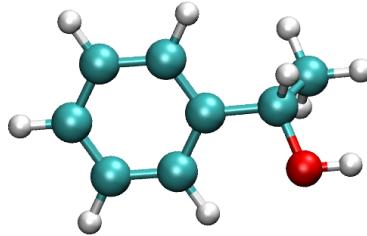
EingenValues - Molecule B

146.173	442.909	530.735
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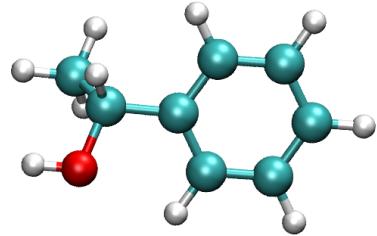
Equal



Molecule A test-R.out\_G09\_inversion



Molecule B test-S.out\_G09\_inversion



Inertia Tensor - Molecule A

146.29	5.10969	-3.31735
5.10969	442.839	1.31631
-3.31735	1.31631	530.688

Inertia Tensor - Molecule B

146.29	-5.10969	3.31735
-5.10969	442.839	1.31631
3.31735	1.31631	530.688

EingenVectors - Molecule A

0.999813	-0.017259	0.00868483
-0.0173824	-0.999746	0.014335
-0.00843522	0.0144833	0.99986

EingenVectors - Molecule B

-0.999813	-0.017259	0.00868483
-0.0173824	0.999746	-0.014335
0.00843522	0.0144833	0.99986

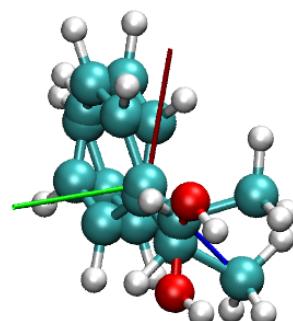
EingenValues - Molecule A

146.173	442.909	530.735
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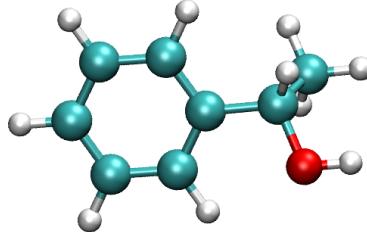
EingenValues - Molecule B

146.173	442.909	530.735
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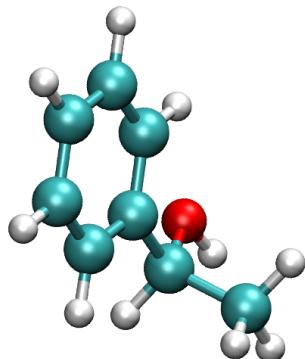
Enantiomers



Molecule A test-R\_out\_G09\_inversion



Molecule B test-S\_out\_G09\_rot-45-45-45



Inertia Tensor - Molecule A

146.29	5.10969	-3.31735
5.10969	442.839	1.31631
-3.31735	1.31631	530.688

Inertia Tensor - Molecule B

435.116	83.1261	142.506
83.1261	374.791	-97.314
142.506	-97.314	309.91

EingenVectors - Molecule A

0.999813	-0.017259	0.00868483
-0.0173824	-0.999746	0.014335
-0.00843522	0.0144833	0.99986

EingenVectors - Molecule B

0.495022	-0.486446	-0.719947
0.125483	0.859929	-0.494748
-0.859771	-0.15457	-0.486725

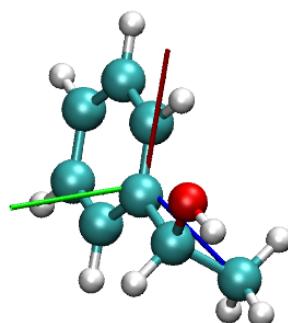
EingenValues - Molecule A

146.173	442.909	530.735
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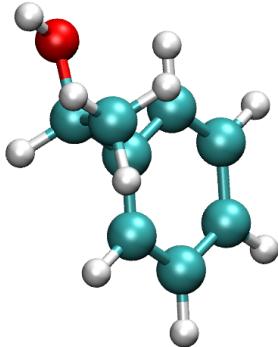
EingenValues - Molecule B

146.173	442.909	530.735
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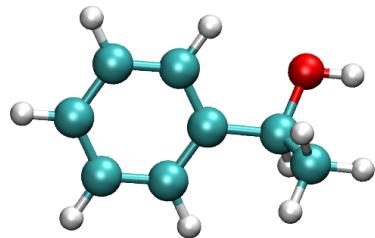
Equal



Molecule A test-R\_out\_G09\_rot-45-45-45



Molecule B test-S\_out\_G09



Inertia Tensor - Molecule A

430.951	89.0849	141.239
89.0849	367.04	-98.5816
141.239	-98.5816	321.828

Inertia Tensor - Molecule B

146.29	-5.10986	3.31731
-5.10986	442.839	1.31633
3.31731	1.31633	530.688

EingenVectors - Molecule A

0.504792	-0.513366	-0.694003
0.142865	0.842546	-0.519332
-0.851337	-0.163006	-0.498652

EingenVectors - Molecule B

-0.999813	-0.0172596	0.00868475
-0.017383	0.999746	-0.0143352
0.00843513	0.0144835	0.99986

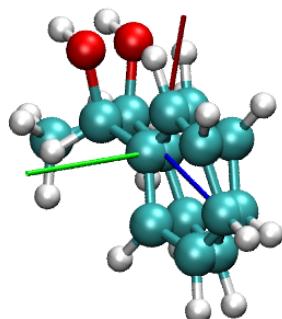
EingenValues - Molecule A

146.173	442.909	530.735
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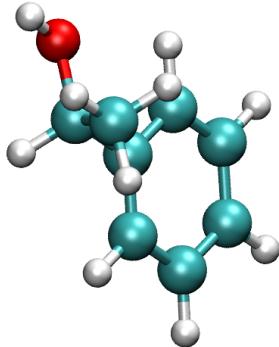
EingenValues - Molecule B

146.173	442.909	530.735
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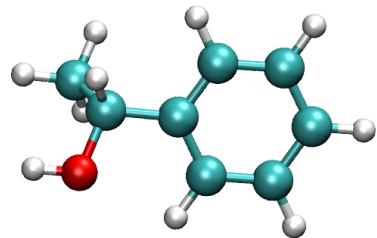
Enantiomers



Molecule A test-R.out\_G09\_rot-45-45-45



Molecule B test-S.out\_G09\_inversion



Inertia Tensor - Molecule A

430.951	89.0849	141.239
89.0849	367.04	-98.5816
141.239	-98.5816	321.828

Inertia Tensor - Molecule B

146.29	-5.10969	3.31735
-5.10969	442.839	1.31631
3.31735	1.31631	530.688

EingenVectors - Molecule A

0.504792	-0.513366	-0.694003
0.142865	0.842546	-0.519332
-0.851337	-0.163006	-0.498652

EingenVectors - Molecule B

-0.999813	-0.017259	0.00868483
-0.0173824	0.999746	-0.014335
0.00843522	0.0144833	0.99986

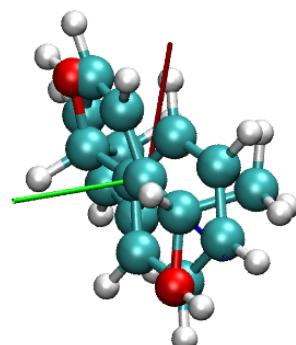
EingenValues - Molecule A

146.173	442.909	530.735
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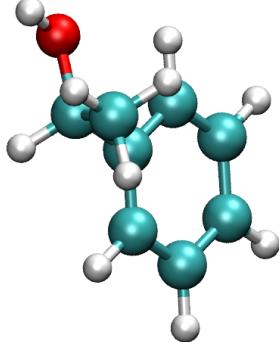
EingenValues - Molecule B

146.173	442.909	530.735
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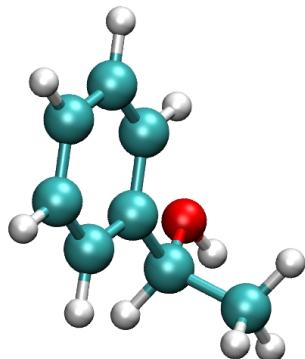
Equal



Molecule A test-R\_out\_G09\_rot-45-45-45



Molecule B test-S\_out\_G09\_rot-45-45-45



Inertia Tensor - Molecule A

430.951	89.0849	141.239
89.0849	367.04	-98.5816
141.239	-98.5816	321.828

Inertia Tensor - Molecule B

435.116	83.1261	142.506
83.1261	374.791	-97.314
142.506	-97.314	309.91

EingenVectors - Molecule A

0.504792	-0.513366	-0.694003
0.142865	0.842546	-0.519332
-0.851337	-0.163006	-0.498652

EingenVectors - Molecule B

0.495022	-0.486446	-0.719947
0.125483	0.859929	-0.494748
-0.859771	-0.15457	-0.486725

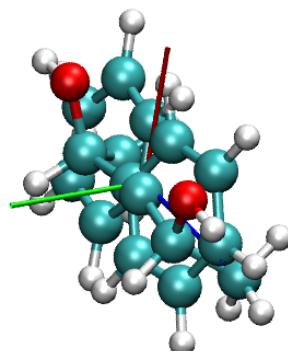
EingenValues - Molecule A

146.173	442.909	530.735
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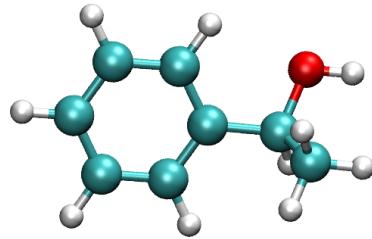
EingenValues - Molecule B

146.173	442.909	530.735
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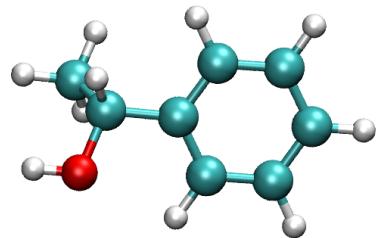
Enantiomers



Molecule A test-S\_out\_G09



Molecule B test-S\_out\_G09\_inversion



Inertia Tensor - Molecule A

146.29	-5.10986	3.31731
-5.10986	442.839	1.31633
3.31731	1.31633	530.688

Inertia Tensor - Molecule B

146.29	-5.10969	3.31735
-5.10969	442.839	1.31631
3.31735	1.31631	530.688

EingenVectors - Molecule A

-0.999813	-0.0172596	0.00868475
-0.017383	0.999746	-0.0143352
0.00843513	0.0144835	0.99986

EingenVectors - Molecule B

-0.999813	-0.017259	0.00868483
-0.0173824	0.999746	-0.014335
0.00843522	0.0144833	0.99986

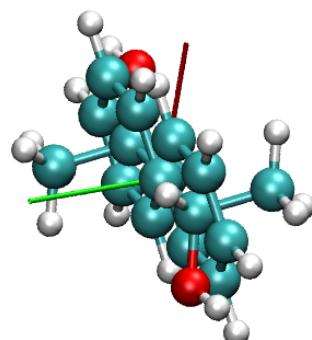
EingenValues - Molecule A

146.173	442.909	530.735
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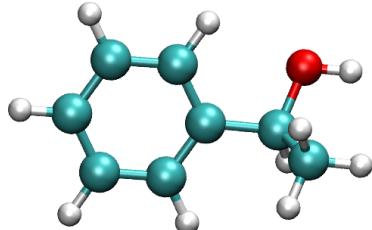
EingenValues - Molecule B

146.173	442.909	530.735
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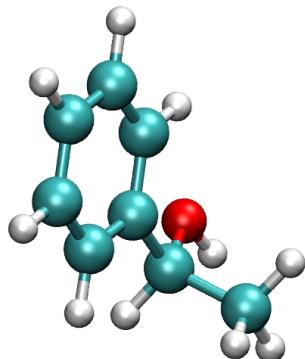
Enantiomers



Molecule A test-S\_out\_G09



Molecule B test-S\_out\_G09\_rot-45-45-45



Inertia Tensor - Molecule A

146.29	-5.10986	3.31731
-5.10986	442.839	1.31633
3.31731	1.31633	530.688

Inertia Tensor - Molecule B

435.116	83.1261	142.506
83.1261	374.791	-97.314
142.506	-97.314	309.91

EingenVectors - Molecule A

-0.999813	-0.0172596	0.00868475
-0.017383	0.999746	-0.0143352
0.00843513	0.0144835	0.99986

EingenVectors - Molecule B

0.495022	-0.486446	-0.719947
0.125483	0.859929	-0.494748
-0.859771	-0.15457	-0.486725

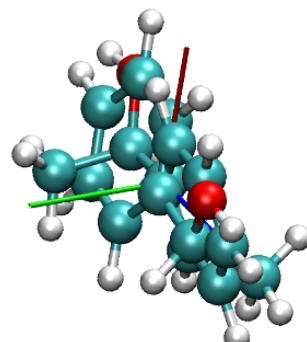
EingenValues - Molecule A

146.173	442.909	530.735
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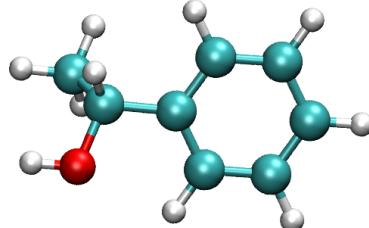
EingenValues - Molecule B

146.173	442.909	530.735
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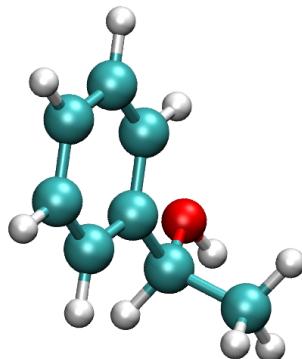
Equal



Molecule A test-S\_out\_G09\_inversion



Molecule B test-S\_out\_G09\_rot-45-45-45



Inertia Tensor - Molecule A

146.29	-5.10969	3.31735
-5.10969	442.839	1.31631
3.31735	1.31631	530.688

Inertia Tensor - Molecule B

435.116	83.1261	142.506
83.1261	374.791	-97.314
142.506	-97.314	309.91

EingenVectors - Molecule A

-0.999813	-0.017259	0.00868483
-0.0173824	0.999746	-0.014335
0.00843522	0.0144833	0.99986

EingenVectors - Molecule B

0.495022	-0.486446	-0.719947
0.125483	0.859929	-0.494748
-0.859771	-0.15457	-0.486725

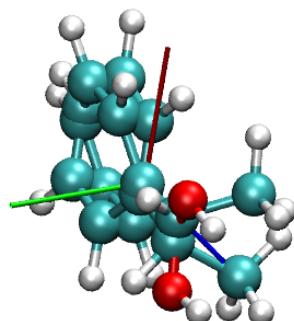
EingenValues - Molecule A

146.173	442.909	530.735
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EingenValues - Molecule B

146.173	442.909	530.735
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Enantiomers



#	Moléculas	Restultado esperado	Resultado programa
1	r-2-chlorobutane_out_G09_inversion E = -618.057081944 Freq =115.2921	Enantiomers	Enantiomers RMS = 0.02719433
	r-2-chlorobutane_rotated_out_G09 E = -618.057081944 Freq =115.2921		
2	r-2-chlorobutane_out_G09_inversion E = -618.057081944 Freq =115.2921	Equal	Equal RMS = 4.366941E-07
	s-2-chlorobutane_out_G09 E = -618.057081943 Freq =115.2939		
3	r-2-chlorobutane_out_G09_inversion E = -618.057081944 Freq =115.2921	Enantiomers	Enantiomers RMS = 0.2294318
	s-2-chlorobutane_out_G09_inversion E = -618.057081943 Freq =115.2939		
4	r-2-chlorobutane_out_G09_inversion E = -618.057081944 Freq =115.2921	Equal	Equal RMS = 5.673033E-07
	s-2-chlorobutane_rotated_out_G09 E = -618.057081943 Freq =115.2939		
5	r-2-chlorobutane_out_G09 E = -618.057081944 Freq =115.2921	Enantiomers	Enantiomers RMS = 0.02719433
	r-2-chlorobutane_out_G09_inversion E = -618.057081944 Freq =115.2921		
6	r-2-chlorobutane_out_G09 E = -618.057081944 Freq =115.2921	Equal	Equal RMS = 1.236488E-09
	r-2-chlorobutane_rotated_out_G09 E = -618.057081944 Freq =115.2921		
7	r-2-chlorobutane_out_G09 E = -618.057081944 Freq =115.2921	Enantiomers	Enantiomers RMS = 0.2294273
	s-2-chlorobutane_out_G09 E = -618.057081943 Freq =115.2939		

#	Moléculas	Restultado esperado	Resultado programa
8	r-2-chlorobutane_out_G09 E = -618.057081944 Freq =115.2921	Equal	Equal  RMS = 4.044324E-06
	s-2-chlorobutane_out_G09_inversion E = -618.057081943 Freq =115.2939		
9	r-2-chlorobutane_out_G09 E = -618.057081944 Freq =115.2921	Enantiomers	Enantiomers  RMS = 0.2294272
	s-2-chlorobutane_rotated_out_G09 E = -618.057081943 Freq =115.2939		
10	r-2-chlorobutane_rotated_out_G09 E = -618.057081944 Freq =115.2921	Enantiomers	Enantiomers  RMS = 0.2294273
	s-2-chlorobutane_out_G09 E = -618.057081943 Freq =115.2939		
11	r-2-chlorobutane_rotated_out_G09 E = -618.057081944 Freq =115.2921	Equal	Equal  RMS = 4.043088E-06
	s-2-chlorobutane_out_G09_inversion E = -618.057081943 Freq =115.2939		
12	r-2-chlorobutane_rotated_out_G09 E = -618.057081944 Freq =115.2921	Enantiomers	Enantiomers  RMS = 0.2294272
	s-2-chlorobutane_rotated_out_G09 E = -618.057081943 Freq =115.2939		
13	s-2-chlorobutane_out_G09_inversion E = -618.057081943 Freq =115.2939	Enantiomers	Enantiomers  RMS = 0.02719894
	s-2-chlorobutane_rotated_out_G09 E = -618.057081943 Freq =115.2939		
14	s-2-chlorobutane_out_G09 E = -618.057081943 Freq =115.2939	Enantiomers	Enantiomers  RMS = 0.02719881
	s-2-chlorobutane_out_G09_inversion E = -618.057081943 Freq =115.2939		

#	Moléculas	Restultado esperado	Resultado programa
15	s-2-chlorobutane_out_G09 E = -618.057081943 Freq =115.2939	Equal	Equal
	s-2-chlorobutane_rotated_out_G09 E = -618.057081943 Freq =115.2939		
16	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	G_09_Cu_AFTER_DFT E = No Data Freq =No Data		
17	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	G_09_Cu E = No Data Freq =No Data		
18	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	G_10_Cu E = No Data Freq =No Data		
19	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	G_11_Cu E = No Data Freq =No Data		
20	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		
21	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
22	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.12656	<b>Different</b>
	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data		
23	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.14548	<b>Different</b>
	SC_08_Cu E = No Data Freq =No Data		
24	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data		
25	G_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu E = No Data Freq =No Data		
26	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.0120518	<b>Different</b>
	G_08_Cu_AFTER_DFT E = No Data Freq =No Data		
27	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_09_Cu_AFTER_DFT E = No Data Freq =No Data		
28	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_09_Cu E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
29	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_10_Cu E = No Data Freq =No Data		
30	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_11_Cu E = No Data Freq =No Data		
31	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.0885651	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		
32	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		
33	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.13861	<b>Different</b>
	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data		
34	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.15753	<b>Different</b>
	SC_08_Cu E = No Data Freq =No Data		
35	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
36	G_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu E = No Data Freq =No Data		
37	G_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_10_Cu E = No Data Freq =No Data		
38	G_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_11_Cu E = No Data Freq =No Data		
39	G_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		
40	G_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.0504	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		
41	G_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data		
42	G_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Cu E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
43	G_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.613767	<b>Different</b>
	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data		
44	G_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.633937	<b>Different</b>
	SC_09_Cu E = No Data Freq =No Data		
45	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.000633333	<b>Different</b>
	G_09_Cu_AFTER_DFT E = No Data Freq =No Data		
46	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_10_Cu E = No Data Freq =No Data		
47	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_11_Cu E = No Data Freq =No Data		
48	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		
49	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.04976	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
50	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data		
51	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Cu E = No Data Freq =No Data		
52	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.613133	<b>Different</b>
	SC_09_Cu_AFTER_DFT		
	E = No Data Freq =No Data		
53	G_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.633304	<b>Different</b>
	SC_09_Cu E = No Data Freq =No Data		
54	G_10_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_11_Cu E = No Data Freq =No Data		
55	G_10_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		
56	G_10_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Cu_AFTER_DFT		
	E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
57	G_10_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data		
58	G_10_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Cu E = No Data Freq =No Data		
59	G_10_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data		
60	G_10_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu E = No Data Freq =No Data		
61	G_11_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		
62	G_11_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		
63	G_11_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
64	G_11_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Cu E = No Data Freq =No Data		
65	G_11_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data		
66	G_11_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu E = No Data Freq =No Data		
67	lj_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		
68	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.05005	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		
69	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		
70	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
71	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu E = No Data Freq =No Data		
72	SC_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.06896	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		
73	SC_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		
74	SC_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.0189151	<b>Different</b>
	SC_08_Cu_AFTER_DFT E = No Data Freq =No Data		
75	SC_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data		
76	SC_08_Cu E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Cu E = No Data Freq =No Data		
77	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
78	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		RMS = 0.43663
79	SC_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_08_Cu E = No Data Freq =No Data		RMS = nan
80	SC_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_09_Cu_AFTER_DFT E = No Data Freq =No Data		RMS = 0.416459
81	SC_09_Cu E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	SC_09_Cu_AFTER_DFT E = No Data Freq =No Data		RMS = 0.0201704
82	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	G_09_Ni_AFTER_DFT E = No Data Freq =No Data		RMS = nan
83	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	G_09_Ni E = No Data Freq =No Data		RMS = nan
84	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_08 E = No Data Freq =No Data		RMS = 0.0937977

#	Moléculas	Restultado esperado	Resultado programa
85	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.834249	<b>Different</b>
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data		
86	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.877307	<b>Different</b>
	lj_08_Ni E = No Data Freq =No Data		
87	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09 E = No Data Freq =No Data		
88	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		
89	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		
90	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_10 E = No Data Freq =No Data		
91	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
92	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.616743	<b>Different</b>
	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data		
93	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.615117	<b>Different</b>
	SC_08_Ni E = No Data Freq =No Data		
94	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data		
95	G_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Ni E = No Data Freq =No Data		
96	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.339204	<b>Different</b>
	G_08_Ni_AFTER_DFT E = No Data Freq =No Data		
97	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_09_Ni_AFTER_DFT E = No Data Freq =No Data		
98	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	G_09_Ni E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
99	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.245401	<b>Different</b>
	lj_08 E = No Data Freq =No Data		
100	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.17345	<b>Different</b>
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data		
101	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.21651	<b>Different</b>
	lj_08_Ni E = No Data Freq =No Data		
102	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09 E = No Data Freq =No Data		
103	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		
104	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		
105	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_10 E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
106	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		
107	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.955946	<b>Different</b>
	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data		
108	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.95432	<b>Different</b>
	SC_08_Ni E = No Data Freq =No Data		
109	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data		
110	G_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Ni E = No Data Freq =No Data		
111	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08 E = No Data Freq =No Data		
112	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
113	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Ni E = No Data Freq =No Data		
114	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.7602	<b>Different</b>
	lj_09 E = No Data Freq =No Data		
115	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.977533	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		
116	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.971333	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		
117	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_10 E = No Data Freq =No Data		
118	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		
119	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
120	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Ni E = No Data Freq =No Data		
121	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.950759	<b>Different</b>
	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data		
122	G_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.943696	<b>Different</b>
	SC_09_Ni E = No Data Freq =No Data		
123	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.0662296	<b>Different</b>
	G_09_Ni_AFTER_DFT E = No Data Freq =No Data		
124	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08 E = No Data Freq =No Data		
125	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data		
126	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Ni E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
127	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.826433	<b>Different</b>
	lj_09 E = No Data Freq =No Data		
128	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.04376	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		
129	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.03756	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		
130	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_10 E = No Data Freq =No Data		
131	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		
132	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data		
133	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_08_Ni E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
134	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.01699	<b>Different</b>
	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data		
135	G_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 1.00993	<b>Different</b>
	SC_09_Ni E = No Data Freq =No Data		
136	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09 E = No Data Freq =No Data		
137	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		
138	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		
139	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_10 E = No Data Freq =No Data		
140	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
141	lj_08_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data	RMS = 0.01393	
142	lj_08_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_09 E = No Data Freq =No Data	RMS = nan	
143	lj_08_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data	RMS = nan	
144	lj_08_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_09_Ni E = No Data Freq =No Data	RMS = nan	
145	lj_08_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_10 E = No Data Freq =No Data	RMS = nan	
146	lj_08_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_11 E = No Data Freq =No Data	RMS = nan	
147	lj_08 E = No Data Freq =No Data	Without comparison	Different
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data	RMS = 0.985035	

#	Moléculas	Restultado esperado	Resultado programa
148	lj_08 E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.765642	Different
	lj_08_Ni E = No Data Freq =No Data		
149	lj_08 E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	Different
	lj_09 E = No Data Freq =No Data		
150	lj_08 E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	Different
	lj_09_Ni_AFTER_DFT		
	E = No Data Freq =No Data		
151	lj_08 E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	Different
	lj_09_Ni E = No Data Freq =No Data		
	E = No Data Freq =No Data		
152	lj_08 E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	Different
	lj_10 E = No Data Freq =No Data		
	E = No Data Freq =No Data		
153	lj_08 E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	Different
	lj_11 E = No Data Freq =No Data		
	E = No Data Freq =No Data		
154	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	Different
	lj_10 E = No Data Freq =No Data		
	E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
155	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data	Without comparison	Different
	lj_11 E = No Data Freq =No Data	RMS = nan	
156	lj_09_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data	RMS = 0.0062	
157	lj_09_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_10 E = No Data Freq =No Data	RMS = nan	
158	lj_09_Ni E = No Data Freq =No Data	Without comparison	Different
	lj_11 E = No Data Freq =No Data	RMS = nan	
159	lj_09 E = No Data Freq =No Data	Without comparison	Different
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data	RMS = 0.0922	
160	lj_09 E = No Data Freq =No Data	Without comparison	Different
	lj_09_Ni E = No Data Freq =No Data	RMS = 0.0984	
161	lj_09 E = No Data Freq =No Data	Without comparison	Different
	lj_10 E = No Data Freq =No Data	RMS = nan	

#	Moléculas	Restultado esperado	Resultado programa
162	lj_09 E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		
163	lj_10 E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		
164	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.604223	<b>Different</b>
	lj_08 E = No Data Freq =No Data		
165	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.217506	<b>Different</b>
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data		
166	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.366882	<b>Different</b>
	lj_08_Ni E = No Data Freq =No Data		
167	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09 E = No Data Freq =No Data		
168	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
169	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		
170	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_10 E = No Data Freq =No Data		
171	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		
172	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data		
173	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Ni E = No Data Freq =No Data		
174	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.602596	<b>Different</b>
	lj_08 E = No Data Freq =No Data		
175	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.219132	<b>Different</b>
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
176	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.368509	<b>Different</b>
	lj_08_Ni E = No Data Freq =No Data		
177	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09 E = No Data Freq =No Data		
178	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		
179	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		
180	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_10 E = No Data Freq =No Data		
181	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		
182	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.00162635	<b>Different</b>
	SC_08_Ni_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
183	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data		
184	SC_08_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	SC_09_Ni E = No Data Freq =No Data		
185	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08 E = No Data Freq =No Data		
186	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data		
187	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_08_Ni E = No Data Freq =No Data		
188	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.0992333	<b>Different</b>
	lj_09 E = No Data Freq =No Data		
189	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.0267741	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
190	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		RMS = 0.0205741
191	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_10 E = No Data Freq =No Data		RMS = nan
192	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_11 E = No Data Freq =No Data		RMS = nan
193	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_08 E = No Data Freq =No Data		RMS = nan
194	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_08_Ni_AFTER_DFT E = No Data Freq =No Data		RMS = nan
195	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_08_Ni E = No Data Freq =No Data		RMS = nan
196	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>	<b>Different</b>
	lj_09 E = No Data Freq =No Data		RMS = 0.0921667

#	Moléculas	Restultado esperado	Resultado programa
197	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.033837	<b>Different</b>
	lj_09_Ni_AFTER_DFT E = No Data Freq =No Data		
198	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.027637	<b>Different</b>
	lj_09_Ni E = No Data Freq =No Data		
199	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_10 E = No Data Freq =No Data		
200	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = nan	<b>Different</b>
	lj_11 E = No Data Freq =No Data		
201	SC_09_Ni E = No Data Freq =No Data	<b>Without comparison</b>  RMS = 0.00706296	<b>Different</b>
	SC_09_Ni_AFTER_DFT E = No Data Freq =No Data		
202	3NFAACa E = No Data Freq =No Data	Equal  RMS = 4.41707E-05	Equal
	3NFAACb E = No Data Freq =No Data		
203	3NFAACa E = No Data Freq =No Data	Different  RMS = 0.0334016	Different
	3NFAACc E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
204	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACd E = No Data Freq =No Data		RMS = 0.0888511
205	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACE E = No Data Freq =No Data		RMS = 0.162132
206	3NFAACa E = No Data Freq =No Data	Equal	Equal
	3NFAACf E = No Data Freq =No Data		RMS = 0.001455454
207	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data		RMS = 0.0330848
208	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACH E = No Data Freq =No Data		RMS = 0.064417
209	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.0837021
210	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.0903201

#	Moléculas	Restultado esperado	Resultado programa
211	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0114116
212	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.0362294
213	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.152833
214	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.157182
215	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.219778
216	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.258442
217	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.0186255

#	Moléculas	Restultado esperado	Resultado programa
218	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0149078
219	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.0228438
220	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.118302
221	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0338585
222	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.00146242
223	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0868356
224	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0414826

#	Moléculas	Restultado esperado	Resultado programa
225	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACc E = No Data Freq =No Data		RMS = 0.0881291
226	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACd E = No Data Freq =No Data		RMS = 0.143579
227	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACe E = No Data Freq =No Data		RMS = 0.107404
228	3NFAACb E = No Data Freq =No Data	<b>Equal</b>	<b>Enantiomers</b>
	3NFAACf E = No Data Freq =No Data		
229	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data		RMS = 0.0878122
230	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data		RMS = 0.00968954
231	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.13843

#	Moléculas	Restultado esperado	Resultado programa
232	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.145048
233	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0661391
234	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.018498
235	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.0981054
236	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.102455
237	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.274505
238	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.203714

#	Moléculas	Restultado esperado	Resultado programa
239	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.036102
240	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0398197
241	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.0318836
242	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0635749
243	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.020869
244	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0561899
245	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0321081

#	Moléculas	Restultado esperado	Resultado programa
246	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0132449
247	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACd E = No Data Freq =No Data		RMS = 0.0554495
248	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACe E = No Data Freq =No Data		RMS = 0.195533
249	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACf E = No Data Freq =No Data		RMS = 0.0879682
250	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data		RMS = 0.000316817
251	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data		RMS = 0.0978186
252	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.0503005

#	Moléculas	Restultado esperado	Resultado programa
253	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.0569185
254	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.02199
255	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.069631
256	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.186234
257	3NFAACc E = No Data Freq =No Data	Enantiomers	Enantiomers
	3NFAACn E = No Data Freq =No Data		RMS = 0.01522269
258	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.186376
259	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.291844

#	Moléculas	Restultado esperado	Resultado programa
260	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.0520271
261	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0483094
262	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.0562454
263	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.151704
264	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0672601
265	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0319392
266	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.120237

#	Moléculas	Restultado esperado	Resultado programa
267	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0748842
268	3NFAACd E = No Data Freq =No Data	Equal	Equal
	3NFAACE E = No Data Freq =No Data		RMS = 0.02981604
269	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACf E = No Data Freq =No Data		RMS = 0.143418
270	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data		RMS = 0.0557663
271	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACH E = No Data Freq =No Data		RMS = 0.153268
272	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.00514902
273	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.00146894

#	Moléculas	Restultado esperado	Resultado programa
274	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0774395
275	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.125081
276	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.241684
277	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.246033
278	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.130927
279	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.347293
280	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.107477

#	Moléculas	Restultado esperado	Resultado programa
281	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.103759
282	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.111695
283	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.207153
284	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.12271
285	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0873887
286	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.175687
287	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.130334

#	Moléculas	Restultado esperado	Resultado programa
288	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACf E = No Data Freq =No Data		RMS = 0.107565
289	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data		RMS = 0.195216
290	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data		RMS = 0.0977146
291	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.245834
292	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.252452
293	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.173543
294	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.125902

#	Moléculas	Restultado esperado	Resultado programa
295	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.00929873
296	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.00494937
297	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.381909
298	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.0963103
299	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.143506
300	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.147224
301	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.139288

#	Moléculas	Restultado esperado	Resultado programa
302	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0438293
303	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.128273
304	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.163594
305	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.075296
306	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.120649
307	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data		RMS = 0.0876514
308	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data		RMS = 0.00985042

#	Moléculas	Restultado esperado	Resultado programa
309	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.138269
310	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.144887
311	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0659782
312	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.0183372
313	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.0982663
314	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.102616
315	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.274344

#	Moléculas	Restultado esperado	Resultado programa
316	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.203875
317	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.0359411
318	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0396588
319	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.0317228
320	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0637358
321	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0207081
322	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.056029

#	Moléculas	Restultado esperado	Resultado programa
323	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.032269
324	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.013084
325	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data		RMS = 0.0975018
326	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.0506173
327	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.0572353
328	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0216732
329	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.0693142

#	Moléculas	Restultado esperado	Resultado programa
330	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.185918
331	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.190267
332	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.186693
333	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.291527
334	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACC E = No Data Freq =No Data		RMS = 0.0517103
335	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0479926
336	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.0559286

#	Moléculas	Restultado esperado	Resultado programa
337	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.151387
338	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0669433
339	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0316224
340	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.11992
341	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0745674
342	3NFAACh E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.148119
343	3NFAACh E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.154737

#	Moléculas	Restultado esperado	Resultado programa
344	3NFAACh E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data	RMS = 0.0758286	
345	3NFAACh E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data	RMS = 0.0281876	
346	3NFAACh E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data	RMS = 0.0884159	
347	3NFAACh E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data	RMS = 0.0927652	
348	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data	RMS = 0.284195	
349	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data	RMS = 0.194025	
350	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data	RMS = 0.0457915	

#	Moléculas	Restultado esperado	Resultado programa
351	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0495092
352	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.0415732
353	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0538853
354	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0305585
355	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0658794
356	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0224186
357	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0229344

#	Moléculas	Restultado esperado	Resultado programa
358	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.00661796
359	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0722905
360	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.119932
361	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.236535
362	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.240884
363	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.136076
364	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.342144

#	Moléculas	Restultado esperado	Resultado programa
365	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.102328
366	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0986099
367	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.106546
368	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.202004
369	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.117561
370	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0822397
371	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.170538

#	Moléculas	Restultado esperado	Resultado programa
372	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.125185
373	3NFAACj E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0789084
374	3NFAACj E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.126549
375	3NFAACj E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.243153
376	3NFAACj E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.247502
377	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.129458
378	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.348762

#	Moléculas	Restultado esperado	Resultado programa
379	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.108946
380	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.105228
381	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.113164
382	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.208622
383	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.124179
384	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0888577
385	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.177156

#	Moléculas	Restultado esperado	Resultado programa
386	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.131803
387	3NFAACk E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.047641
388	3NFAACk E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.164244
389	3NFAACk E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.168594
390	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.208366
391	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.269854
392	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.0300371

#	Moléculas	Restultado esperado	Resultado programa
393	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0263194
394	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.0342554
395	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.129714
396	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0452701
397	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.00994921
398	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0982472
399	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0528942

#	Moléculas	Restultado esperado	Resultado programa
400	3NFAACl E = No Data Freq =No Data	Enantiomers	Enantiomers RMS = 0.07729889
	3NFAACm E = No Data Freq =No Data		
401	3NFAACl E = No Data Freq =No Data	Different	Different RMS = 0.120953
	3NFAACn E = No Data Freq =No Data		
402	3NFAACl E = No Data Freq =No Data	Different	Different RMS = 0.256007
	4NFAACa E = No Data Freq =No Data		
403	3NFAACl E = No Data Freq =No Data	Different	Different RMS = 0.222213
	4NFAACb E = No Data Freq =No Data		
404	3NFAACl E = No Data Freq =No Data	Different	Different RMS = 0.0176039
	4NFAACc E = No Data Freq =No Data		
405	3NFAACl E = No Data Freq =No Data	Different	Different RMS = 0.0213216
	4NFAACd E = No Data Freq =No Data		
406	3NFAACl E = No Data Freq =No Data	Different	Different RMS = 0.0133856
	4NFAACe E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
407	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0820729
408	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.00237094
409	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0376918
410	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0506062
411	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0052532
412	3NFAACm E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.00434937
413	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.372611

#	Moléculas	Restultado esperado	Resultado programa
414	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.105609
415	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.134207
416	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.137925
417	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.129989
418	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0345305
419	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.118974
420	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.154295

#	Moléculas	Restultado esperado	Resultado programa
421	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0659973
422	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.111135
423	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.37696
424	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.10126
425	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACC E = No Data Freq =No Data		RMS = 0.138557
426	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.142274
427	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.134338

#	Moléculas	Restultado esperado	Resultado programa
428	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data	RMS = 0.0388799	
429	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.123324	
430	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.158645	
431	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data	RMS = 0.0703467	
432	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data	RMS = 0.1157	
433	4NFAACa E = No Data Freq =No Data	Enantiomers	Enantiomers
	4NFAACb E = No Data Freq =No Data	RMS = 0.485443	
434	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data	RMS = 0.238403	

#	Moléculas	Restultado esperado	Resultado programa
435	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.234686
436	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.242622
437	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.33808
438	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.253636
439	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.218315
440	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.306613
441	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.26126

#	Moléculas	Restultado esperado	Resultado programa
442	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.239816
443	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.243534
444	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.235598
445	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.14014
446	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.224583
447	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.259904
448	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.171606

#	Moléculas	Restultado esperado	Resultado programa
449	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.216959
450	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.00371771
451	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.00421832
452	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0996768
453	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.015233
454	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0200879
455	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0682101

#	Moléculas	Restultado esperado	Resultado programa
456	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0228571
457	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.00793602
458	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.103395
459	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0189507
460	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0163702
461	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0719278
462	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0265748

#	Moléculas	Restultado esperado	Resultado programa
463	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data	RMS = 0.0954585	
464	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.0110146	
465	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.0243062	
466	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data	RMS = 0.0639918	
467	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data	RMS = 0.0186388	
468	4NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.0844439	
469	4NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.119765	

#	Moléculas	Restultado esperado	Resultado programa
470	4NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0314668
471	4NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0768197
472	4NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0353209
473	4NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0529771
474	4NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.00762414
475	4NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.088298
476	4NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.042945

#	Moléculas	Restultado esperado	Resultado programa
477	4NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.045353
478	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	Different	Different
	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018		RMS = 0.0199855
479	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	Different	Different
	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018		RMS = 0.019986
480	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	Different	Different
	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103		RMS = 0.331901
481	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	Different	Different
	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103		RMS = 0.211483
482	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	Different	Different
	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725		RMS = 0.476729
483	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	Different	Different
	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725		RMS = 0.47673

#	Moléculas	Restultado esperado	Resultado programa
484	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752	RMS = 0.289298	
485	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	Different	Different
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752	RMS = 0.289298	
486	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Equal	Enantiomers
	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	RMS = 1.152282E-18	
487	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018	RMS = 0.269312	
488	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018	RMS = 0.269312	
489	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	RMS = 0.0426031	
490	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103	RMS = 0.0778147	

#	Moléculas	Restultado esperado	Resultado programa
491	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725	RMS = 0.766027	
492	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725	RMS = 0.766028	
493	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752	RMS = 1.15228E-18	
494	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752	RMS = 1.15228E-18	
495	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018	Different	Different
	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	RMS = 0.311915	
496	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018	Different	Different
	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103	RMS = 0.191497	
497	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018	Different	Different
	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725	RMS = 0.496715	

#	Moléculas	Restultado esperado	Resultado programa
498	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018	Different	Different
	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725	RMS = 0.496716	
499	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752	RMS = 0.269312	
500	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018	Different	Different
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752	RMS = 0.269312	
501	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018	Equal	Equal
	2,3-dimethyl-butane_out_G09_inversion E = -237.082490952 Freq =58.6018	RMS = 1.773561E-07	
502	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018	Different	Different
	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	RMS = 0.311916	
503	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018	Different	Different
	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103	RMS = 0.191498	
504	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018	Different	Different
	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725	RMS = 0.496715	

#	Moléculas	Restultado esperado	Resultado programa
505	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018	Different	Different
	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725		RMS = 0.496715
506	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752		RMS = 0.269312
507	2,3-dimethyl-butane_out_G09 E = -237.082490952 Freq =58.6018	Different	Different
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752		RMS = 0.269312
508	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103	Different	Different
	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725		RMS = 0.688213
509	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103	Different	Different
	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725		RMS = 0.688213
510	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752		RMS = 0.0778147
511	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103	Different	Different
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752		RMS = 0.0778147

#	Moléculas	Restultado esperado	Resultado programa
512	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Enantiomers	Enantiomers RMS = 0.1203334
	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103		
513	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Different	Different RMS = 0.80863
	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725		
514	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Different	Different RMS = 0.808631
	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725		
515	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Different	Different RMS = 0.0426031
	hexane_out_G09 E = -237.085500432 Freq =72.0752		
516	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Different	Different RMS = 0.0426031
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752		
517	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725	Different	Different RMS = 0.766028
	hexane_out_G09 E = -237.085500432 Freq =72.0752		
518	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725	Different	Different RMS = 0.766028
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752		

#	Moléculas	Restultado esperado	Resultado programa
519	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725	Equal	Equal
	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725		RMS = 2.333815E-07
520	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752		RMS = 0.766027
521	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725	Different	Different
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752		RMS = 0.766027
522	hexane_out_G09 E = -237.085500432 Freq =72.0752	Equal	Equal
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752		RMS = 0
523	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Equal	Equal
	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793		RMS = 0.0989238
524	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777		RMS = nan
525	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777		RMS = nan

#	Moléculas	Restultado esperado	Resultado programa
526	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777	RMS = nan	
527	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	RMS = 0.390641	
528	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268	RMS = 0.390642	
529	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	RMS = nan	
530	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	RMS = nan	
531	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777	RMS = nan	
532	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	RMS = 0.489568	

#	Moléculas	Restultado esperado	Resultado programa
533	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		RMS = 0.489569
534	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Equal	Equal
	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793		RMS = 0.0922148 Warning: Degeneracy
535	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Equal	Equal
	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793		RMS = 0.00670901 Warning: Degeneracy
536	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777		RMS = nan
537	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777		RMS = nan
538	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		RMS = nan
539	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268		RMS = 0.48286

#	Moléculas	Restultado esperado	Resultado programa
540	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		RMS = 0.48286
541	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09 E = -197.772988492 Freq =208.9793		RMS = 0.092204 Warning: Degeneracy
542	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793		RMS = 1.07659E-05 Warning: Degeneracy
543	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793		RMS = 0.0989131 Warning: Degeneracy
544	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816		RMS = 0.0214957 Warning: Degeneracy
545	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777		RMS = nan
546	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777		RMS = nan

#	Moléculas	Restultado esperado	Resultado programa
547	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		RMS = nan
548	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268		RMS = 0.390652
549	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		RMS = 0.390653
550	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09 E = -197.772988492 Freq =208.9793		
551	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793		
552	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793		
553	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777		

#	Moléculas	Restultado esperado	Resultado programa
554	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777		RMS = nan
555	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		RMS = nan
556	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268		RMS = 0.369158
557	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		RMS = 0.369159
558	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09 E = -197.772988492 Freq =208.9793		RMS = 6.59223E-06 Warning: Degeneracy
559	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793		RMS = 0.0922214 Warning: Degeneracy
560	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_out_G09_rot_x15-y15-z15 E = -197.772988492 Freq =208.9793		RMS = 0.00670242 Warning: Degeneracy

#	Moléculas	Restultado esperado	Resultado programa
561	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816		RMS = 0.0922106 Warning: Degeneracy
562	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Equal	Equal
	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816		RMS = 0.113706 Warning: Degeneracy
563	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777		RMS = nan
564	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777		RMS = nan
565	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		RMS = nan
566	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268		RMS = 0.482866
567	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		RMS = 0.482867

#	Moléculas	Restultado esperado	Resultado programa
568	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	Equal	Equal  RMS = 2.339753E-05
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		
569	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	Different	Different  RMS = nan
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268		
570	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	Different	Different  RMS = nan
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		
571	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777	Different	Different  RMS = nan
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268		
572	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777	Different	Different  RMS = nan
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		
573	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	Equal	Equal  RMS = 2.339753E-05
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777		
574	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	Equal	Equal  RMS = 1.188202E-12
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		

#	Moléculas	Restultado esperado	Resultado programa
575	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	RMS = nan	
576	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268	RMS = nan	
577	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	Equal	Equal
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268	RMS = 7.27607E-07 Warning: Degeneracy	
578	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	RMS = nan	
579	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	RMS = nan	
580	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954	RMS = nan	
581	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954	RMS = nan	

#	Moléculas	Restultado esperado	Resultado programa
582	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596	RMS = nan	
583	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596	RMS = nan	
584	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Equal	Equal
	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549		RMS = 0
585	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	RMS = nan	
586	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	RMS = nan	
587	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954	RMS = nan	
588	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954	RMS = nan	

#	Moléculas	Restultado esperado	Resultado programa
589	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596	RMS = nan	
590	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596	RMS = nan	
591	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	Equal	Enantiomers
	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954	RMS = 0.8973984	
592	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	Equal	Enantiomers
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954	RMS = 0.8973979	
593	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	Equal	Equal
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596	RMS = 0	
594	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	Equal	Equal
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596	RMS = 0	
595	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	Equal	Equal
	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	RMS = 0	

#	Moléculas	Restultado esperado	Resultado programa
596	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	<b>Equal</b>	<b>Enantiomers</b>  RMS = 0.8973984
	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954		
597	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	<b>Equal</b>	<b>Enantiomers</b>  RMS = 0.8973979
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954		
598	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	Equal	Equal  RMS = 0
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596		
599	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	Equal	Equal  RMS = 0
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596		
600	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954	<b>Equal</b>	<b>Enantiomers</b>  RMS = 0.0001075617
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596		
601	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954	<b>Equal</b>	<b>Enantiomers</b>  RMS = 0.0001075617
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596		
602	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954	Equal	Equal  RMS = 6.620476E-08
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954		

#	Moléculas	Restultado esperado	Resultado programa
603	Tetrabenzoporphyrin_rotated02.out_G09 E = -1604.15788879 Freq =19.3954	<b>Equal</b>	<b>Enantiomers</b>  <b>RMS = 0.0001074955</b>
	Tetrabenzoporphyrin_rotated.out_G09 E = -1604.15793928 Freq =20.2596		
604	Tetrabenzoporphyrin_rotated02.out_G09 E = -1604.15788879 Freq =19.3954	<b>Equal</b>	<b>Enantiomers</b>  <b>RMS = 0.0001074955</b>
	Tetrabenzoporphyrin_rotated.out_G09_inversion E = -1604.15793928 Freq =20.2596		
605	Tetrabenzoporphyrin_rotated.out_G09 E = -1604.15793928 Freq =20.2596	Equal	Equal  RMS = 0
	Tetrabenzoporphyrin_rotated.out_G09_inversion E = -1604.15793928 Freq =20.2596		
606	R-R-R-Fructuose.out_G09 E = -687.366006448 Freq =36.7188	Different	Different  RMS = 0.449321
	R-R-S-Fructuose.out_G09 E = -687.367479320 Freq =43.3327		
607	R-R-R-Fructuose.out_G09 E = -687.366006448 Freq =36.7188	Different	Different  RMS = 0.274434
	R-S-R-Fructuose.out_G09 E = -687.362461360 Freq =34.8257		
608	R-R-R-Fructuose.out_G09 E = -687.366006448 Freq =36.7188	Different	Different  RMS = 0.404519
	R-S-S-Fructuose.out_G09 E = -687.363689916 Freq =34.8064		
609	R-R-R-Fructuose.out_G09 E = -687.366006448 Freq =36.7188	Different	Different  RMS = 0.299091
	S-R-R-Fructuose.out_G09 E = -687.363690093 Freq =34.7777		

#	Moléculas	Restultado esperado	Resultado programa
610	R-R-R-Fructuose_out_G09 E = -687.366006448 Freq =36.7188	Different	Different
	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =		RMS = 0.269535
611	R-R-R-Fructuose_out_G09 E = -687.366006448 Freq =36.7188	Different	Different
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371		RMS = 0.327879
612	R-R-R-Fructuose_out_G09 E = -687.366006448 Freq =36.7188	Different	Different
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992		RMS = 0.402361
613	R-R-S-Fructuose_out_G09 E = -687.367479320 Freq =43.3327	Different	Different
	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257		RMS = 0.174888
614	R-R-S-Fructuose_out_G09 E = -687.367479320 Freq =43.3327	Different	Different
	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064		RMS = 0.0448022
615	R-R-S-Fructuose_out_G09 E = -687.367479320 Freq =43.3327	Different	Different
	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777		RMS = 0.15023
616	R-R-S-Fructuose_out_G09 E = -687.367479320 Freq =43.3327	Different	Different
	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =		RMS = 0.179786

#	Moléculas	Restultado esperado	Resultado programa
617	R-R-S-Fructuose_out_G09 E = -687.367479320 Freq =43.3327	Enantiomers	Enantiomers  <b>RMS = 0.0005551068</b>
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371		
618	R-R-S-Fructuose_out_G09 E = -687.367479320 Freq =43.3327	Different	Different  <b>RMS = 0.0469601</b>
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992		
619	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Different	Different  <b>RMS = 0.130085</b>
	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064		
620	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Different	Different  <b>RMS = 0.0246573</b>
	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777		
621	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Enantiomers	Enantiomers  <b>RMS = 0.005799255</b>
	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =		
622	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Different	Different  <b>RMS = 0.0534457</b>
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371		
623	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Different	Different  <b>RMS = 0.127928</b>
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992		

#	Moléculas	Restultado esperado	Resultado programa
624	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064	Enantiomers	Enantiomers  <b>RMS = 0.0001020726</b>
	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777		
625	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064	Different	Different  <b>RMS = 0.134984</b>
	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =		
626	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064	Different	Different  <b>RMS = 0.0766398</b>
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371		
627	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064	Different	Different  <b>RMS = 0.00215791</b>
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992		
628	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777	Different	Different  <b>RMS = 0.029556</b>
	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =		
629	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777	Different	Different  <b>RMS = 0.0287884</b>
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371		
630	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777	Different	Different  <b>RMS = 0.10327</b>
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992		

#	Moléculas	Restultado esperado	Resultado programa
631	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =	Different	Different
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371	RMS = 0.0583444	
632	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =	Different	Different
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992	RMS = 0.132826	
633	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371	Different	Different
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992	RMS = 0.0744819	
634	r-enan_out_G09_inversion_output E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers
	r-enan_rotated_out_G09 E = -9590.12967553 Freq =134.7377		
635	r-enan_out_G09_inversion_output E = -9590.12967553 Freq =134.7377	Equal	Equal
	s-enan_out_G09 E = -9590.12967522 Freq =134.6541		
636	r-enan_out_G09_inversion_output E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers
	s-enan_out_G09_inversion_output E = -9590.12967522 Freq =134.6541		
637	r-enan_out_G09_inversion_output E = -9590.12967553 Freq =134.7377	Equal	Equal
	s-enan_rotated_out_G09 E = -9590.12967522 Freq =134.6541		

#	Moléculas	Restultado esperado	Resultado programa
638	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers RMS = 0.01735201
	r-enan_out_G09_inversion_output E = -9590.12967553 Freq =134.7377		
639	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Equal	Equal RMS = 0
	r-enan_rotated_out_G09 E = -9590.12967553 Freq =134.7377		
640	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers RMS = 0.00506593
	s-enan_out_G09 E = -9590.12967522 Freq =134.6541		
641	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Equal	Equal RMS = 3.832848E-06
	s-enan_out_G09_inversion_output E = -9590.12967522 Freq =134.6541		
642	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers RMS = 0.005065924
	s-enan_rotated_out_G09 E = -9590.12967522 Freq =134.6541		
643	r-enan_rotated_out_G09 E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers RMS = 0.00506593
	s-enan_out_G09 E = -9590.12967522 Freq =134.6541		
644	r-enan_rotated_out_G09 E = -9590.12967553 Freq =134.7377	Equal	Equal RMS = 3.832848E-06
	s-enan_out_G09_inversion_output E = -9590.12967522 Freq =134.6541		

#	Moléculas	Restultado esperado	Resultado programa
645	r-enan_rotated_out_G09 E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers  RMS = 0.005065924
	s-enan_rotated_out_G09 E = -9590.12967522 Freq =134.6541		
646	s-enan_out_G09_inversion_output E = -9590.12967522 Freq =134.6541	Enantiomers	Enantiomers  RMS = 0.01734936
	s-enan_rotated_out_G09 E = -9590.12967522 Freq =134.6541		
647	s-enan_out_G09 E = -9590.12967522 Freq =134.6541	Enantiomers	Enantiomers  RMS = 0.01734936
	s-enan_out_G09_inversion_output E = -9590.12967522 Freq =134.6541		
648	s-enan_out_G09 E = -9590.12967522 Freq =134.6541	Equal	Equal  RMS = 6.301958E-09
	s-enan_rotated_out_G09 E = -9590.12967522 Freq =134.6541		
649	test-R_out_G09_inversion E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers  RMS = 0.1261689
	test-R_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428		
650	test-R_out_G09_inversion E = -386.195553794 Freq =38.2428	Equal	Equal  RMS = 1.131338E-07
	test-S_out_G09 E = -386.195553794 Freq =38.2428		
651	test-R_out_G09_inversion E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers  RMS = 2.547026E-17
	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428		

#	Moléculas	Restultado esperado	Resultado programa
652	test-R_out_G09_inversion E = -386.195553794 Freq =38.2428	Equal	Equal
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	RMS = 1.575741E-07	
653	test-R_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers
	test-S_out_G09 E = -386.195553794 Freq =38.2428	RMS = 0.1189346	
654	test-R_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	Equal	Equal
	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428	RMS = 1.229453E-06	
655	test-R_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	RMS = 0.1261691	
656	test-R_out_G09 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers
	test-R_out_G09_inversion E = -386.195553794 Freq =38.2428	RMS = 0.2451035	
657	test-R_out_G09 E = -386.195553794 Freq =38.2428	Equal	Equal
	test-R_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	RMS = 1.324403E-06	
658	test-R_out_G09 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers
	test-S_out_G09 E = -386.195553794 Freq =38.2428	RMS = 3.820539E-17	

#	Moléculas	Restultado esperado	Resultado programa
659	test-R_out_G09 E = -386.195553794 Freq =38.2428	Equal	Equal  <b>RMS = 9.494985E-08</b>
	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428		
660	test-R_out_G09 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers  <b>RMS = 0.2451037</b>
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428		
661	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers  <b>RMS = 1.575741E-07</b>
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428		
662	test-S_out_G09 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers  <b>RMS = 0.2451035</b>
	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428		
663	test-S_out_G09 E = -386.195553794 Freq =38.2428	Equal	Equal  <b>RMS = 2.749179E-07</b>
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428		

## 2. Extras

Durante la realización de este reporte me surgió la necesidad de crear un par de scripts que puedan ayudar para el trabajo y el empleo de esté programa. La tarea del script *script-Make\_All\_Comparations.bsh* es realizar todas las comparaciones posibles en una carpeta que contenga varias geometrías en el formato de archivo XYZ, guardando el resultado en otro archivo.

El otro script es *translate\_comparatation2Latex.bsh* que utiliza la salida del anterior script para crear un resumen de las comparaciones y traducirlas a un formato personalizado de latex y, de esta manera, poder visualizar con mayor facilidad las comparaciones.

Actualmente el script sigue en desarrollo y se encuentra en el repositorio del programa.