



BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

FACULTAD DE CIENCIAS QUÍMICAS
LABORATORIO DE FISICOQUÍMICA TEÓRICA

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

18 de febrero de 2019

1. Resultados

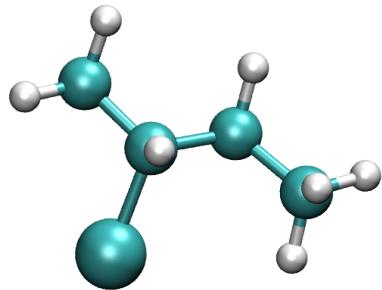
1.1. Pruebas realizadas

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.

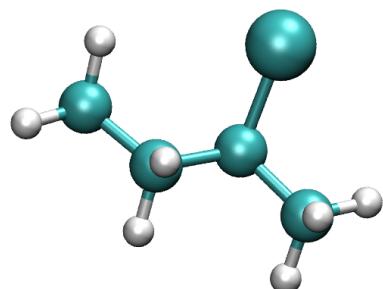
AsymmetricEnantiomers Número 1

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

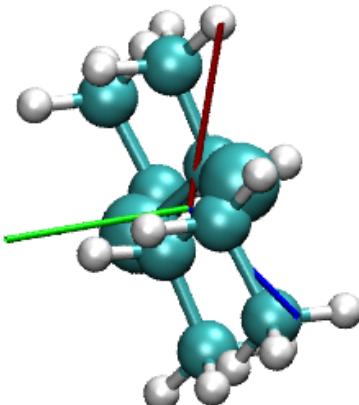
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

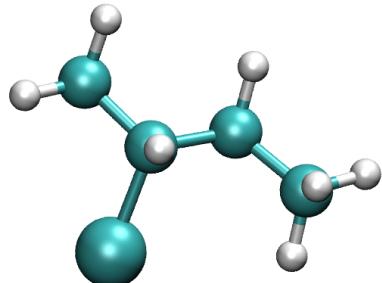
112.224	165.623	257.016
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Enantiomers



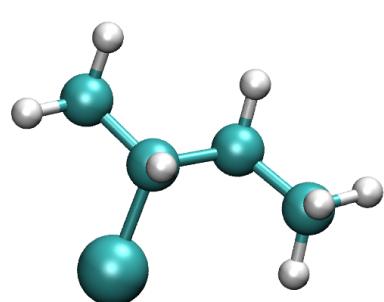
AsymmetricEnantiomers Número 2

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

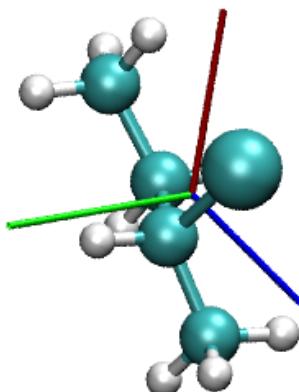
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

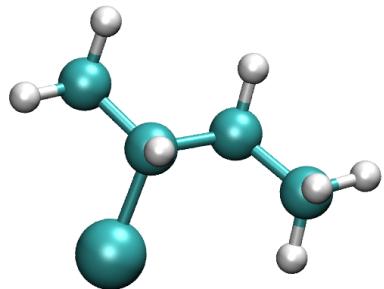
112.224	165.623	257.016
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Equal

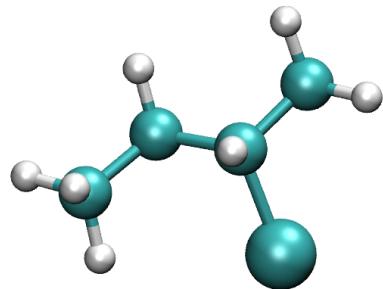


AsymmetricEnantiomers Número 3

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

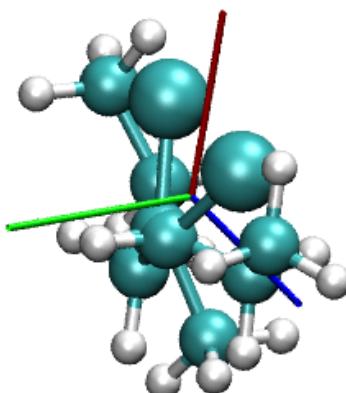
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

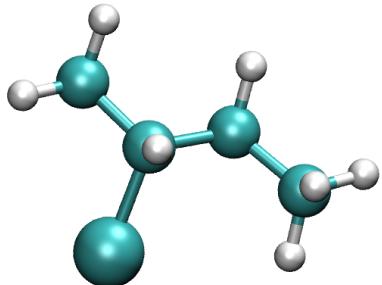
112.224	165.624	257.017
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Enantiomers



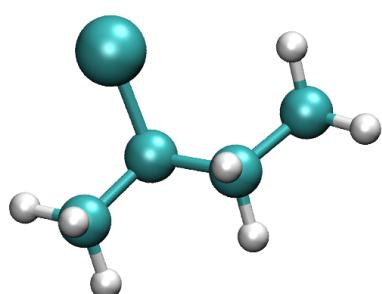
AsymmetricEnantiomers Número 4

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

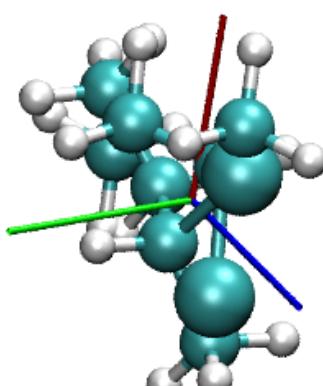
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

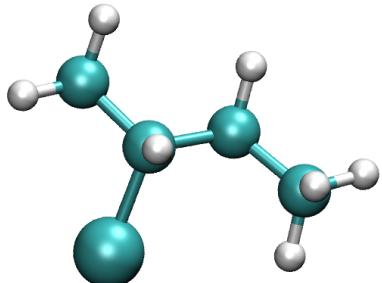
112.224	165.624	257.018
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Equal



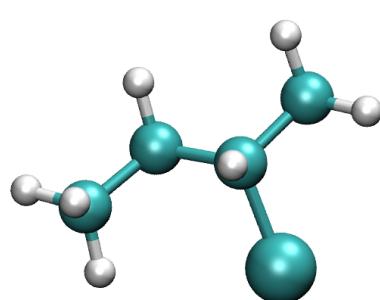
AsymmetricEnantiomers Número 5

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

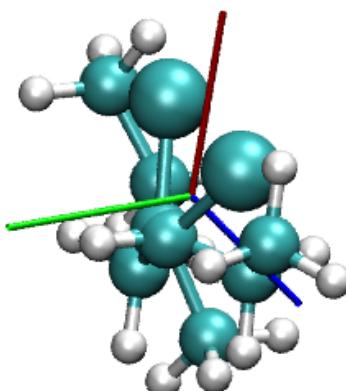
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

112.224	165.624	257.017
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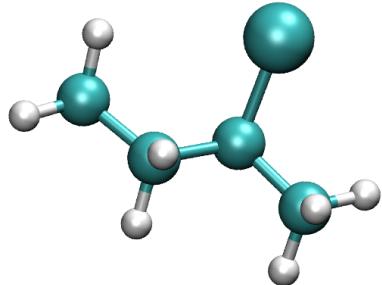
Enantiomers



AsymmetricEnantiomers Número 6

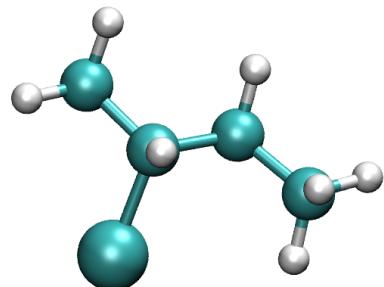
Molecule A

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

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

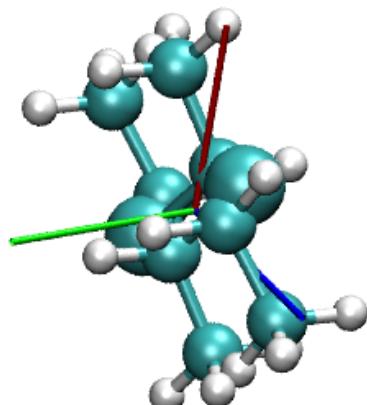
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

112.224	165.623	257.016
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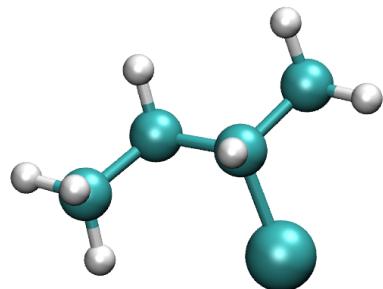
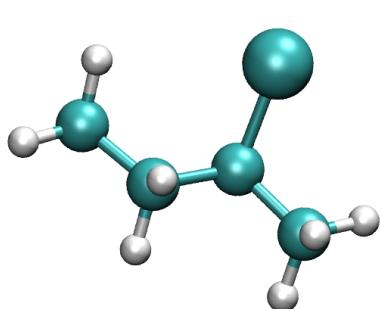
Enantiomers



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

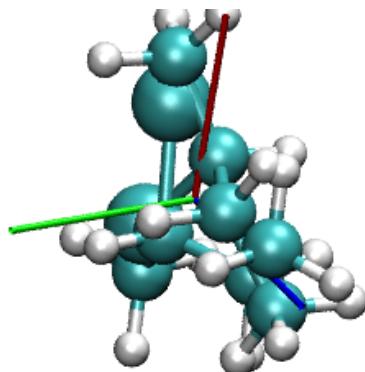
EingenVectors - Molecule A		
-0.986829	-0.161756	-0.00158103
0.161764	-0.986785	-0.00941017
-3.79835e-05	-0.00954198	0.999954

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

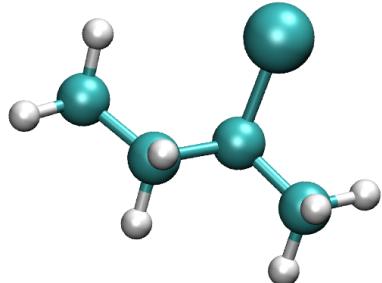
Equal



AsymmetricEnantiomers Número 8

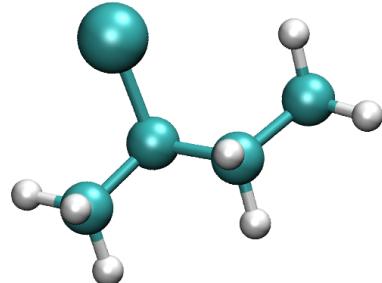
Molecule A

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

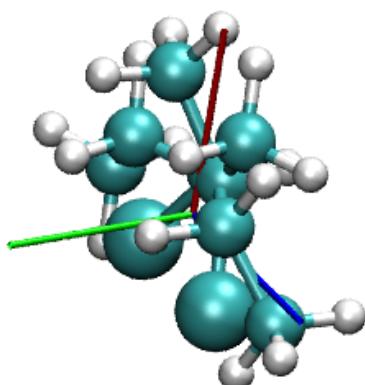
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

112.224	165.624	257.018
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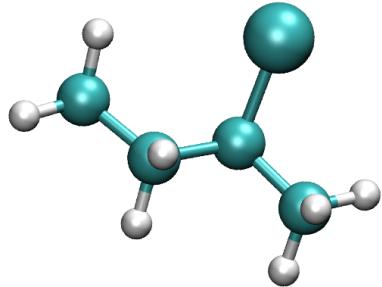
Enantiomers



AsymmetricEnantiomers Número 9

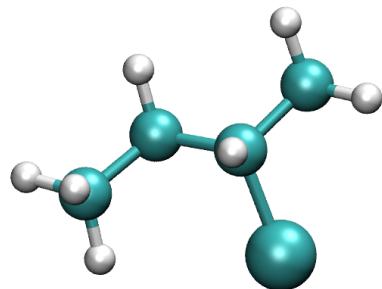
Molecule A

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

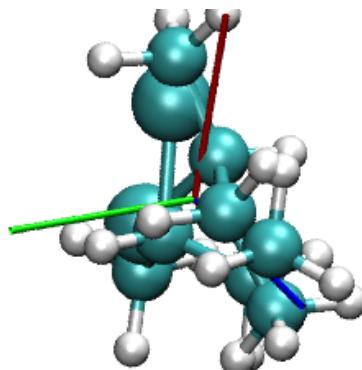
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

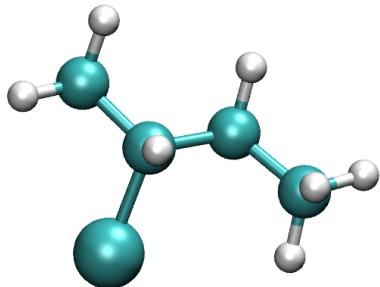
112.224	165.624	257.017
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Equal

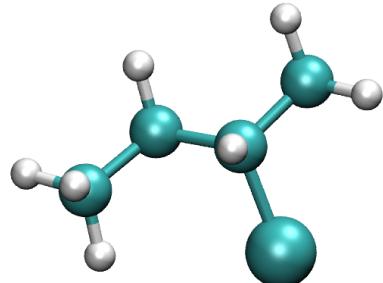


AsymmetricEnantiomers Número 10

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

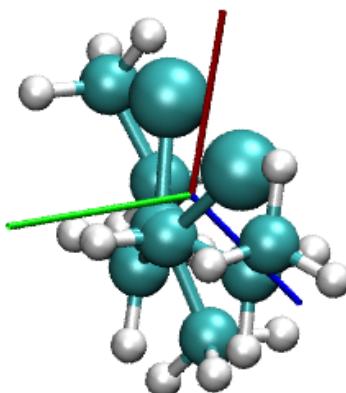
EingenVectors - Molecule A		
-0.986829	-0.161759	-0.00158112
0.161767	-0.986784	-0.00941025
-3.80279e-05	-0.00954208	0.999954

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

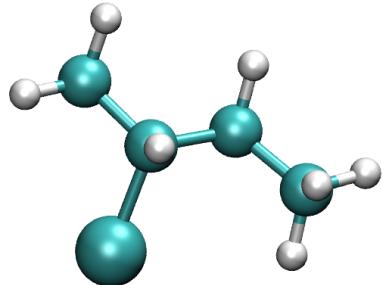
Enantiomers



AsymmetricEnantiomers Número 11

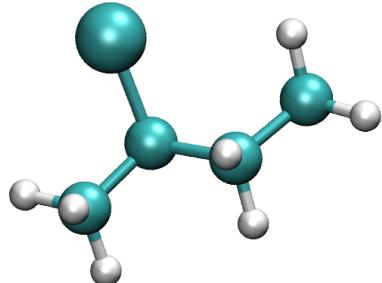
Molecule A

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

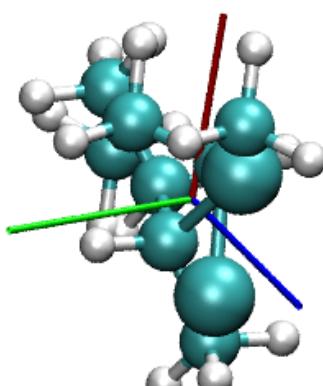
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

112.224	165.624	257.018
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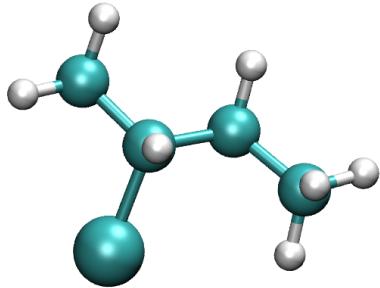
Equal



AsymmetricEnantiomers Número 12

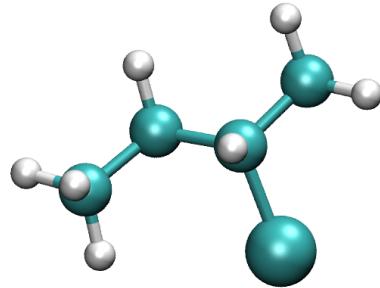
Molecule A

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

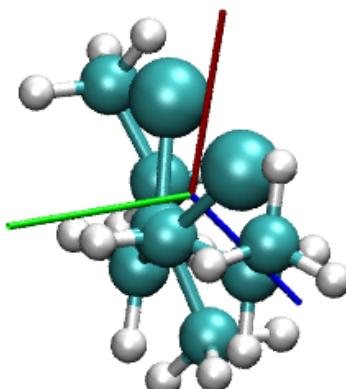
EingenValues - Molecule A

112.224	165.623	257.016
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EingenValues - Molecule B

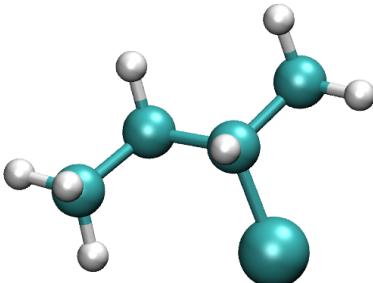
112.224	165.624	257.017
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Enantiomers



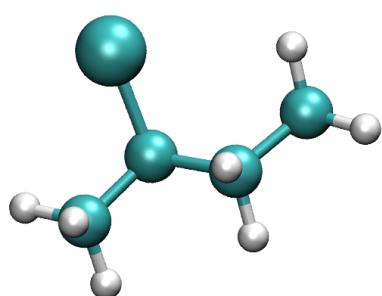
AsymmetricEnantiomers Número 13

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

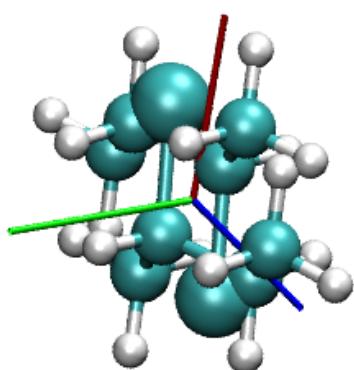
EingenValues - Molecule A

112.224	165.624	257.017
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EingenValues - Molecule B

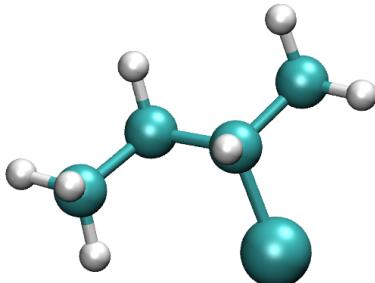
112.224	165.624	257.018
---------	---------	---------

Enantiomers



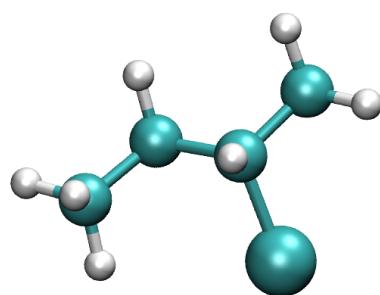
AsymmetricEnantiomers Número 14

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

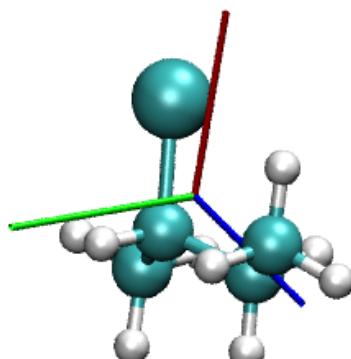
EingenValues - Molecule A

112.224	165.624	257.017
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EingenValues - Molecule B

112.224	165.624	257.017
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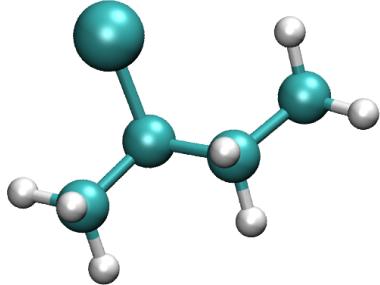
Equal



AsymmetricEnantiomers Número 15

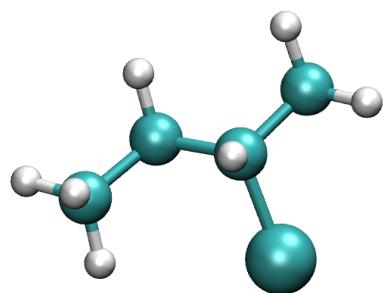
Molecule A

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

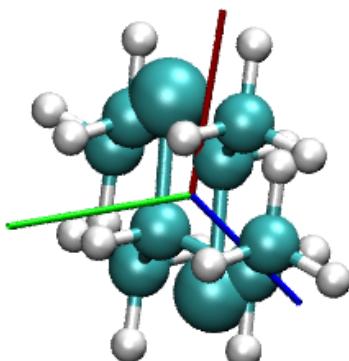
EingenValues - Molecule A

112.224	165.624	257.018
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EingenValues - Molecule B

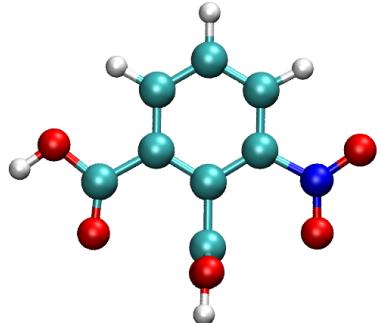
112.224	165.624	257.017
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Enantiomers

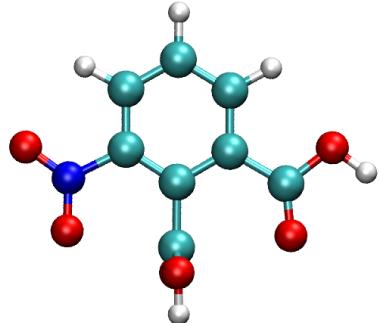


FireTest Número 16

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

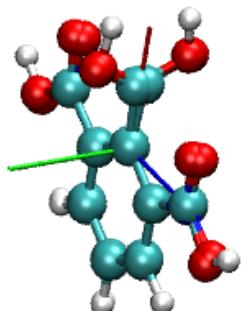
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

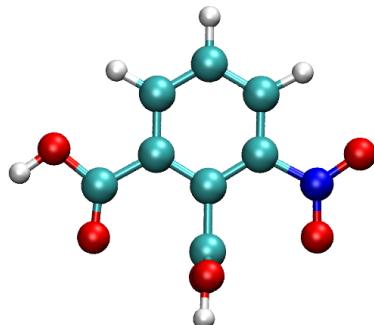
530.103	915.738	1361.08
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Equal

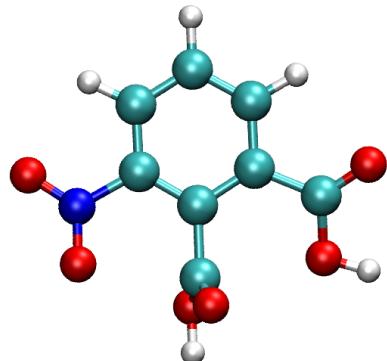


FireTest Número 17

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

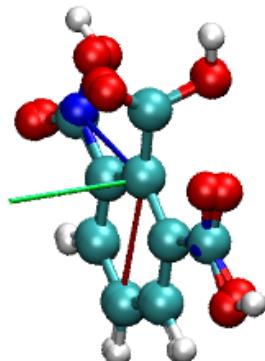
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

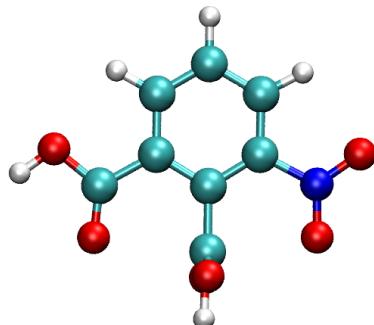
531.402	913.293	1353.16
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Different

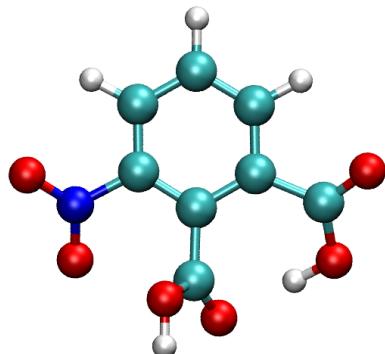


FireTest Número 18

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

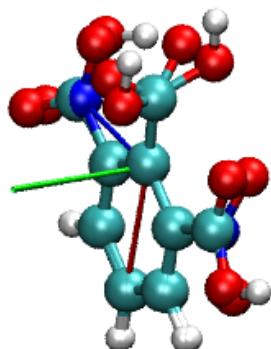
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

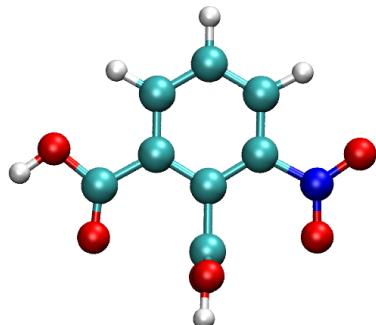
524.175	935.342	1359.19
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Different

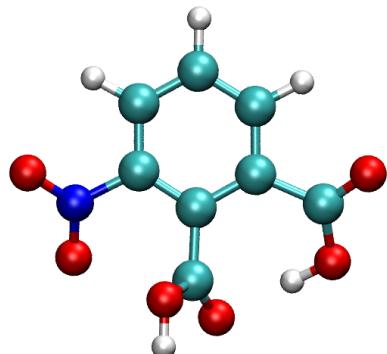


FireTest Número 19

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

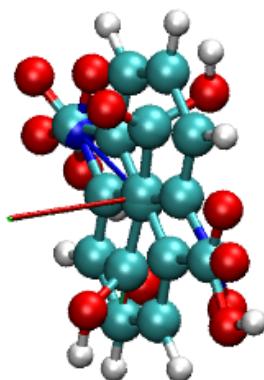
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

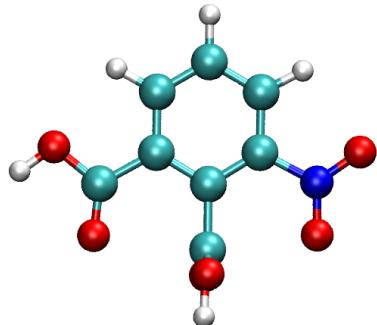
524.162	935.308	1359.22
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Different

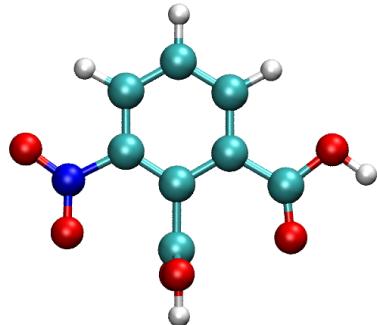


FireTest Número 20

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

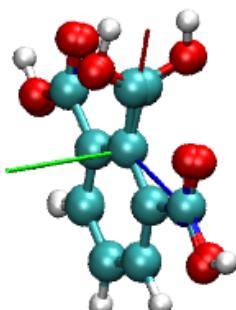
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

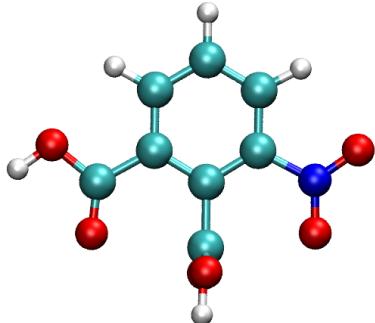
530.045	915.527	1360.79
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Equal

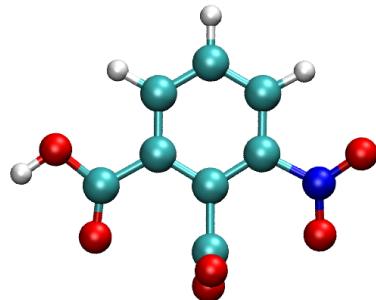


FireTest Número 21

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

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

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

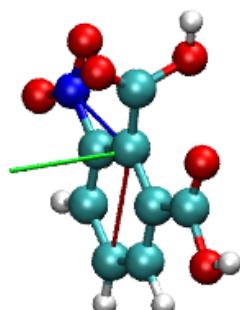
EigenValues - Molecule A

530.124	915.807	1361.14
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EigenValues - Molecule B

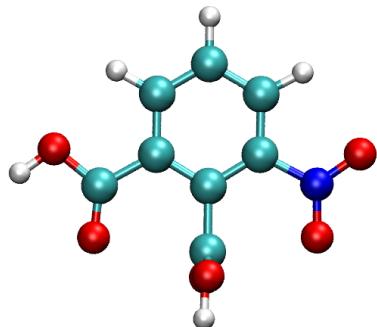
532.89	918.442	1356.93
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Different

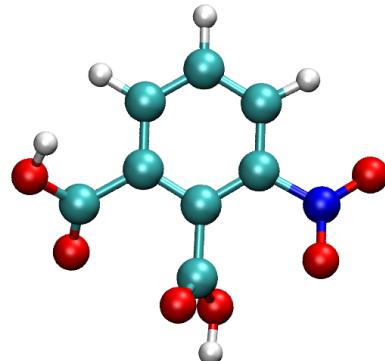


FireTest Número 22

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

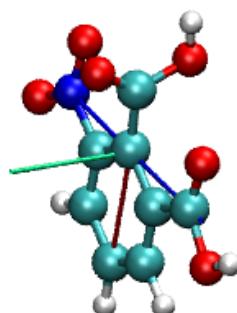
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

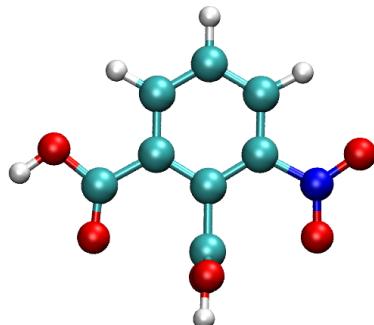
528.663	924.928	1336.12
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Different

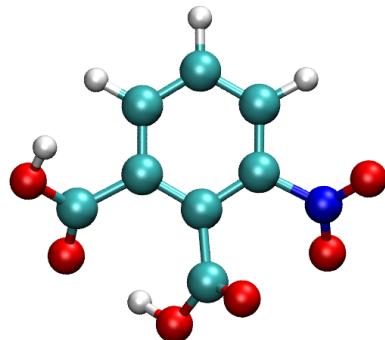


FireTest Número 23

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

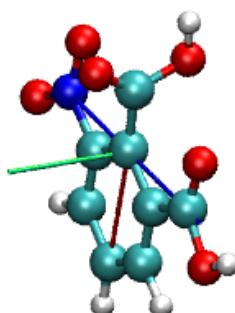
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

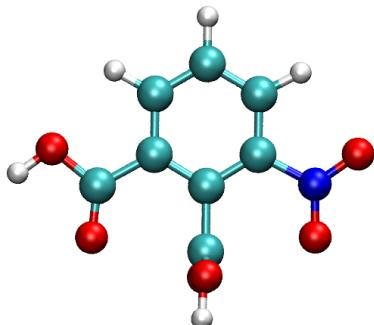
521.475	949.659	1346.18
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Different

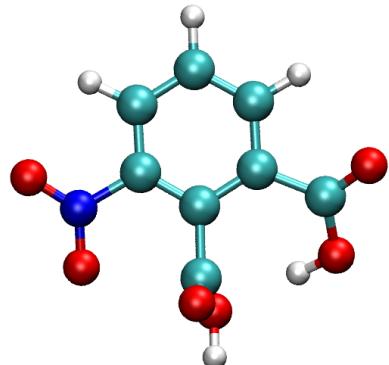


FireTest Número 24

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

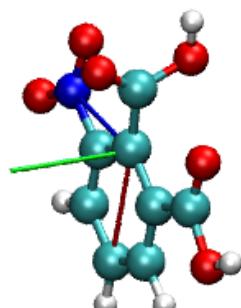
EigenValues - Molecule A

530.124	915.807	1361.14
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EigenValues - Molecule B

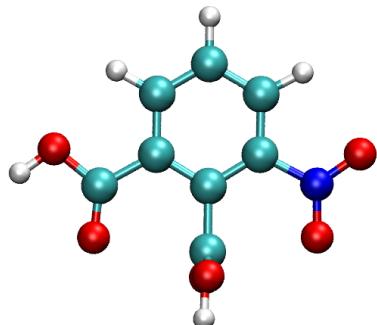
533.726	920.137	1348.3
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Different

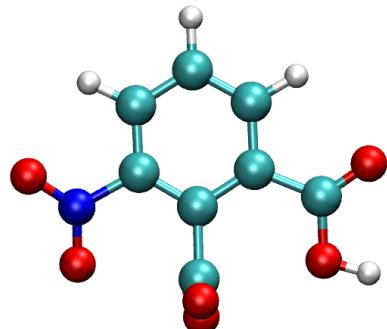


FireTest Número 25

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

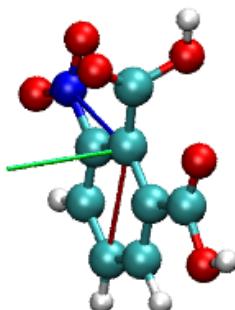
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

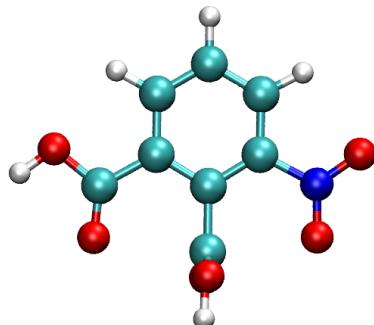
534.81	913.339	1353.78
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Different

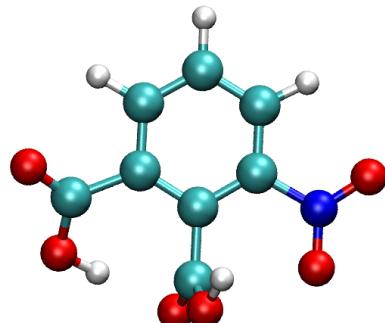


FireTest Número 26

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

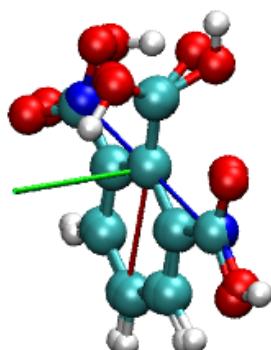
EingenValues - Molecule A

530.124	915.807	1361.14
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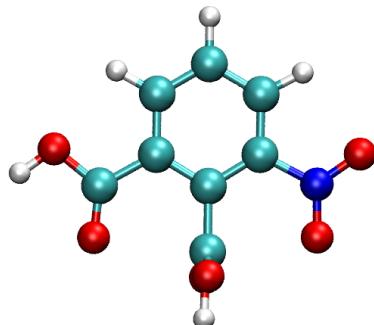
EingenValues - Molecule B

531.691	929.434	1355.4
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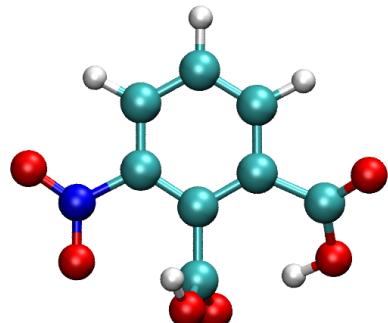
Different



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

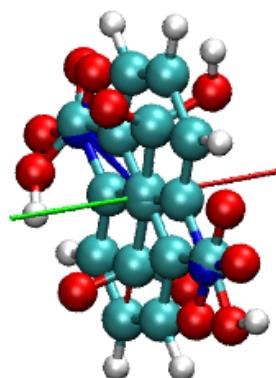
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

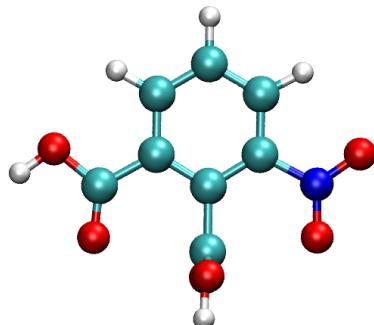
531.698	929.417	1355.4
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Different

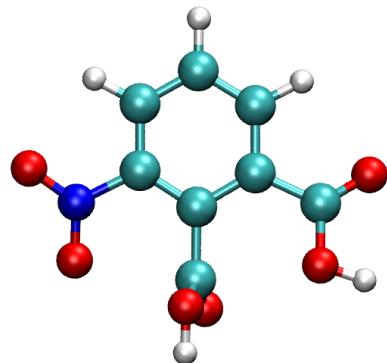


FireTest Número 28

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

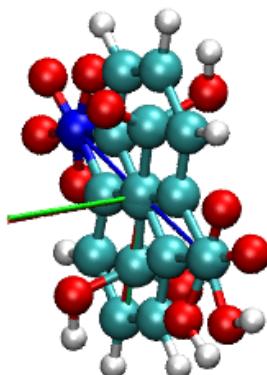
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

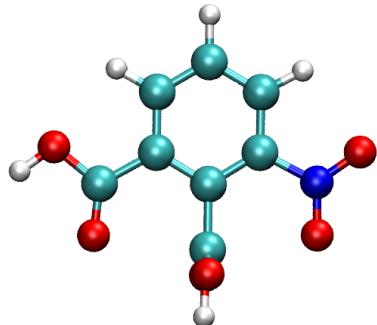
531.43	913.309	1353.35
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Different

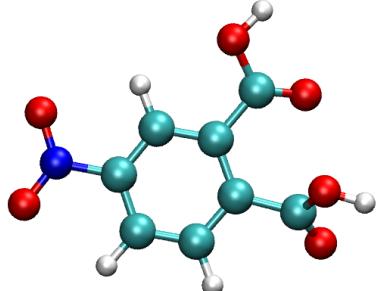


FireTest Número 29

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

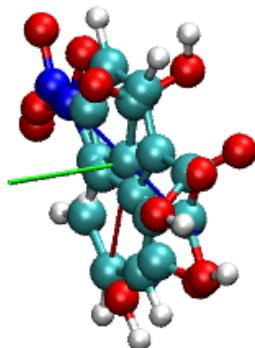
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

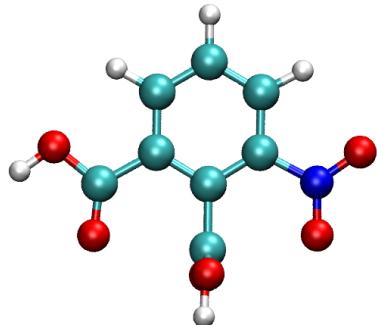
479.363	1242.41	1647.39
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Different

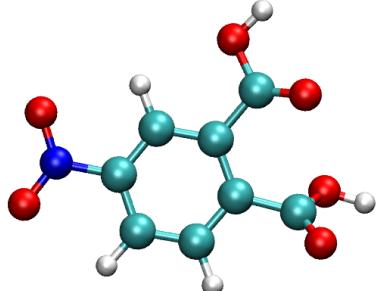


FireTest Número 30

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

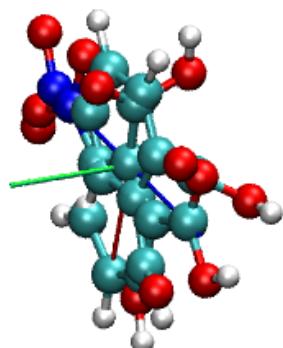
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

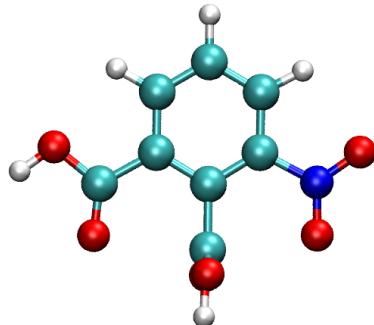
479.308	1242.41	1647.31
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Different

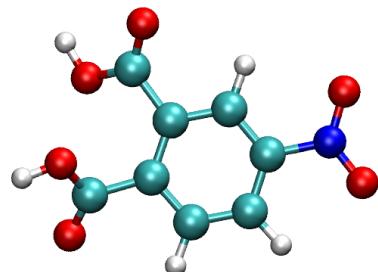


FireTest Número 31

Molecule A 3NFAACa



Molecule B 4NFAACC



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

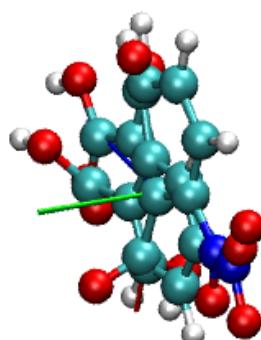
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

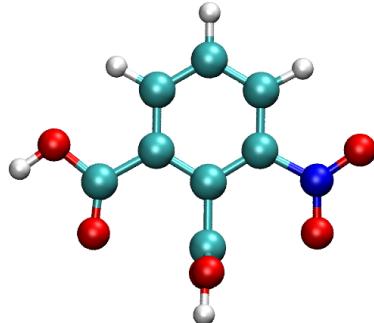
482.027	1240.32	1647.08
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Different

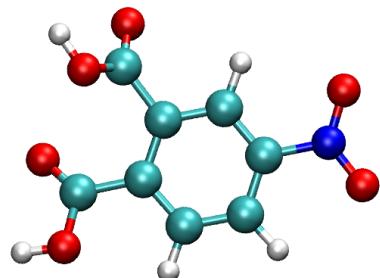


FireTest Número 32

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

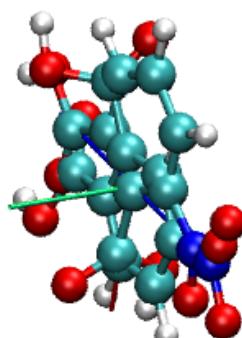
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

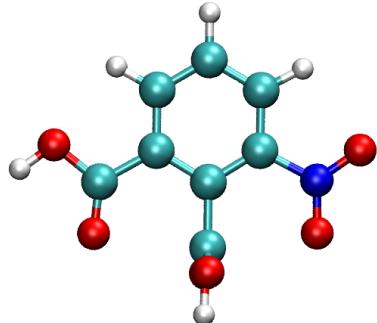
491.663	1231.14	1650.13
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Different

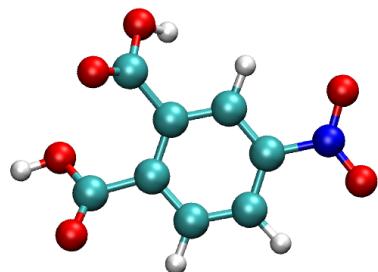


FireTest Número 33

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

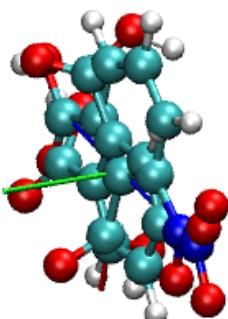
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

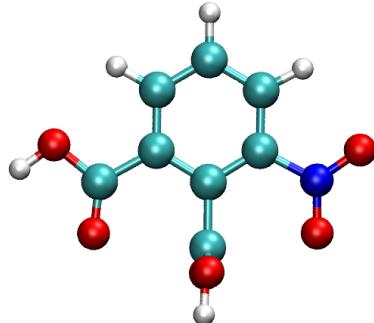
489.011	1233.7	1641.81
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Different

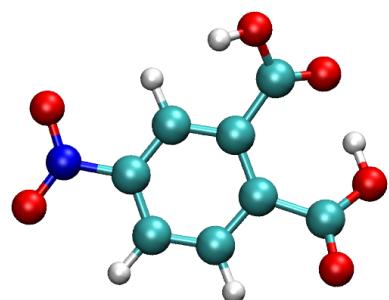


FireTest Número 34

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

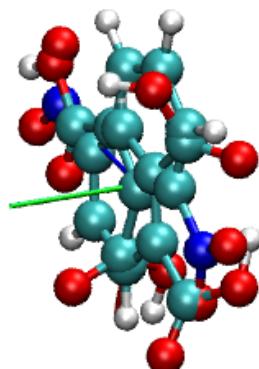
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

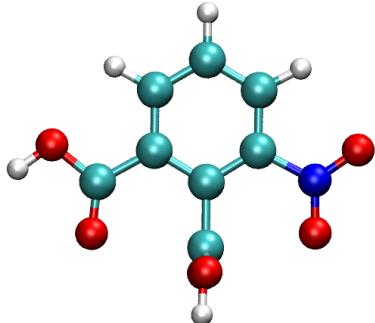
509.668	1219.11	1681.18
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Different

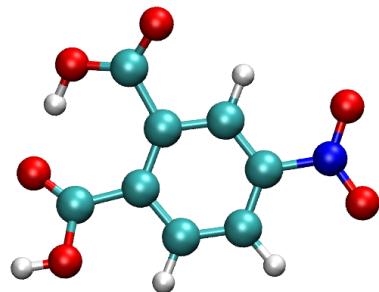


FireTest Número 35

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

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

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

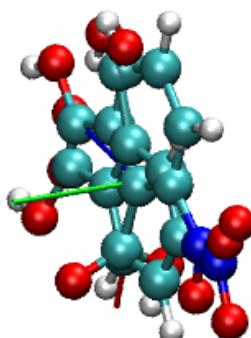
EigenValues - Molecule A

530.124	915.807	1361.14
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EigenValues - Molecule B

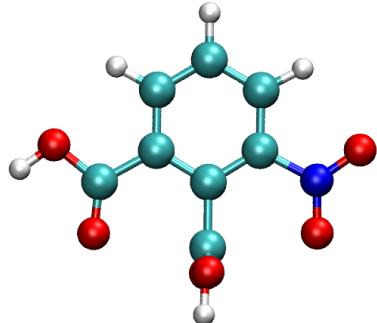
513.751	1208.07	1700.9
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Different

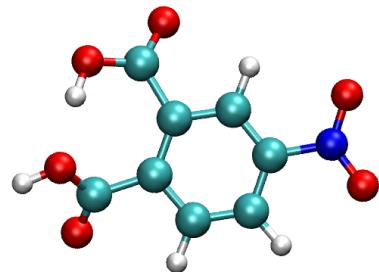


FireTest Número 36

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

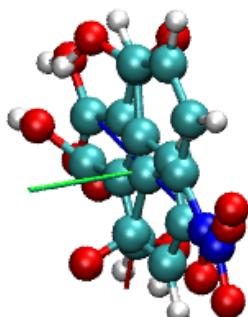
EingenValues - Molecule A

530.124	915.807	1361.14
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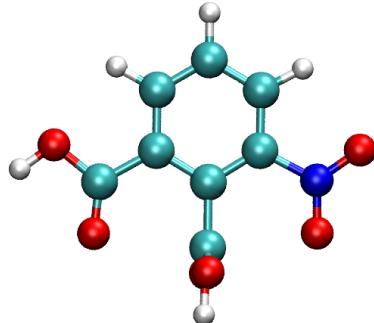
EingenValues - Molecule B

502.409	1232.26	1676.02
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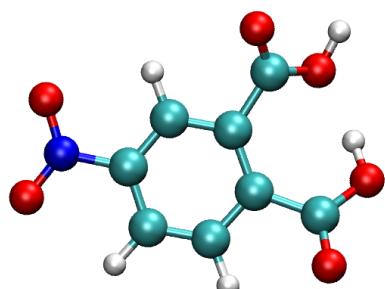
Different



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

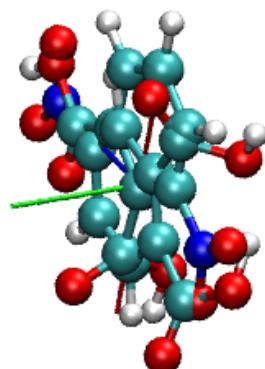
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

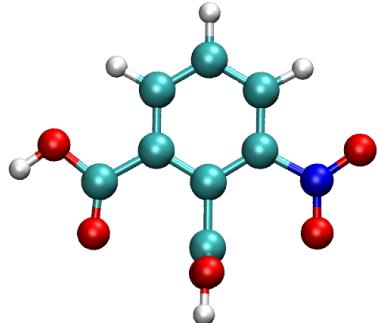
509.897	1225.65	1680.83
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Different

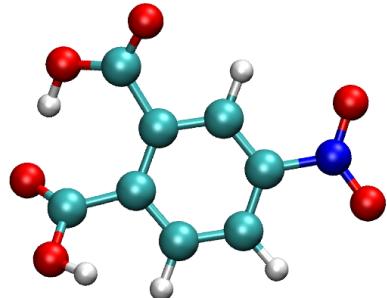


FireTest Número 38

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

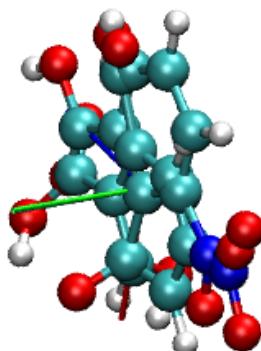
EingenValues - Molecule A

530.124	915.807	1361.14
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EingenValues - Molecule B

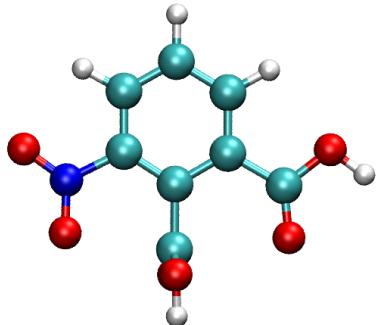
506.607	1222.36	1678.43
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Different

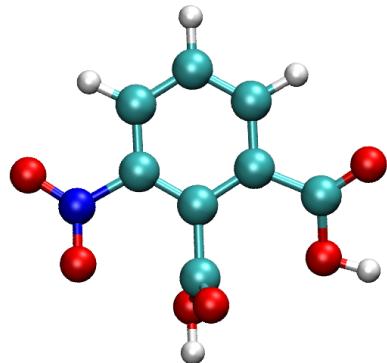


FireTest Número 39

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

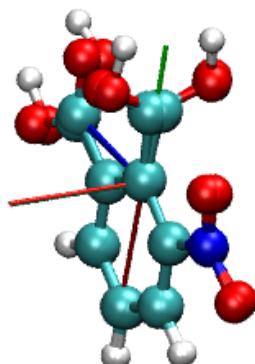
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

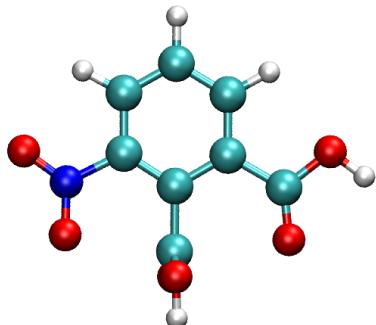
531.402	913.293	1353.16
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Different

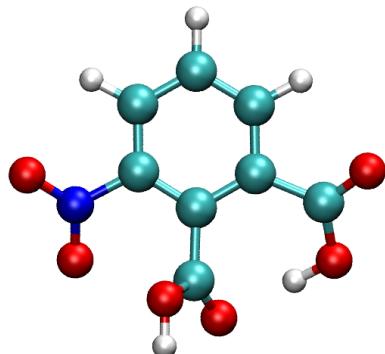


FireTest Número 40

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

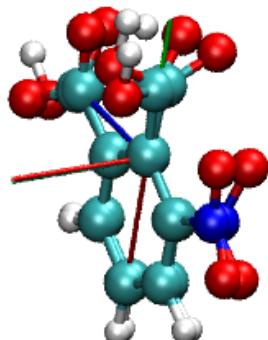
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

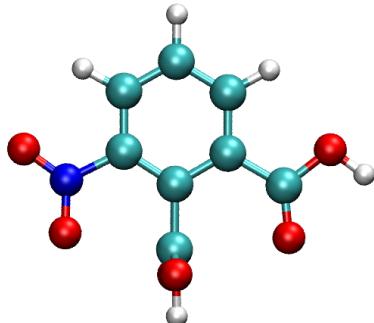
524.175	935.342	1359.19
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Different

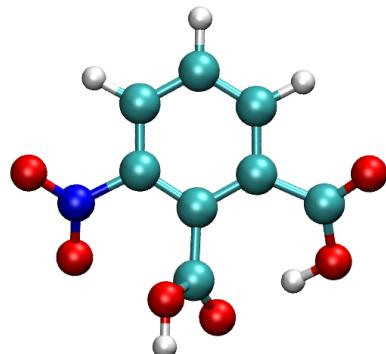


FireTest Número 41

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

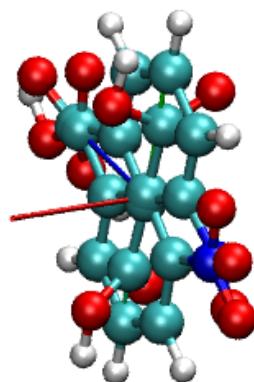
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

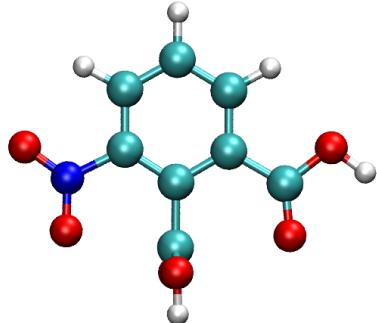
524.162	935.308	1359.22
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Different

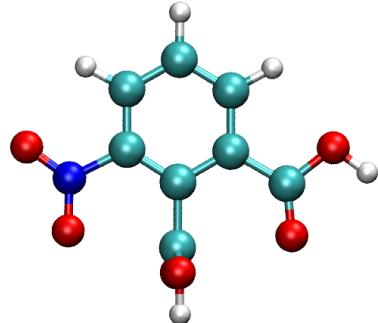


FireTest Número 42

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

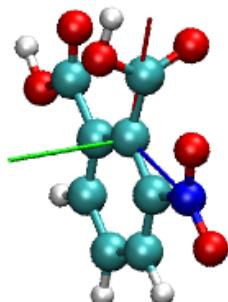
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

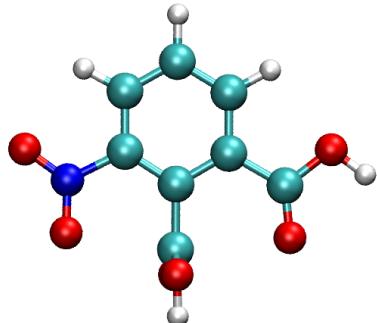
530.045	915.527	1360.79
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Equal

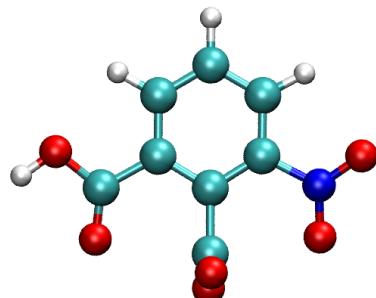


FireTest Número 43

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

EigenVectors - Molecule A

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

EigenVectors - Molecule B

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

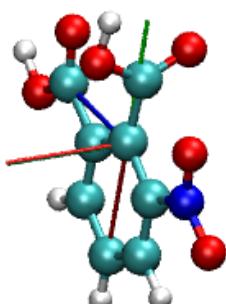
EigenValues - Molecule A

530.103	915.738	1361.08
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EigenValues - Molecule B

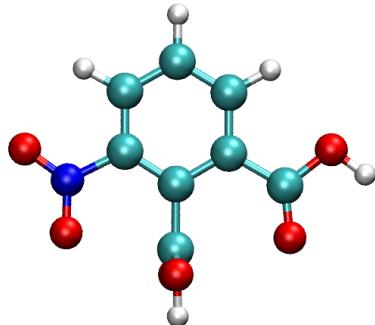
532.89	918.442	1356.93
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Different

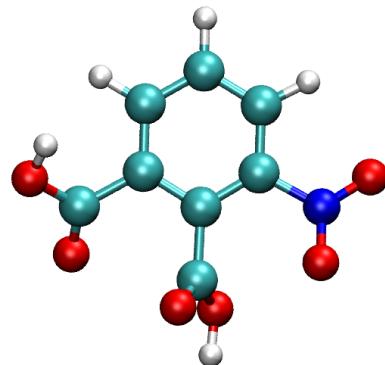


FireTest Número 44

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

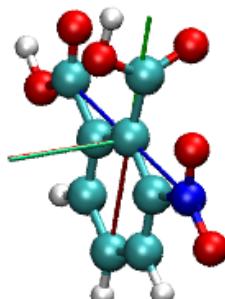
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

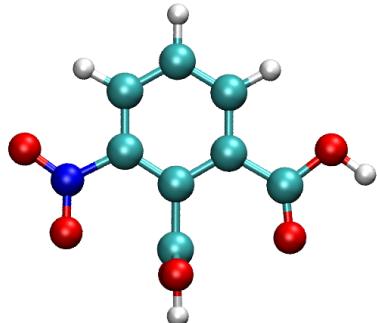
528.663	924.928	1336.12
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Different

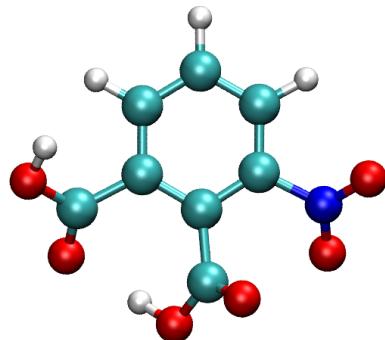


FireTest Número 45

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

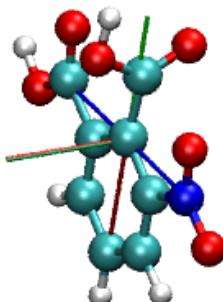
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

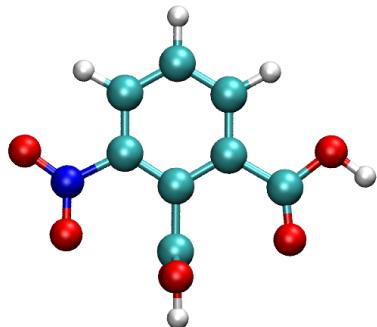
521.475	949.659	1346.18
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Different

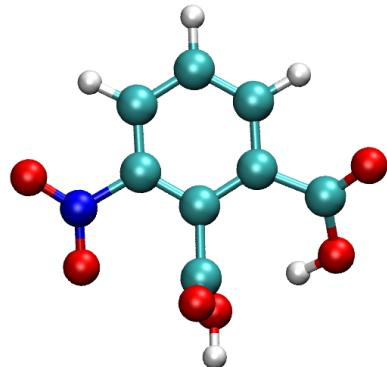


FireTest Número 46

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

EigenVectors - Molecule A

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

EigenVectors - Molecule B

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

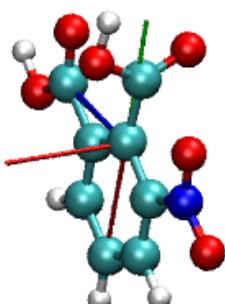
EigenValues - Molecule A

530.103	915.738	1361.08
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EigenValues - Molecule B

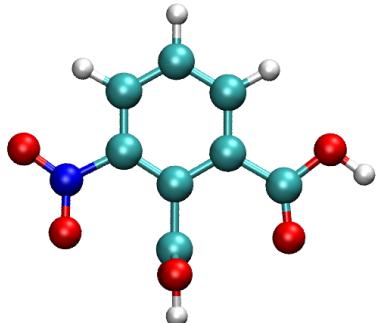
533.726	920.137	1348.3
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Different

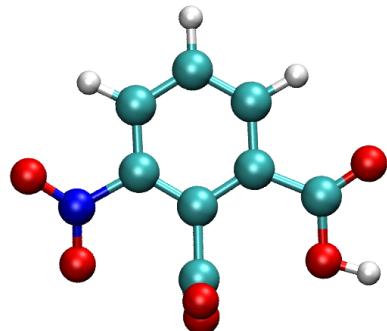


FireTest Número 47

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

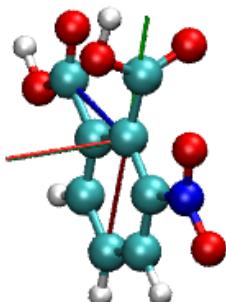
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

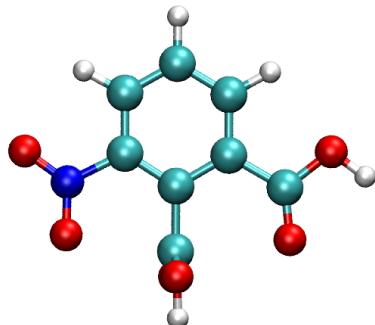
534.81	913.339	1353.78
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Different

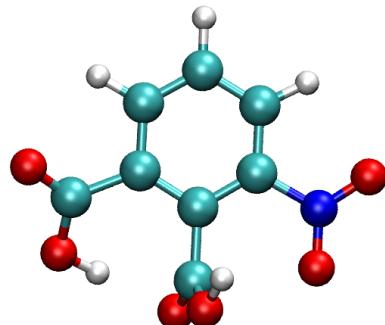


FireTest Número 48

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

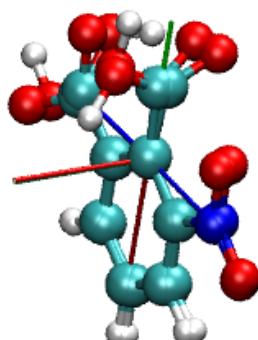
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

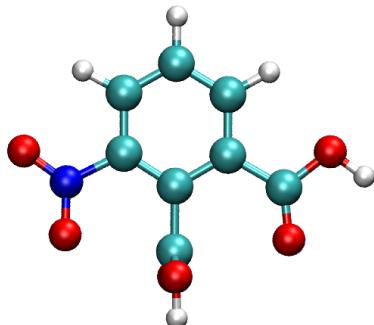
531.691	929.434	1355.4
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Different

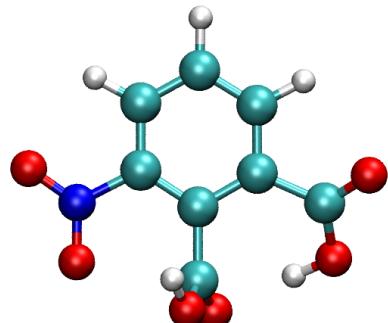


FireTest Número 49

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

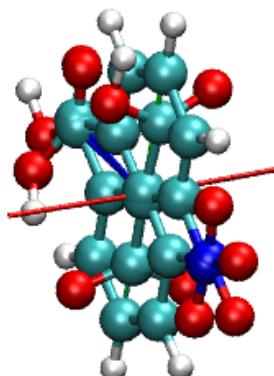
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

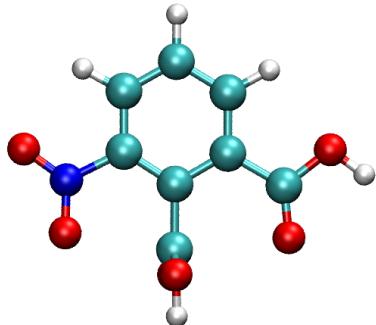
531.698	929.417	1355.4
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Different

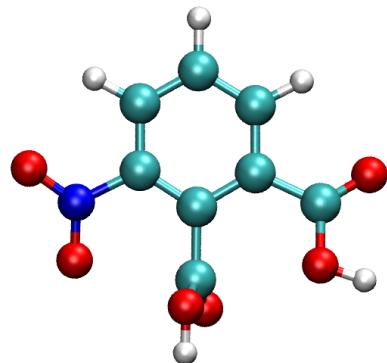


FireTest Número 50

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

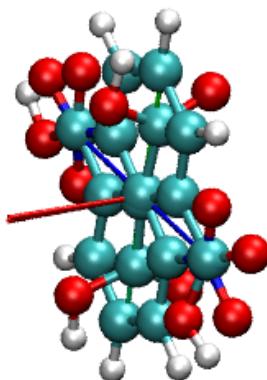
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

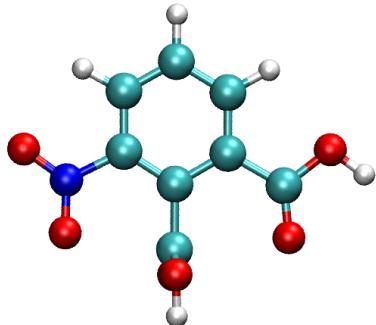
531.43	913.309	1353.35
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Different

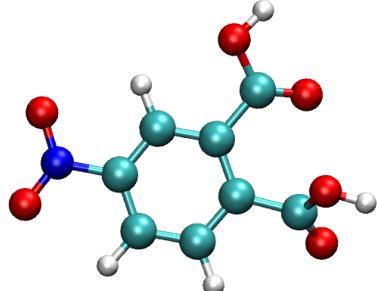


FireTest Número 51

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

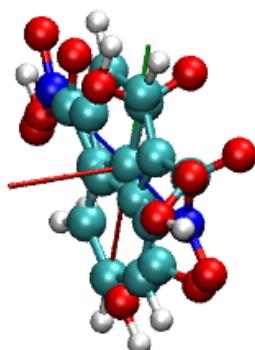
EingenValues - Molecule A

530.103	915.738	1361.08
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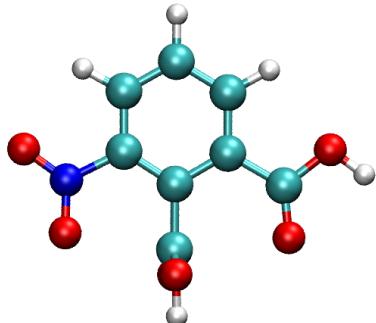
EingenValues - Molecule B

479.363	1242.41	1647.39
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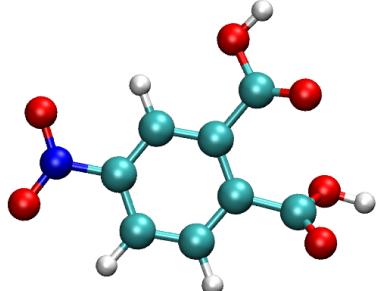
Different



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

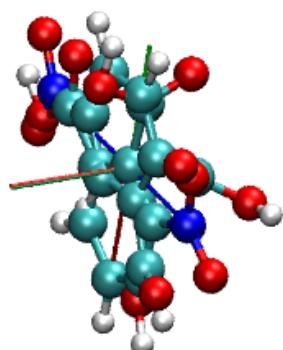
EingenValues - Molecule A

530.103	915.738	1361.08
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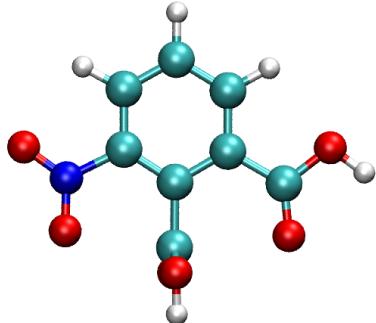
EingenValues - Molecule B

479.308	1242.41	1647.31
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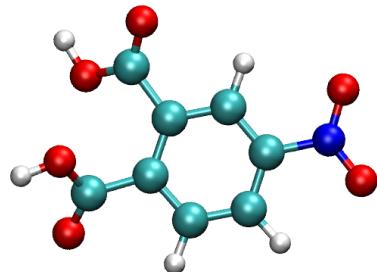
Different



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

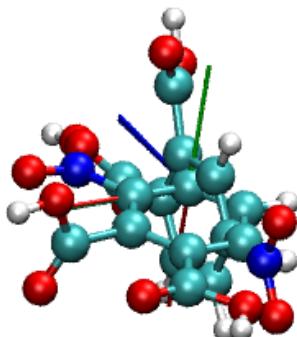
EingenValues - Molecule A

530.103	915.738	1361.08
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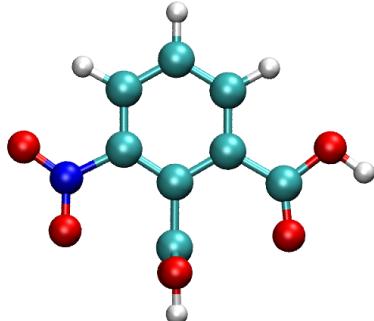
EingenValues - Molecule B

482.027	1240.32	1647.08
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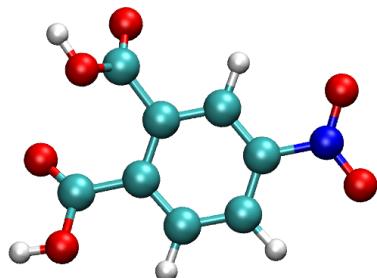
Different



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

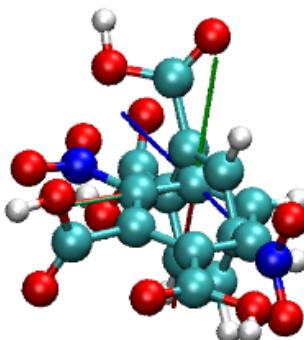
EingenValues - Molecule A

530.103	915.738	1361.08
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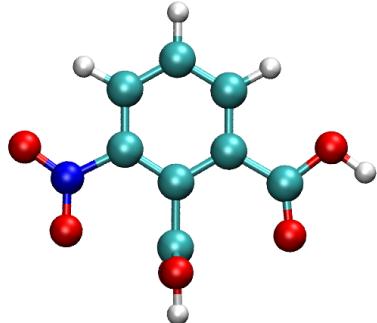
EingenValues - Molecule B

491.663	1231.14	1650.13
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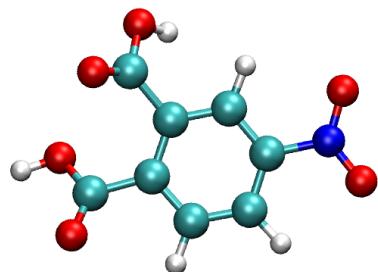
Different



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

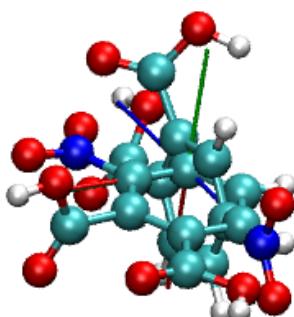
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

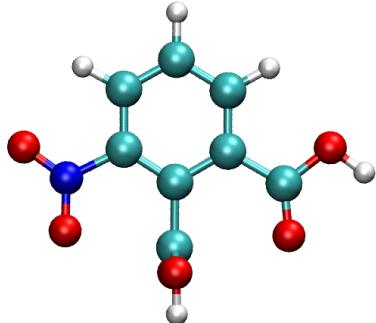
489.011	1233.7	1641.81
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Different

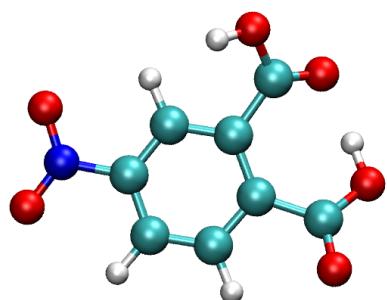


FireTest Número 56

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

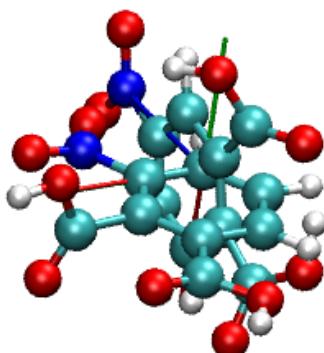
EingenValues - Molecule A

530.103	915.738	1361.08
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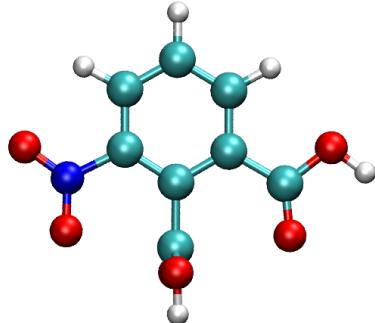
EingenValues - Molecule B

509.668	1219.11	1681.18
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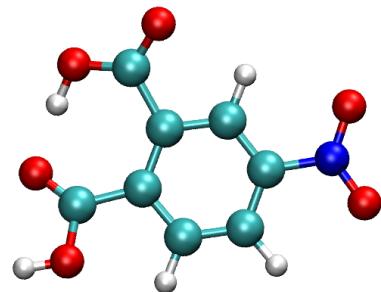
Different



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

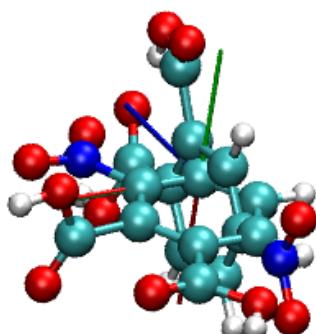
EingenValues - Molecule A

530.103	915.738	1361.08
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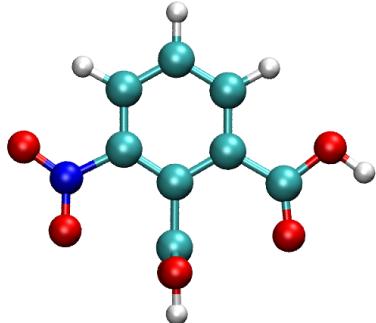
EingenValues - Molecule B

513.751	1208.07	1700.9
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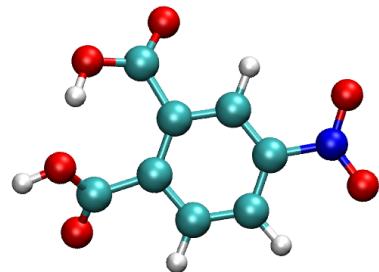
Different



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

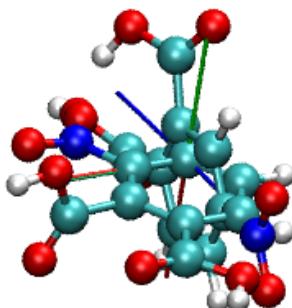
EingenValues - Molecule A

530.103	915.738	1361.08
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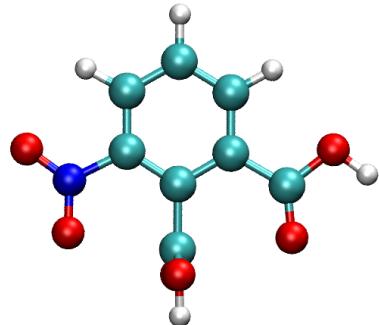
EingenValues - Molecule B

502.409	1232.26	1676.02
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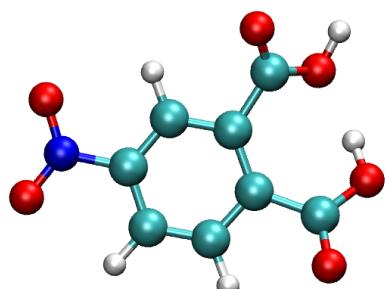
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

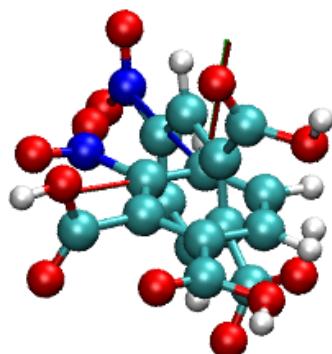
EingenValues - Molecule A

530.103	915.738	1361.08
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EingenValues - Molecule B

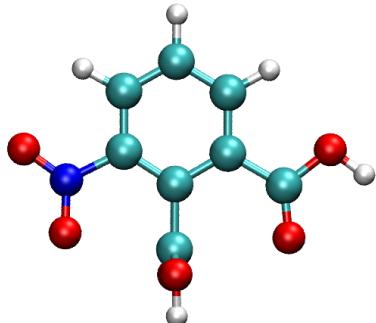
509.897	1225.65	1680.83
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Different

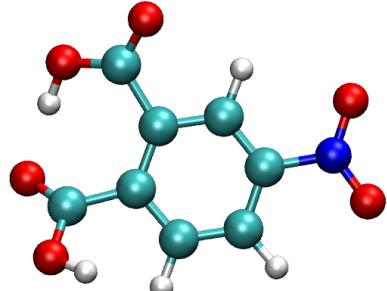


FireTest Número 60

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

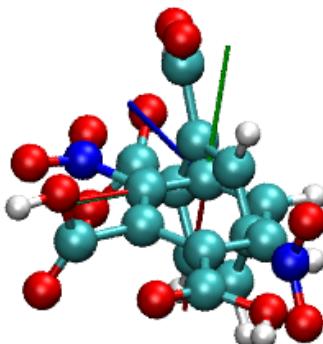
EingenValues - Molecule A

530.103	915.738	1361.08
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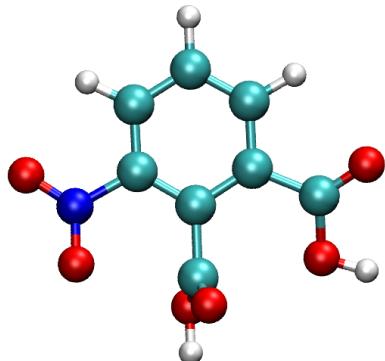
EingenValues - Molecule B

506.607	1222.36	1678.43
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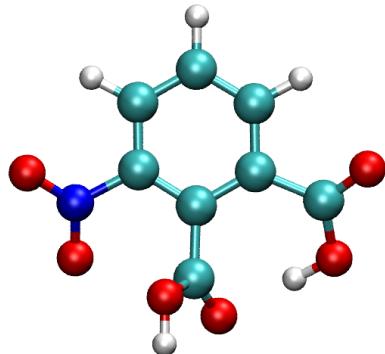
Different



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

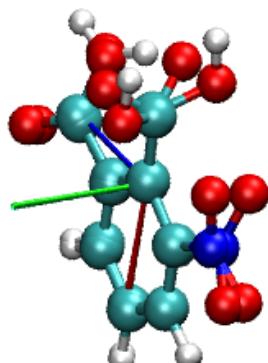
EingenValues - Molecule A

531.402	913.293	1353.16
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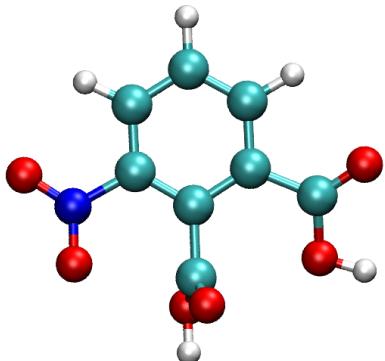
EingenValues - Molecule B

524.175	935.342	1359.19
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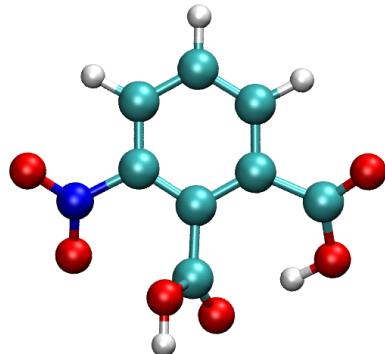
Different



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

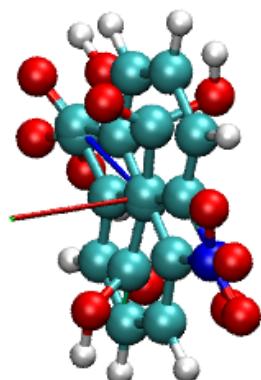
EingenValues - Molecule A

531.402	913.293	1353.16
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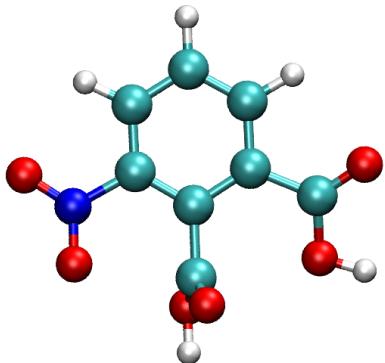
EingenValues - Molecule B

524.162	935.308	1359.22
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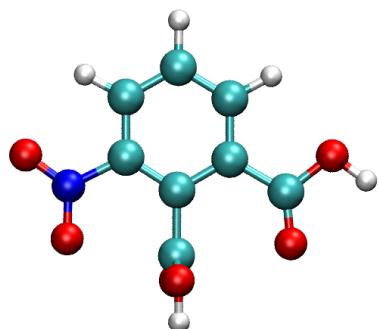
Different



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

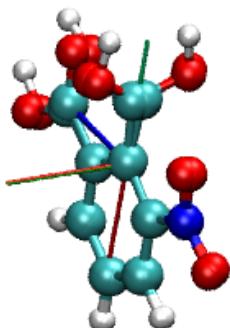
EingenValues - Molecule A

531.402	913.293	1353.16
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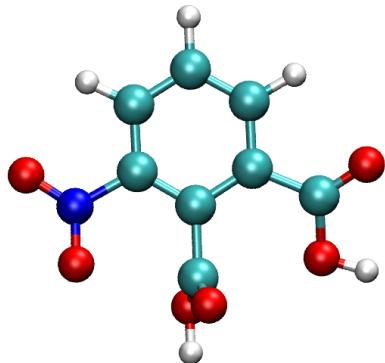
EingenValues - Molecule B

530.045	915.527	1360.79
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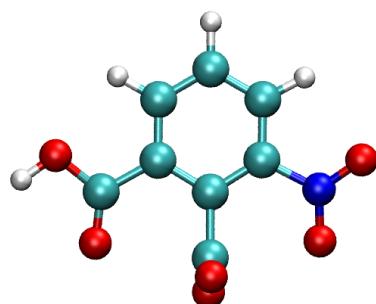
Different



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

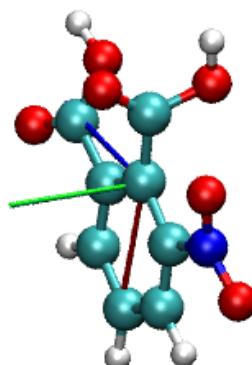
EingenValues - Molecule A

531.402	913.293	1353.16
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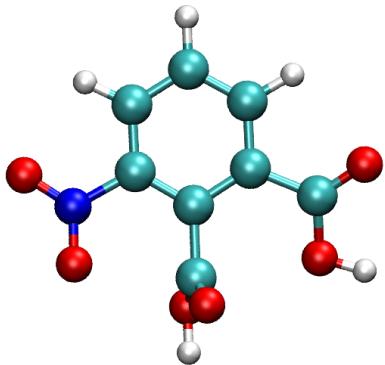
EingenValues - Molecule B

532.89	918.442	1356.93
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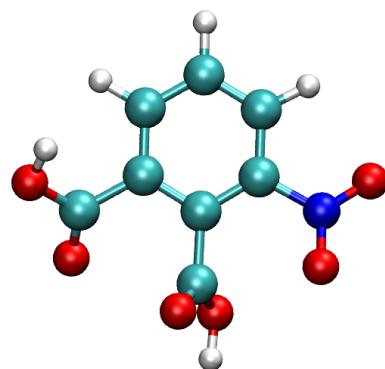
Different



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

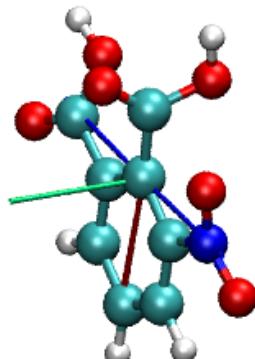
EingenValues - Molecule A

531.402	913.293	1353.16
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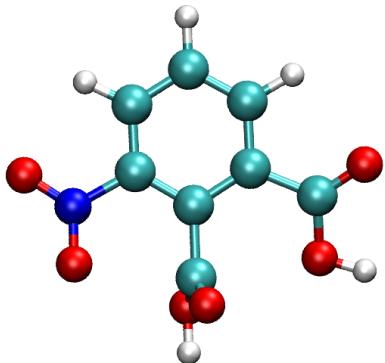
EingenValues - Molecule B

528.663	924.928	1336.12
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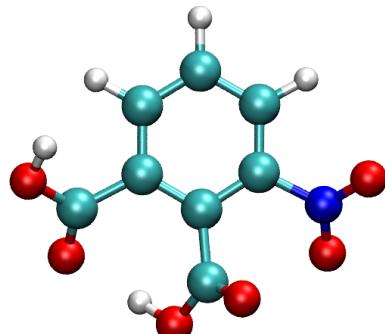
Different



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

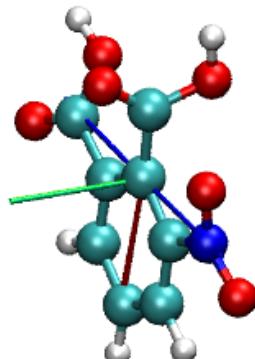
EingenValues - Molecule A

531.402	913.293	1353.16
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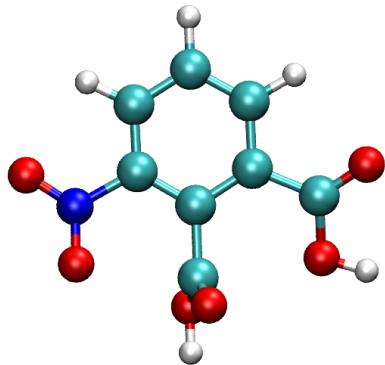
EingenValues - Molecule B

521.475	949.659	1346.18
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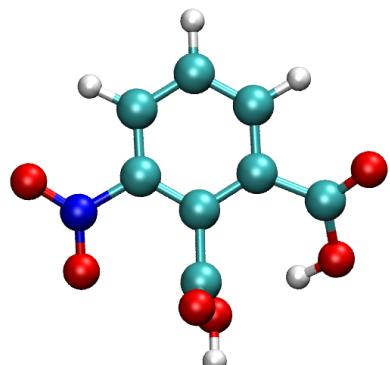
Different



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

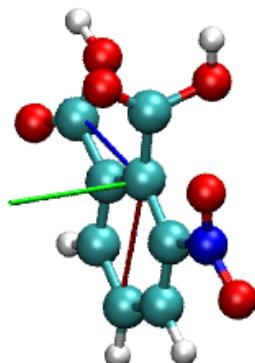
EingenValues - Molecule A

531.402	913.293	1353.16
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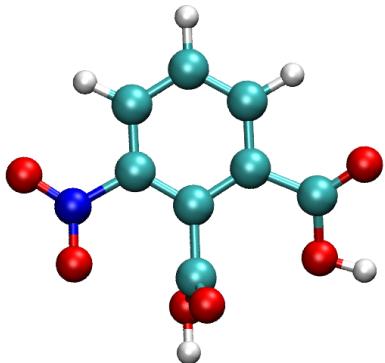
EingenValues - Molecule B

533.726	920.137	1348.3
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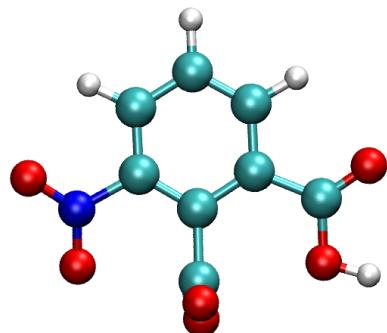
Different



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

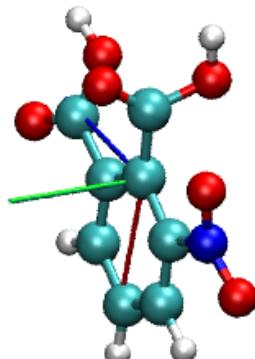
EingenValues - Molecule A

531.402	913.293	1353.16
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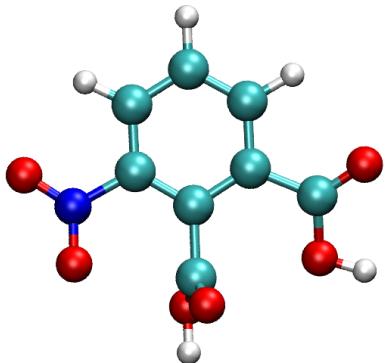
EingenValues - Molecule B

534.81	913.339	1353.78
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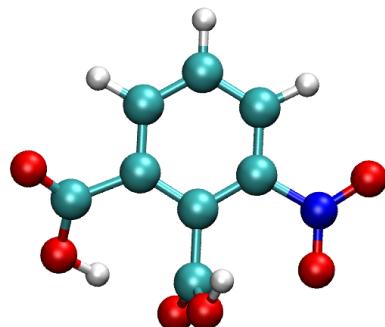
Different



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

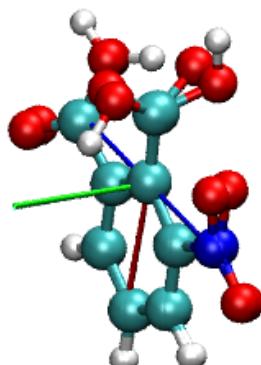
EingenValues - Molecule A

531.402	913.293	1353.16
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EingenValues - Molecule B

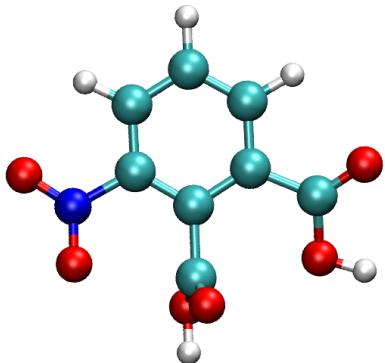
531.691	929.434	1355.4
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Different

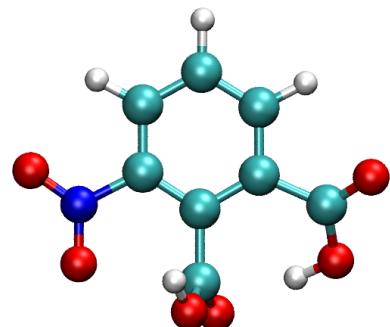


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Molecule A 3NFAACc



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

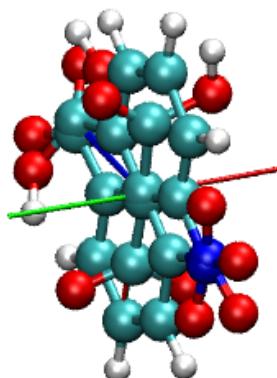
EingenValues - Molecule A

531.402	913.293	1353.16
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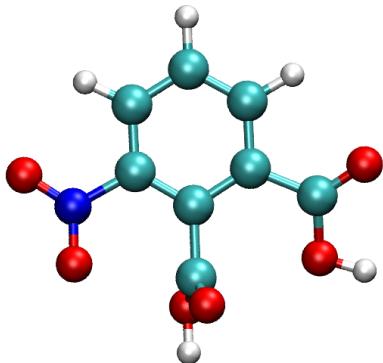
EingenValues - Molecule B

531.698	929.417	1355.4
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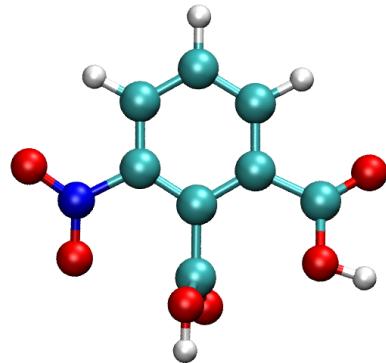
Different



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

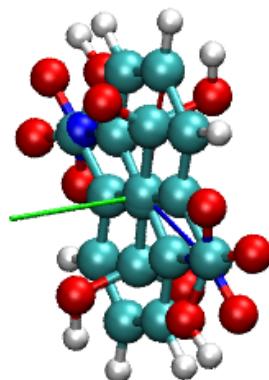
EingenValues - Molecule A

531.402	913.293	1353.16
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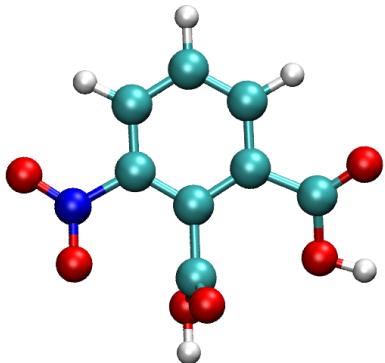
EingenValues - Molecule B

531.43	913.309	1353.35
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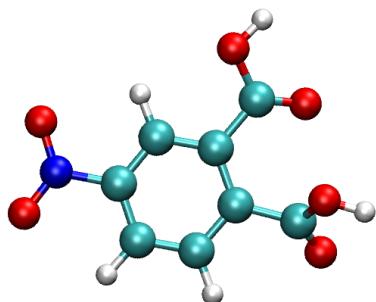
Enantiomers



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

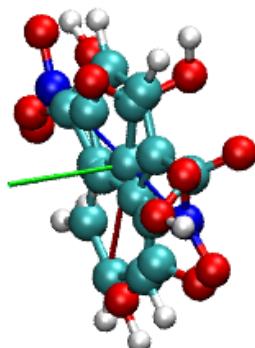
EingenValues - Molecule A

531.402	913.293	1353.16
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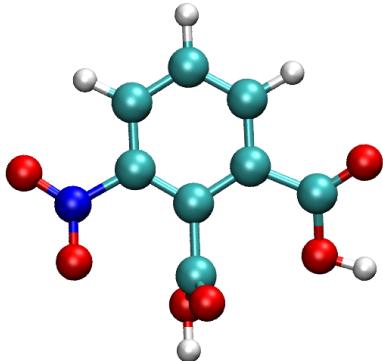
EingenValues - Molecule B

479.363	1242.41	1647.39
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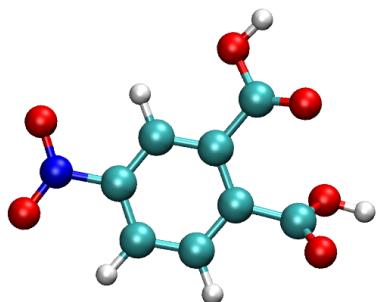
Different



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

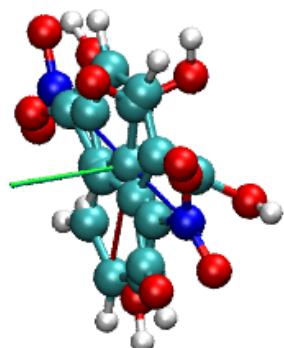
EingenValues - Molecule A

531.402	913.293	1353.16
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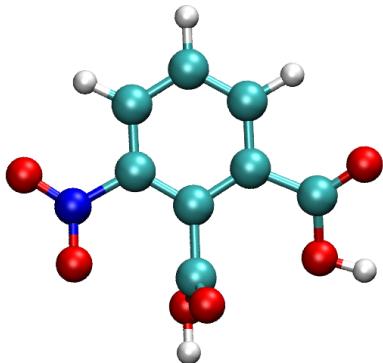
EingenValues - Molecule B

479.308	1242.41	1647.31
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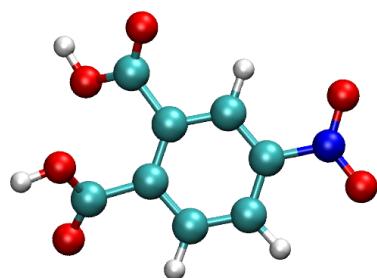
Different



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

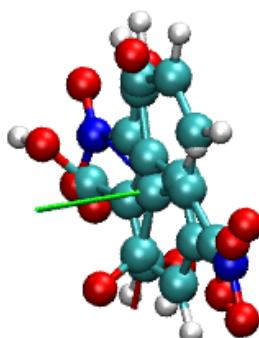
EingenValues - Molecule A

531.402	913.293	1353.16
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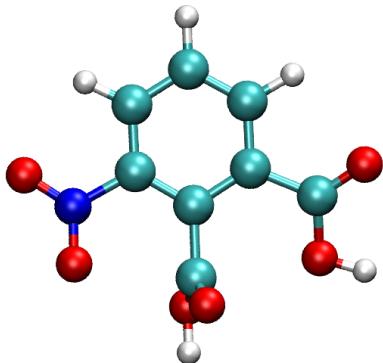
EingenValues - Molecule B

482.027	1240.32	1647.08
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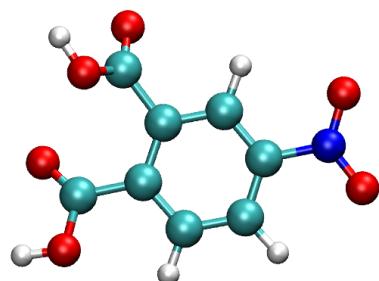
Different



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

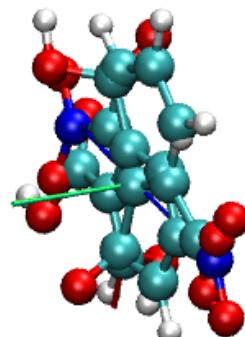
EingenValues - Molecule A

531.402	913.293	1353.16
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EingenValues - Molecule B

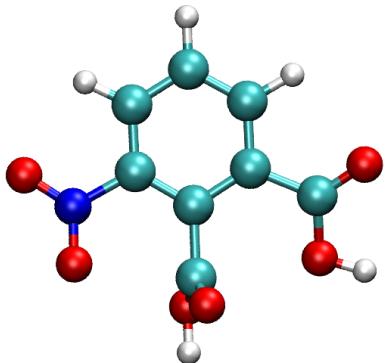
491.663	1231.14	1650.13
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Different

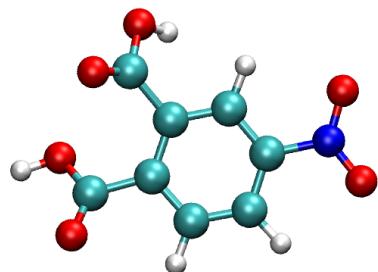


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Molecule A 3NFAACc



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

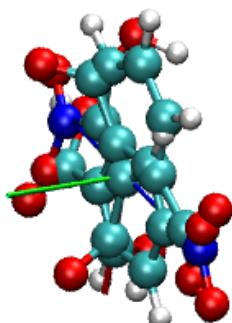
EingenValues - Molecule A

531.402	913.293	1353.16
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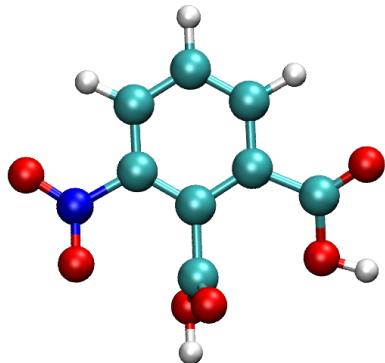
EingenValues - Molecule B

489.011	1233.7	1641.81
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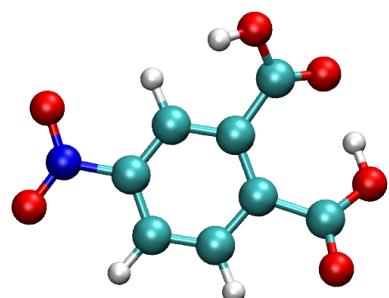
Different



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

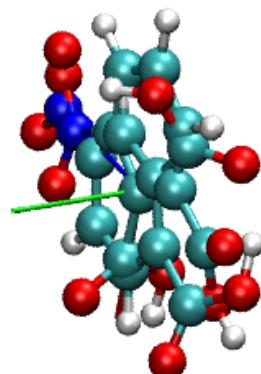
EingenValues - Molecule A

531.402	913.293	1353.16
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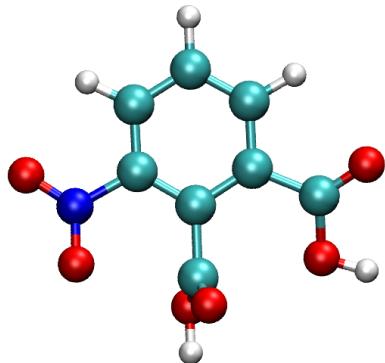
EingenValues - Molecule B

509.668	1219.11	1681.18
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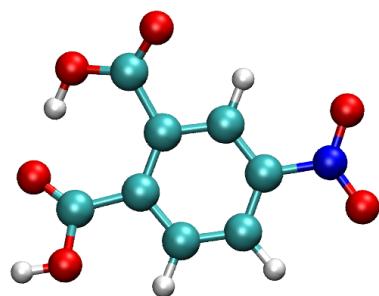
Different



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

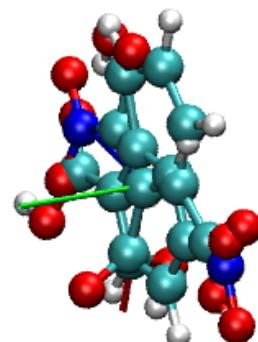
EingenValues - Molecule A

531.402	913.293	1353.16
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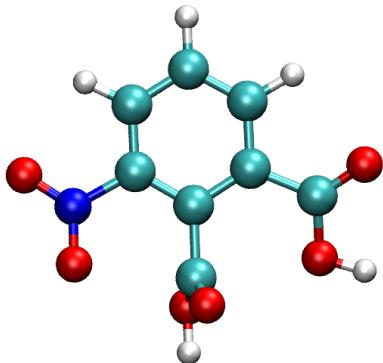
EingenValues - Molecule B

513.751	1208.07	1700.9
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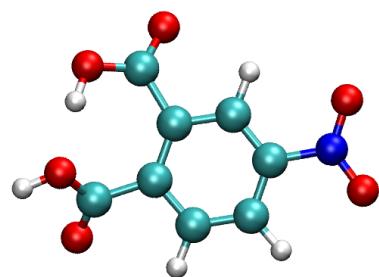
Different



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

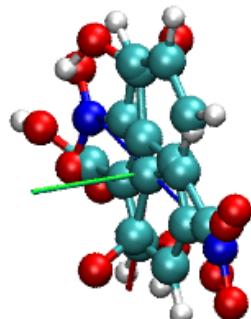
EingenValues - Molecule A

531.402	913.293	1353.16
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EingenValues - Molecule B

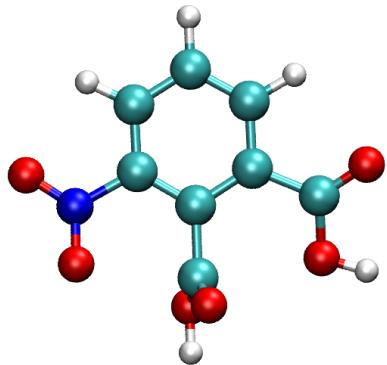
502.409	1232.26	1676.02
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Different

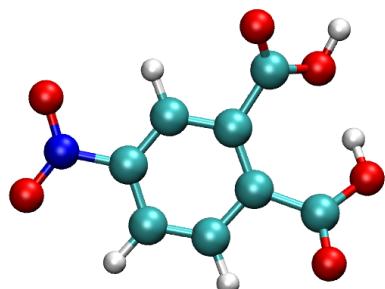


FireTest Número 80

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

EigenVectors - Molecule A

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

EigenVectors - Molecule B

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

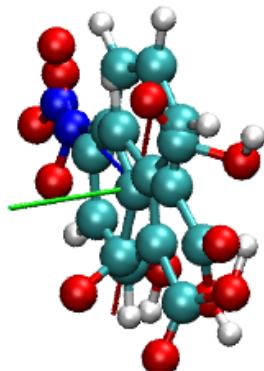
EigenValues - Molecule A

531.402	913.293	1353.16
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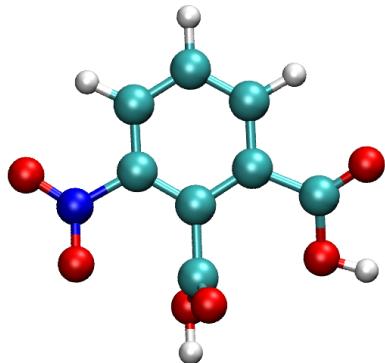
EigenValues - Molecule B

509.897	1225.65	1680.83
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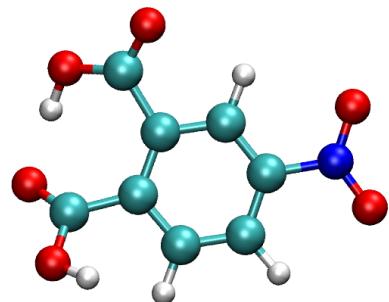
Different



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

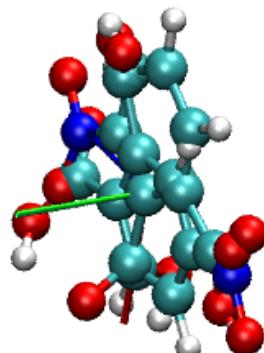
EingenValues - Molecule A

531.402	913.293	1353.16
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EingenValues - Molecule B

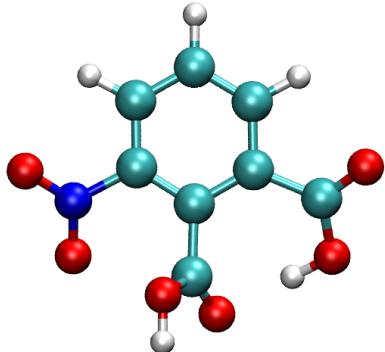
506.607	1222.36	1678.43
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Different

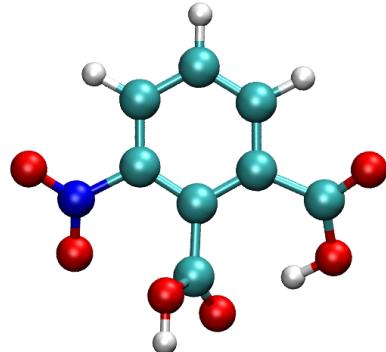


FireTest Número 82

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

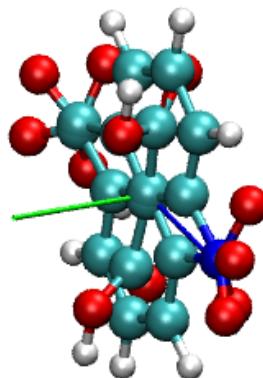
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

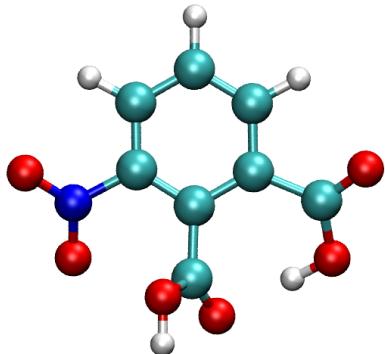
524.162	935.308	1359.22
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Enantiomers

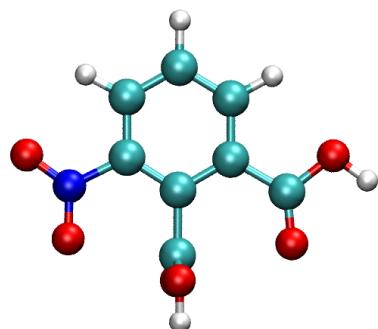


FireTest Número 83

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

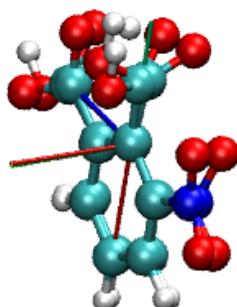
EingenValues - Molecule A

524.175	935.342	1359.19
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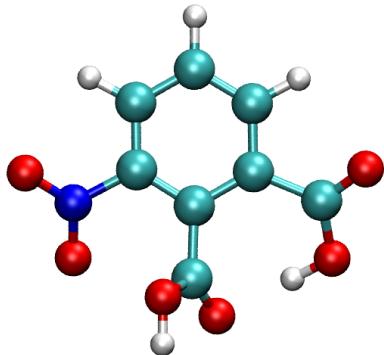
EingenValues - Molecule B

530.045	915.527	1360.79
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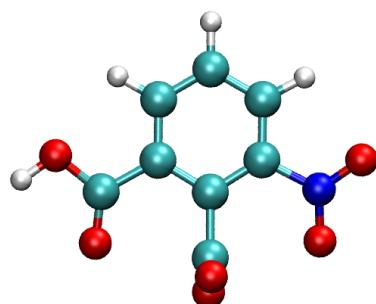
Different



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

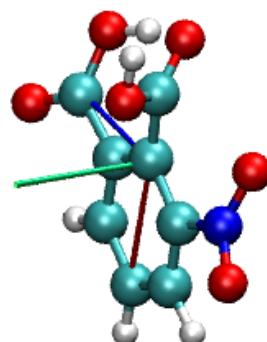
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

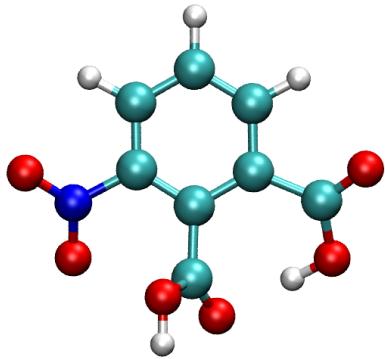
532.89	918.442	1356.93
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Different

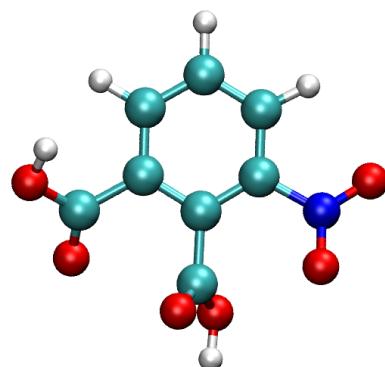


FireTest Número 85

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

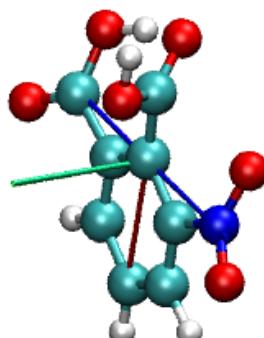
EingenValues - Molecule A

524.175	935.342	1359.19
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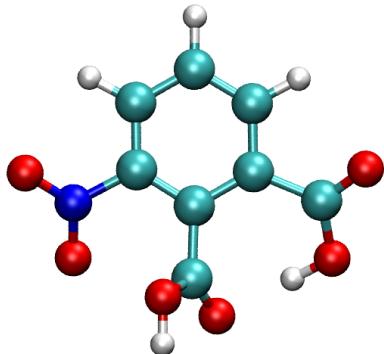
EingenValues - Molecule B

528.663	924.928	1336.12
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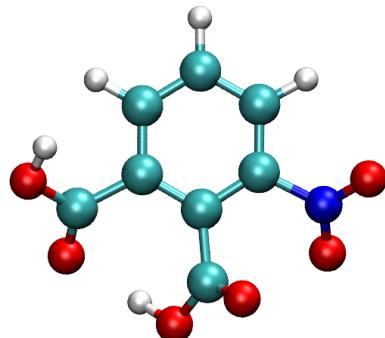
Different



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

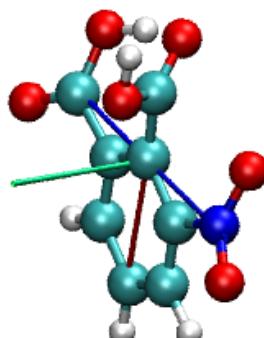
EingenValues - Molecule A

524.175	935.342	1359.19
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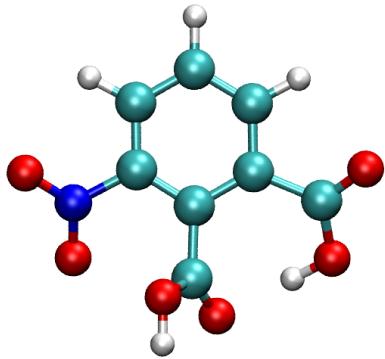
EingenValues - Molecule B

521.475	949.659	1346.18
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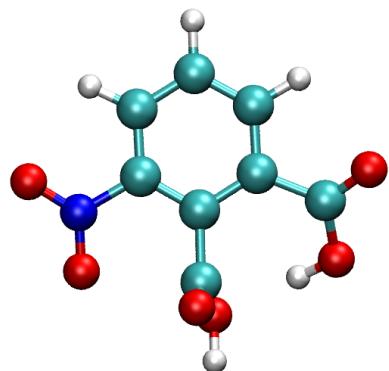
Different



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

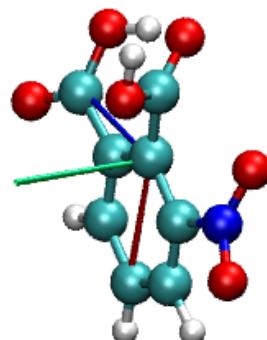
EingenValues - Molecule A

524.175	935.342	1359.19
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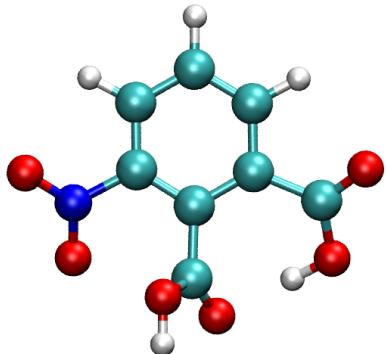
EingenValues - Molecule B

533.726	920.137	1348.3
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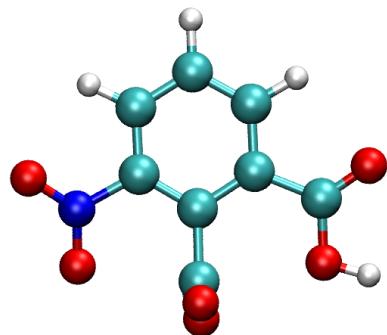
Different



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

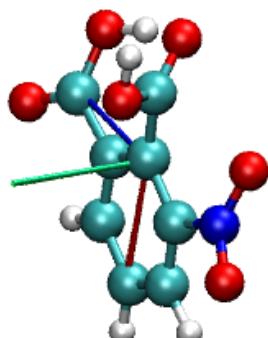
EingenValues - Molecule A

524.175	935.342	1359.19
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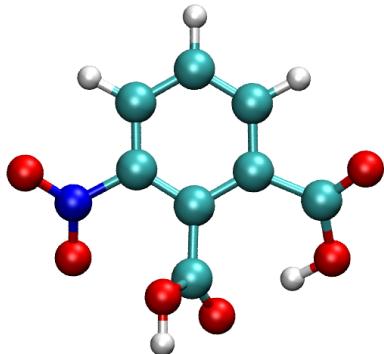
EingenValues - Molecule B

534.81	913.339	1353.78
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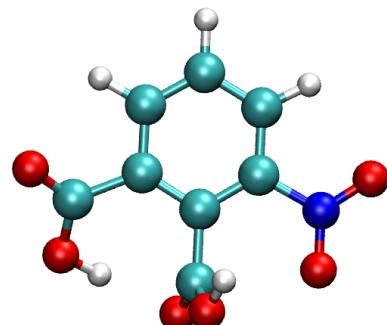
Different



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

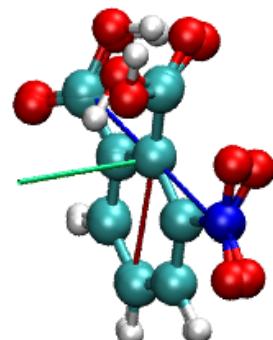
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

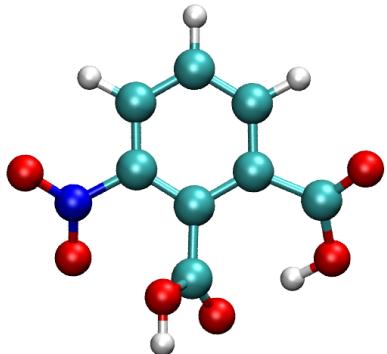
531.691	929.434	1355.4
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Different

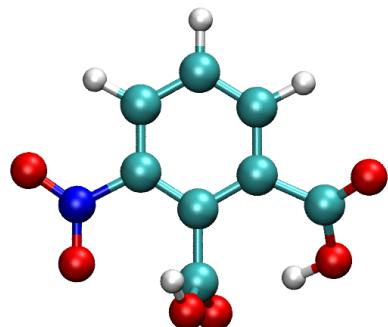


FireTest Número 90

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

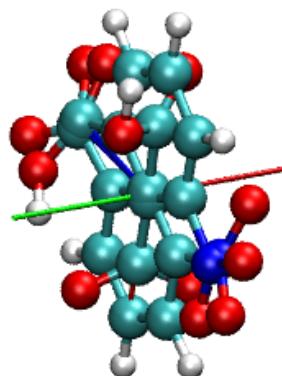
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

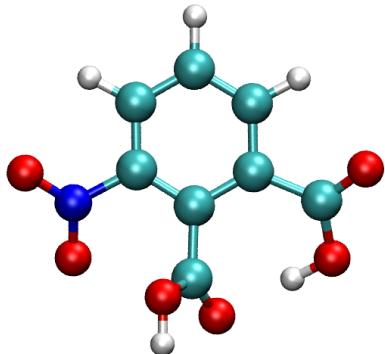
531.698	929.417	1355.4
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Different

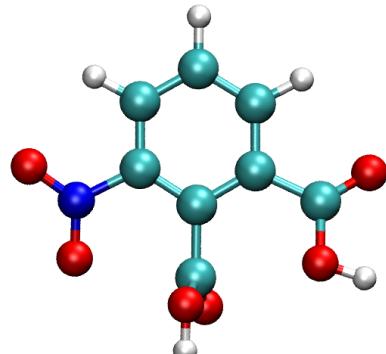


FireTest Número 91

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

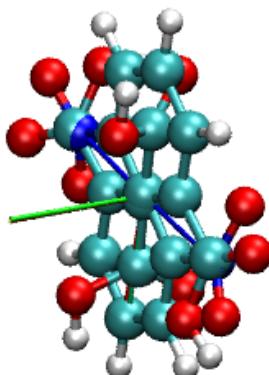
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

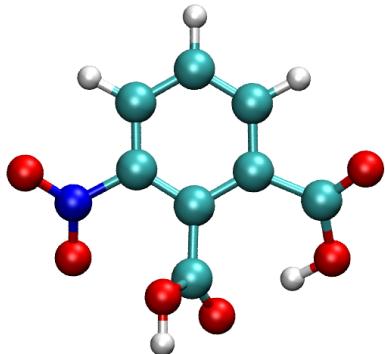
531.43	913.309	1353.35
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Different

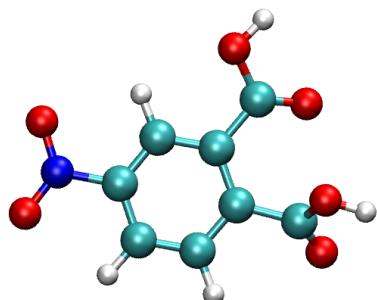


FireTest Número 92

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

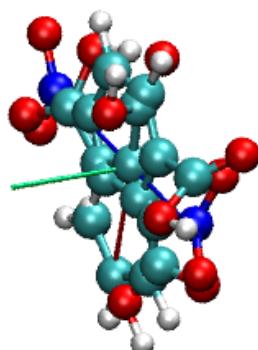
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

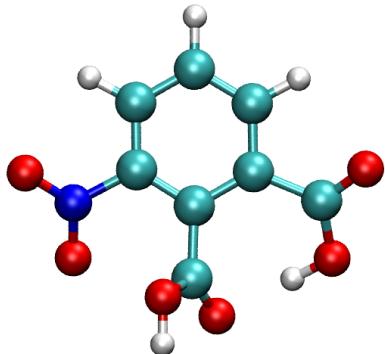
479.363	1242.41	1647.39
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Different

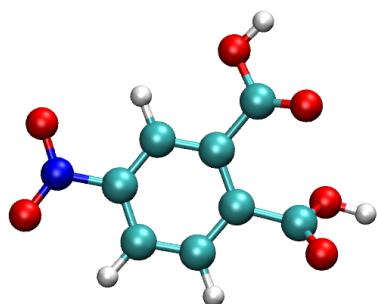


FireTest Número 93

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

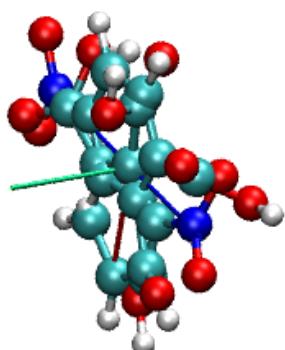
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

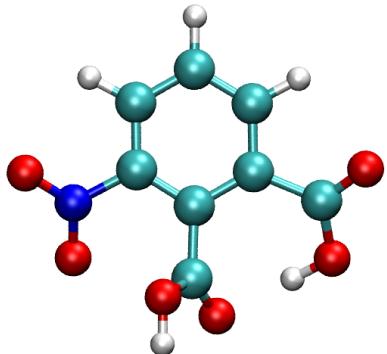
479.308	1242.41	1647.31
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Different

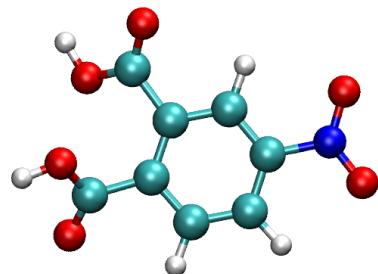


FireTest Número 94

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

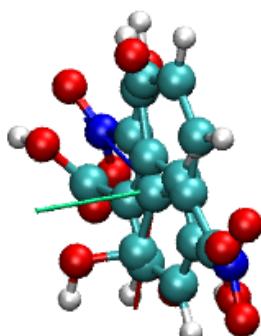
EingenValues - Molecule A

524.175	935.342	1359.19
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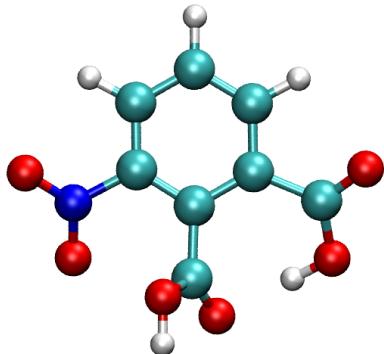
EingenValues - Molecule B

482.027	1240.32	1647.08
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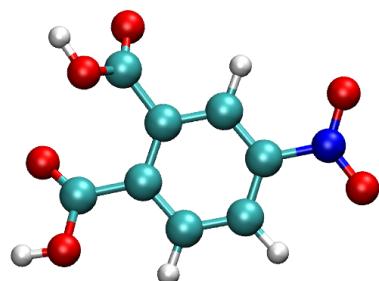
Different



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

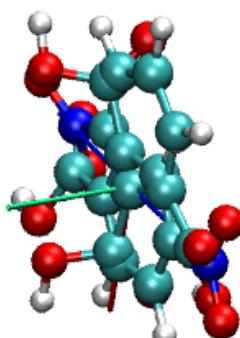
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

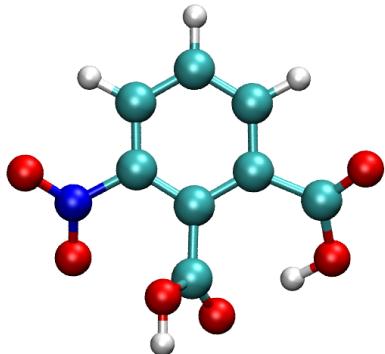
491.663	1231.14	1650.13
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Different

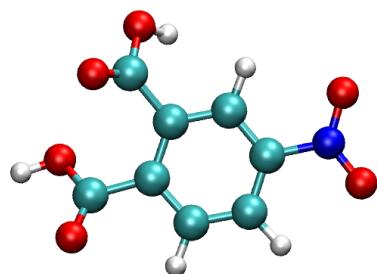


FireTest Número 96

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

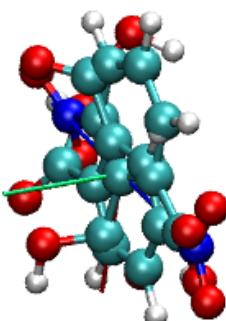
EingenValues - Molecule A

524.175	935.342	1359.19
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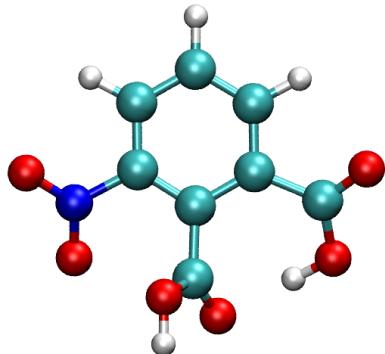
EingenValues - Molecule B

489.011	1233.7	1641.81
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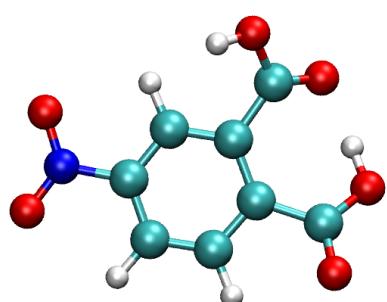
Different



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

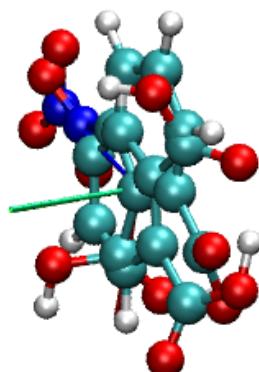
EingenValues - Molecule A

524.175	935.342	1359.19
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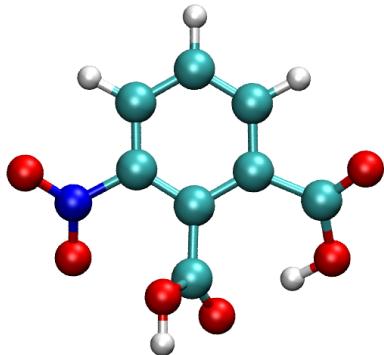
EingenValues - Molecule B

509.668	1219.11	1681.18
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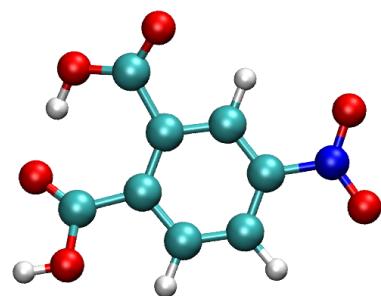
Different



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

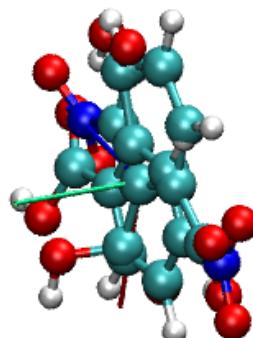
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

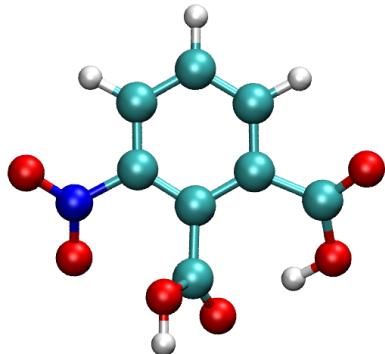
513.751	1208.07	1700.9
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Different

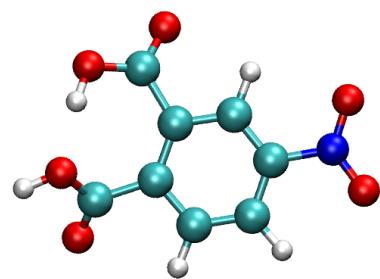


FireTest Número 99

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

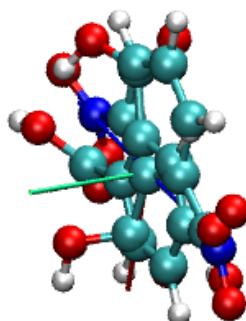
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

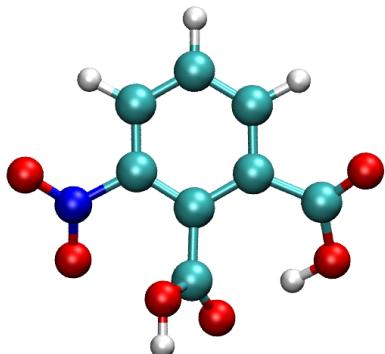
502.409	1232.26	1676.02
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Different

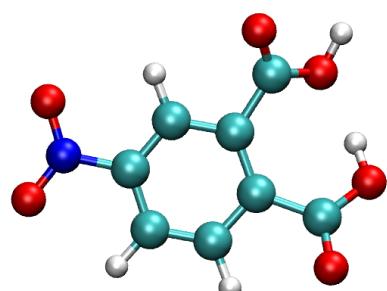


FireTest Número 100

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

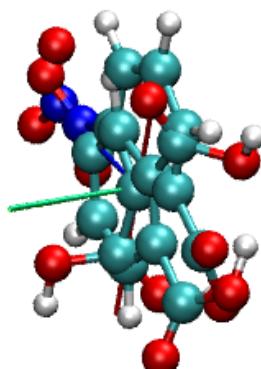
EigenValues - Molecule A

524.175	935.342	1359.19
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EigenValues - Molecule B

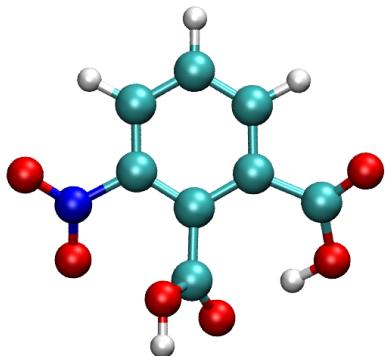
509.897	1225.65	1680.83
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Different

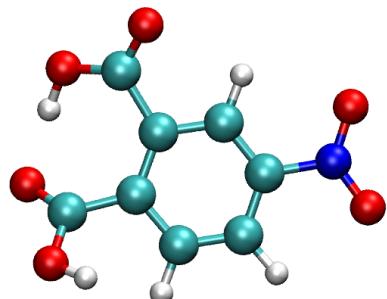


FireTest Número 101

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

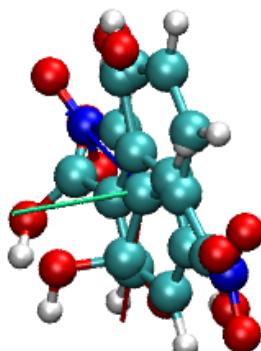
EingenValues - Molecule A

524.175	935.342	1359.19
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EingenValues - Molecule B

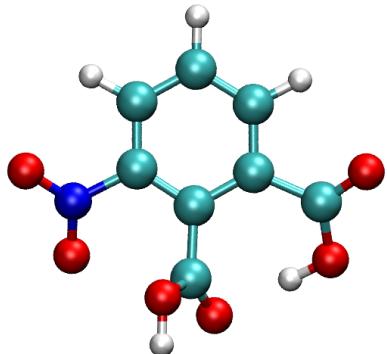
506.607	1222.36	1678.43
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Different

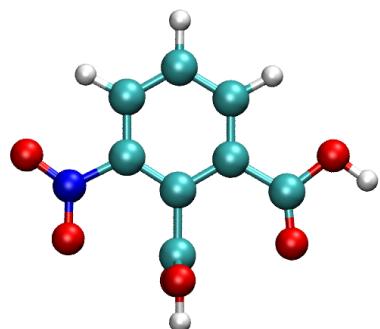


FireTest Número 102

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

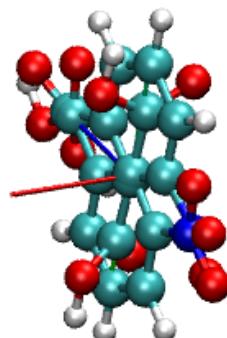
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

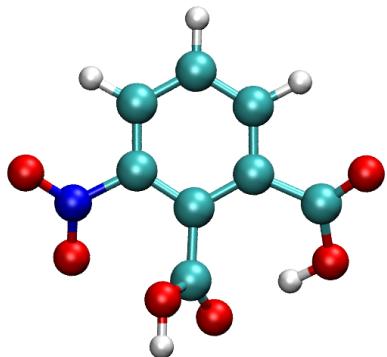
530.045	915.527	1360.79
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Different

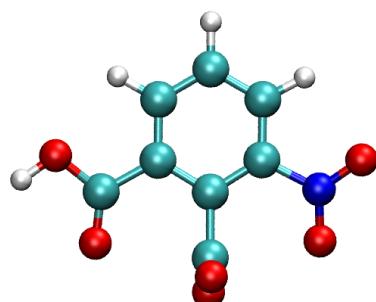


FireTest Número 103

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

EigenVectors - Molecule A

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

EigenVectors - Molecule B

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

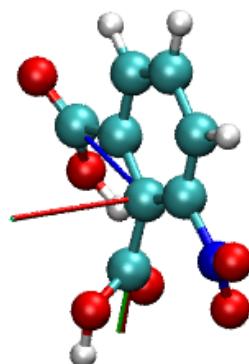
EigenValues - Molecule A

524.162	935.308	1359.22
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EigenValues - Molecule B

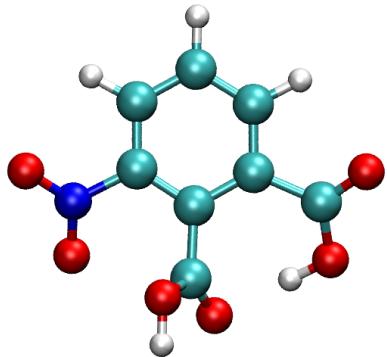
532.89	918.442	1356.93
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Different

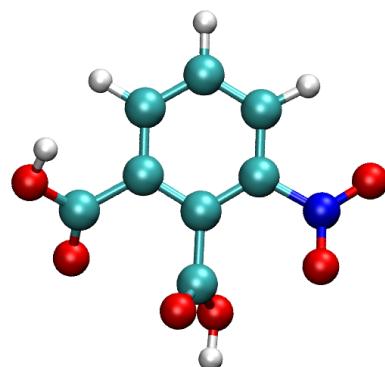


FireTest Número 104

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

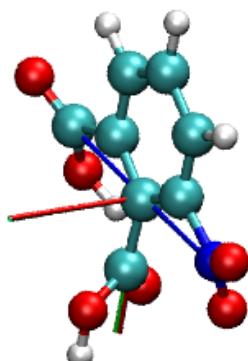
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

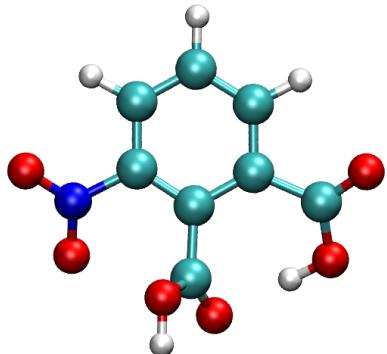
528.663	924.928	1336.12
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Different

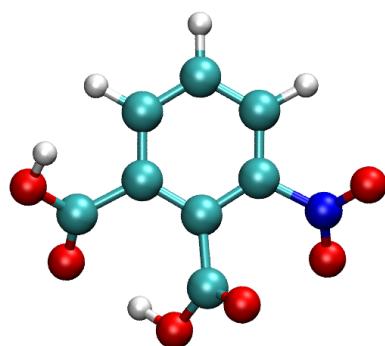


FireTest Número 105

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

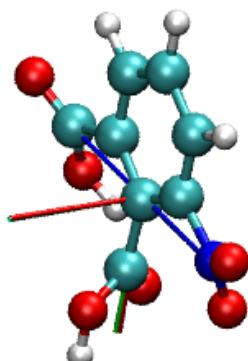
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

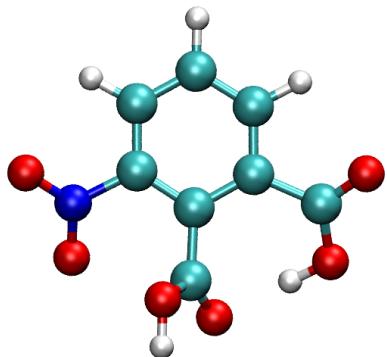
521.475	949.659	1346.18
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Different

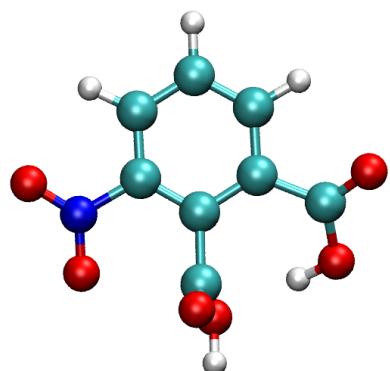


FireTest Número 106

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

EigenVectors - Molecule A

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

EigenVectors - Molecule B

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

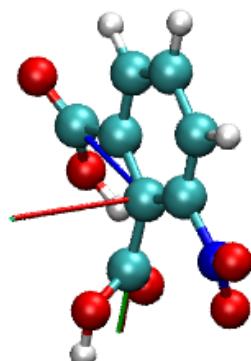
EigenValues - Molecule A

524.162	935.308	1359.22
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EigenValues - Molecule B

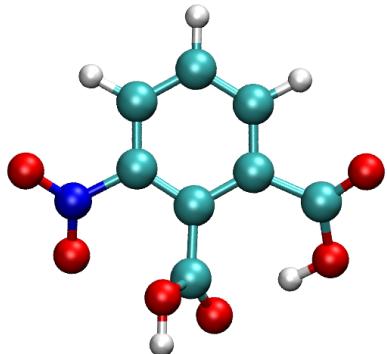
533.726	920.137	1348.3
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Different

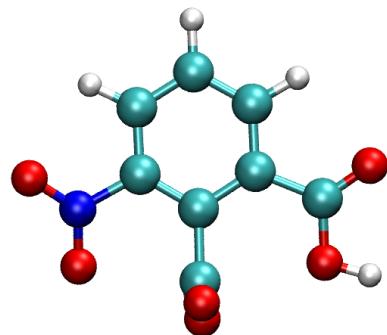


FireTest Número 107

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

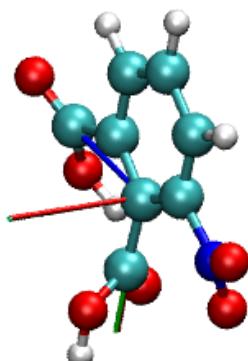
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

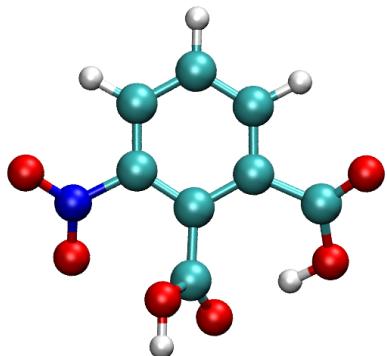
534.81	913.339	1353.78
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Different

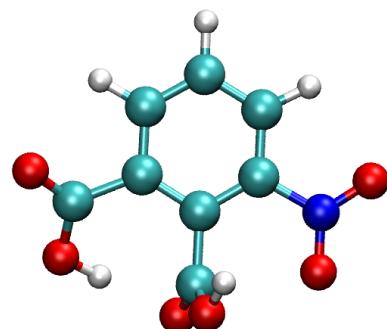


FireTest Número 108

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

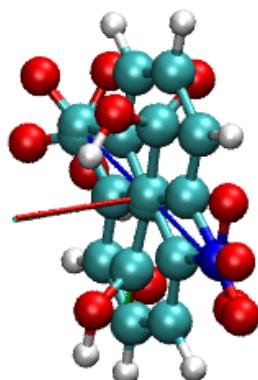
EingenValues - Molecule A

524.162	935.308	1359.22
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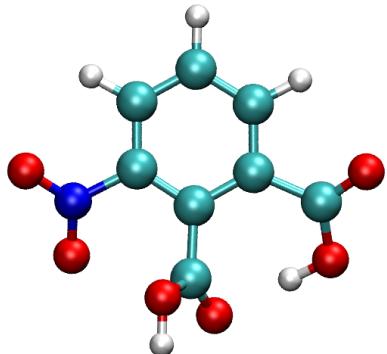
EingenValues - Molecule B

531.691	929.434	1355.4
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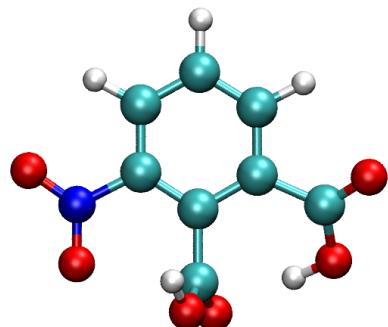
Different



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

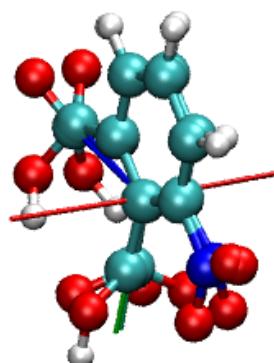
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

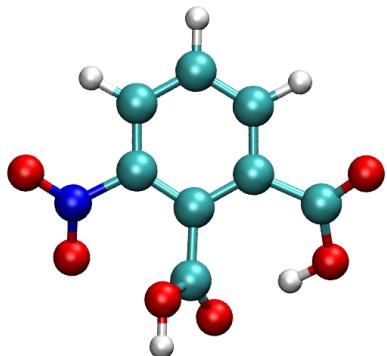
531.698	929.417	1355.4
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Different

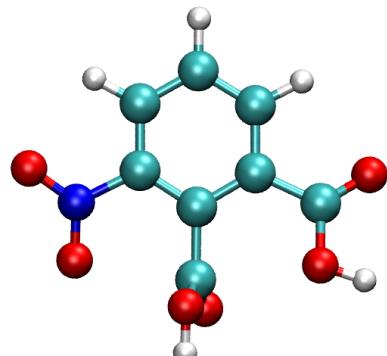


FireTest Número 110

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

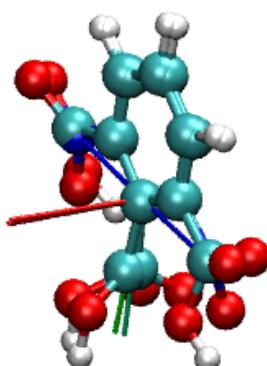
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

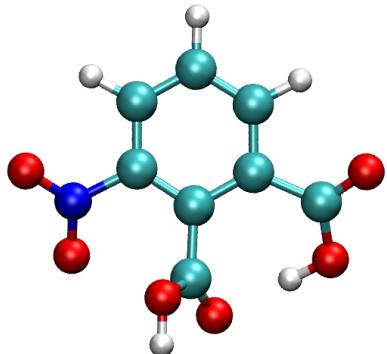
531.43	913.309	1353.35
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Different

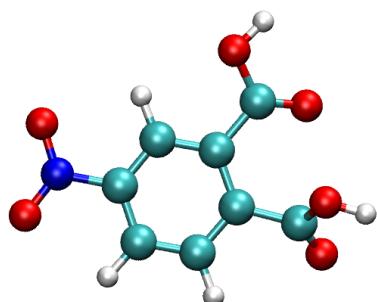


FireTest Número 111

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

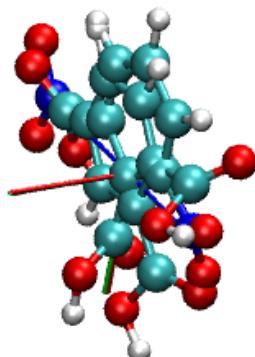
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

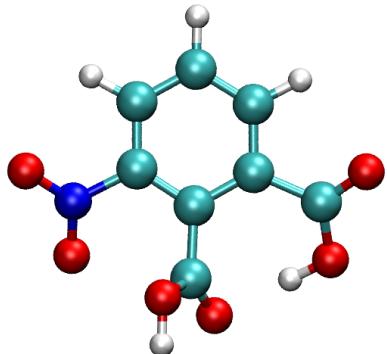
479.363	1242.41	1647.39
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Different

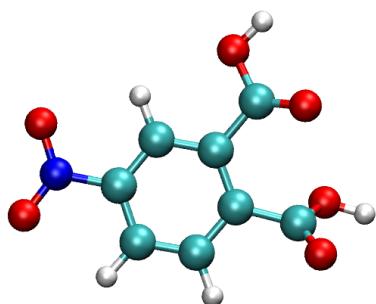


FireTest Número 112

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

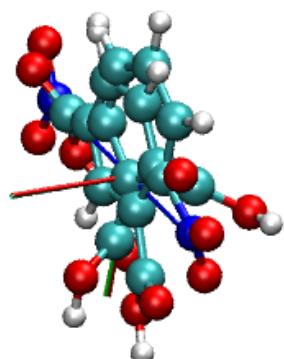
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

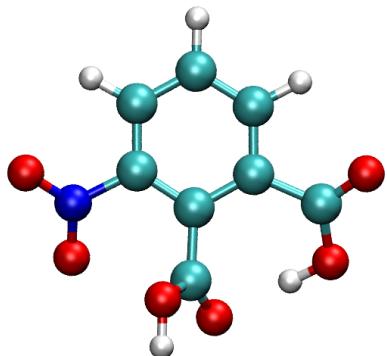
479.308	1242.41	1647.31
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Different

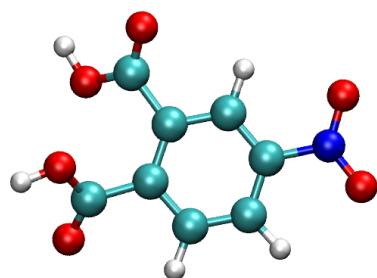


FireTest Número 113

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

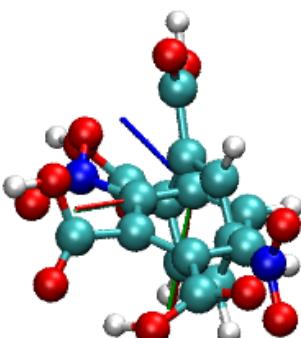
EingenValues - Molecule A

524.162	935.308	1359.22
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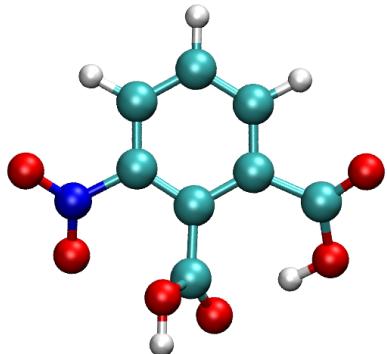
EingenValues - Molecule B

482.027	1240.32	1647.08
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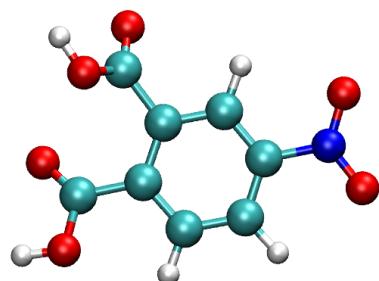
Different



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

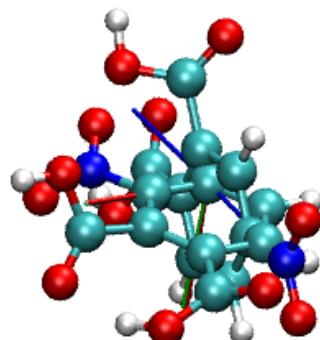
EingenValues - Molecule A

524.162	935.308	1359.22
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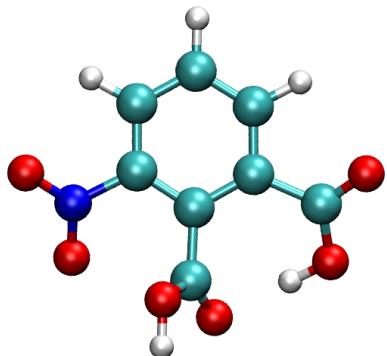
EingenValues - Molecule B

491.663	1231.14	1650.13
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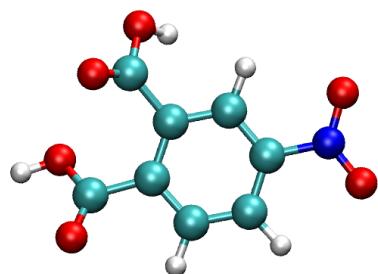
Different



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

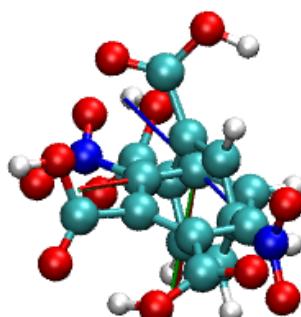
EingenValues - Molecule A

524.162	935.308	1359.22
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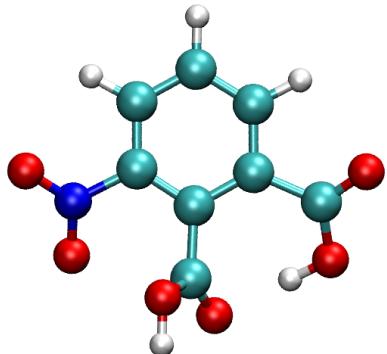
EingenValues - Molecule B

489.011	1233.7	1641.81
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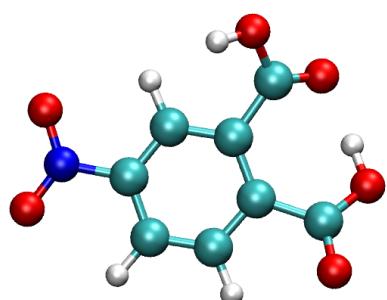
Different



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

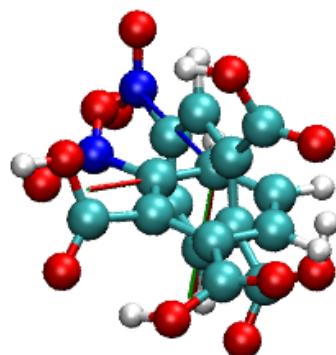
EingenValues - Molecule A

524.162	935.308	1359.22
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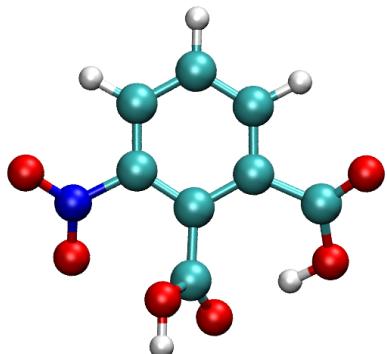
EingenValues - Molecule B

509.668	1219.11	1681.18
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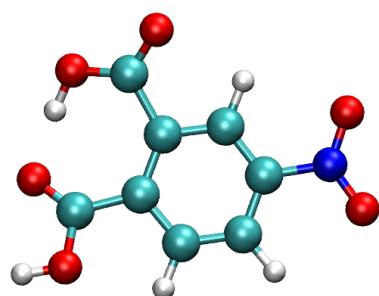
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

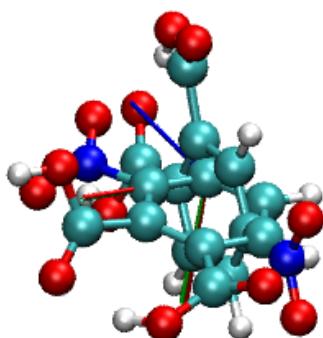
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

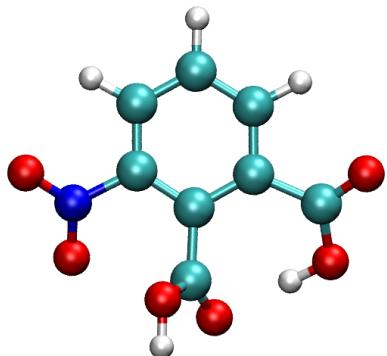
513.751	1208.07	1700.9
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Different

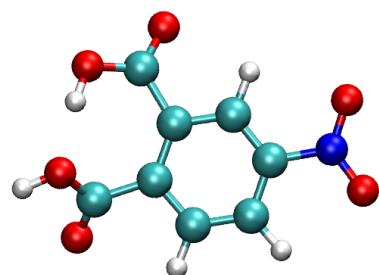


FireTest Número 118

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

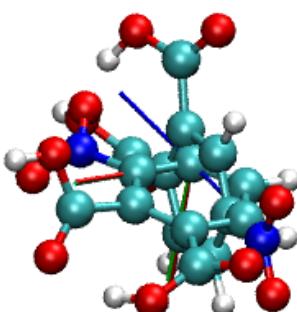
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

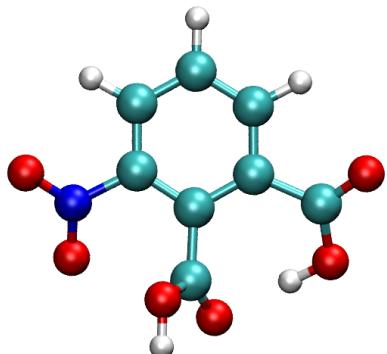
502.409	1232.26	1676.02
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Different

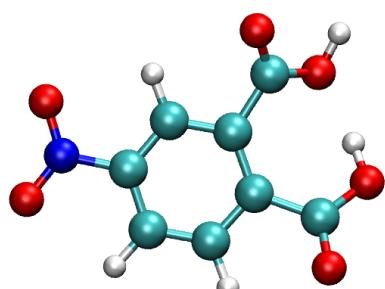


FireTest Número 119

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

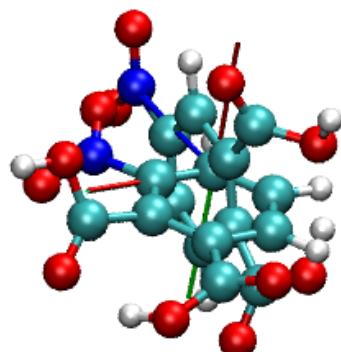
EigenValues - Molecule A

524.162	935.308	1359.22
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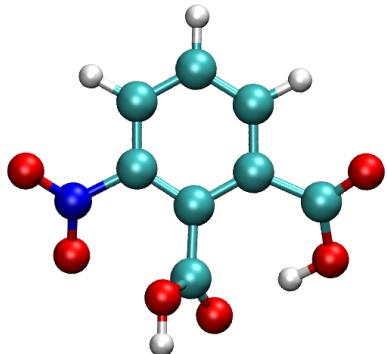
EigenValues - Molecule B

509.897	1225.65	1680.83
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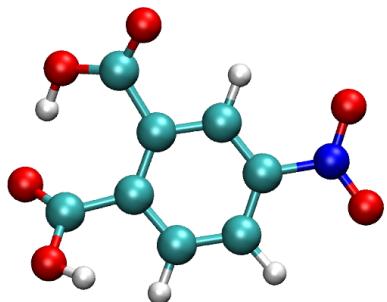
Different



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

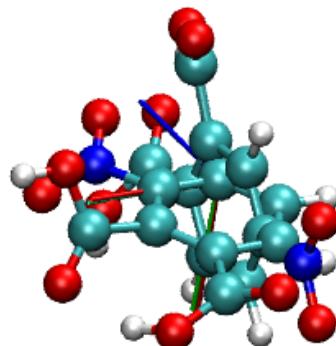
EingenValues - Molecule A

524.162	935.308	1359.22
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EingenValues - Molecule B

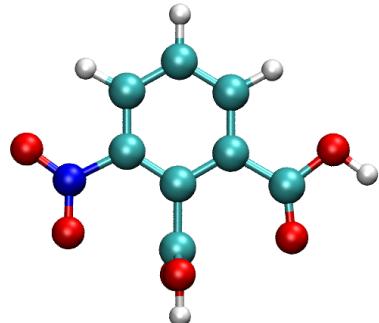
506.607	1222.36	1678.43
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Different

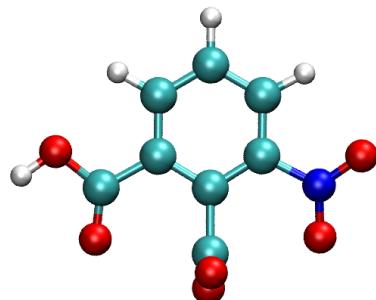


FireTest Número 121

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

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

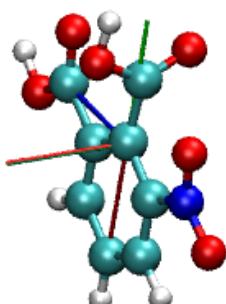
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

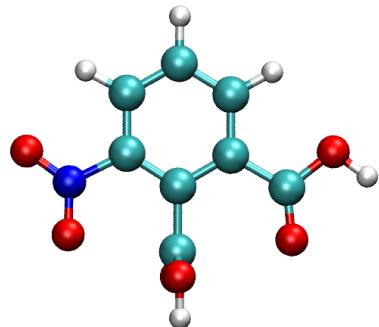
532.89	918.442	1356.93
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Different

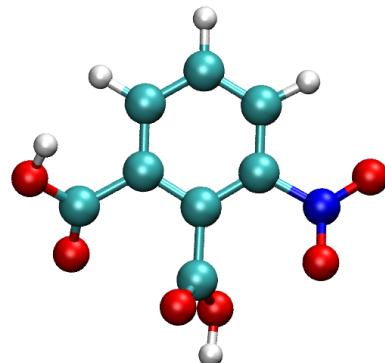


FireTest Número 122

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

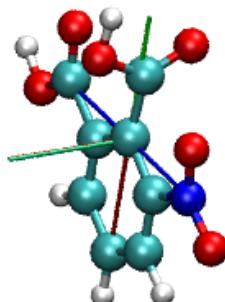
EingenValues - Molecule A

530.045	915.527	1360.79
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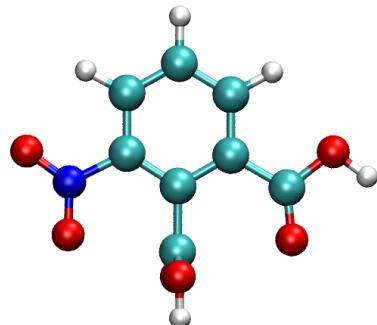
EingenValues - Molecule B

528.663	924.928	1336.12
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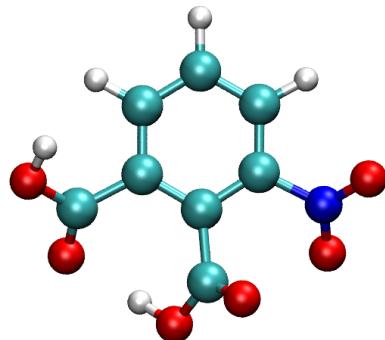
Different



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

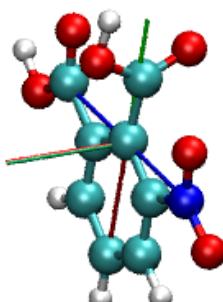
EingenValues - Molecule A

530.045	915.527	1360.79
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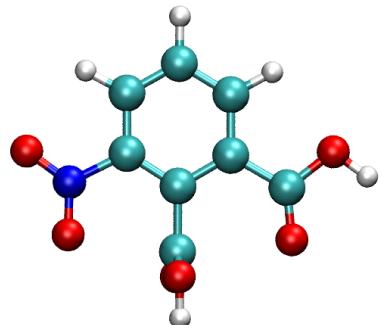
EingenValues - Molecule B

521.475	949.659	1346.18
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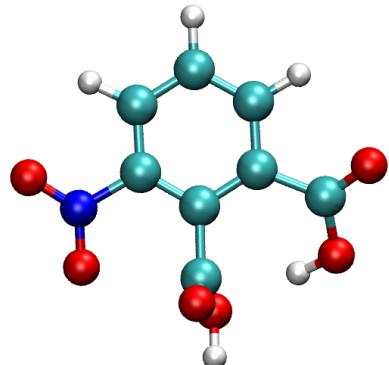
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

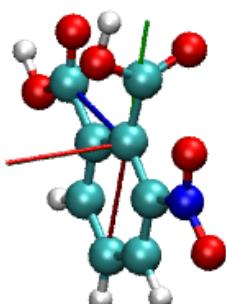
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

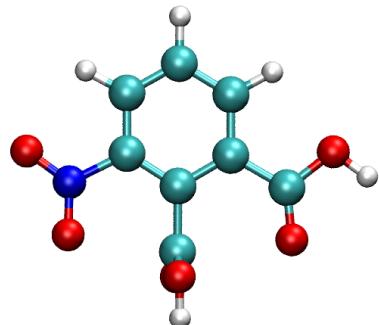
533.726	920.137	1348.3
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Different

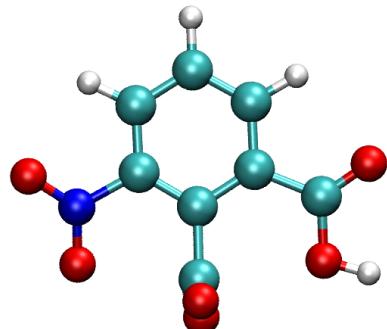


FireTest Número 125

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

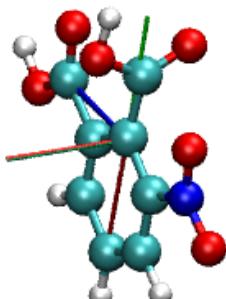
EingenValues - Molecule A

530.045	915.527	1360.79
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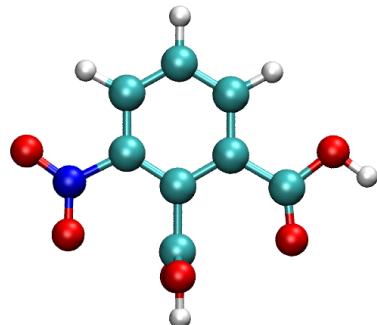
EingenValues - Molecule B

534.81	913.339	1353.78
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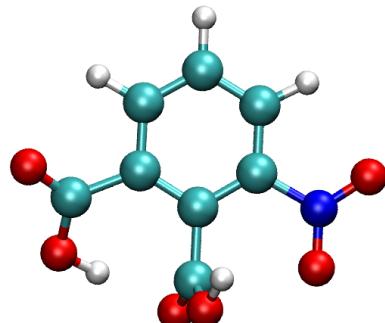
Different



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

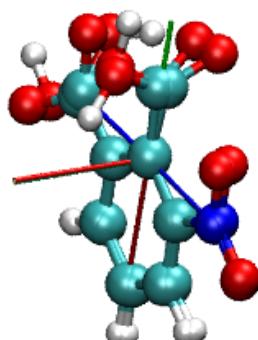
EingenValues - Molecule A

530.045	915.527	1360.79
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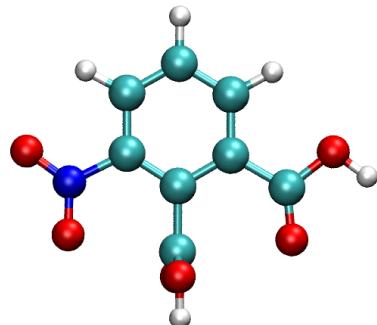
EingenValues - Molecule B

531.691	929.434	1355.4
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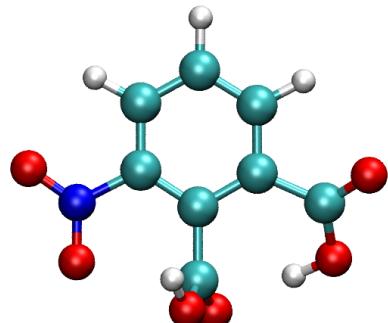
Different



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

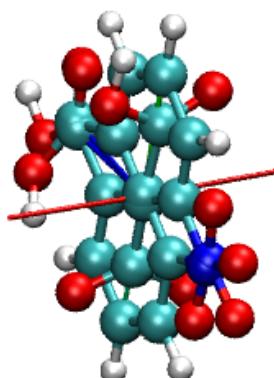
EingenValues - Molecule A

530.045	915.527	1360.79
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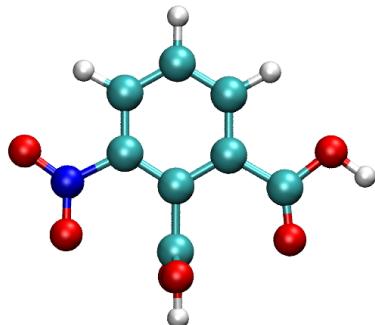
EingenValues - Molecule B

531.698	929.417	1355.4
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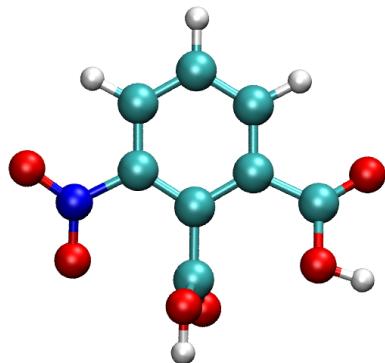
Different



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

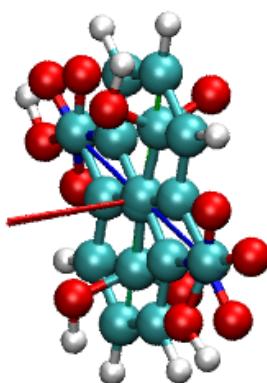
EingenValues - Molecule A

530.045	915.527	1360.79
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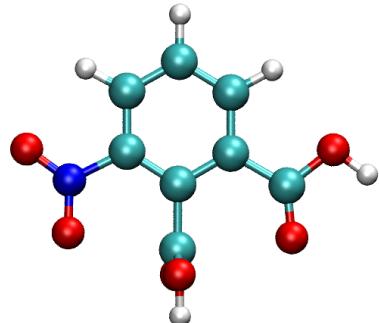
EingenValues - Molecule B

531.43	913.309	1353.35
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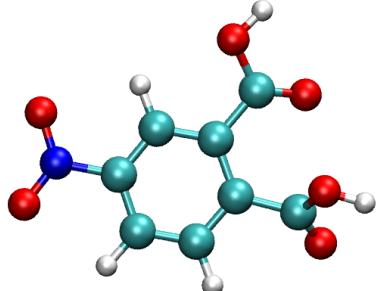
Different



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

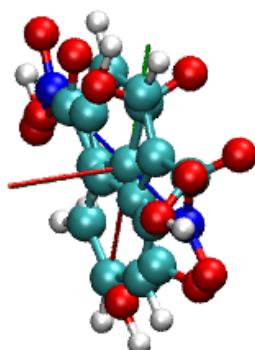
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

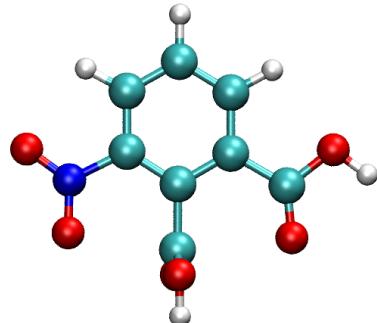
479.363	1242.41	1647.39
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Different

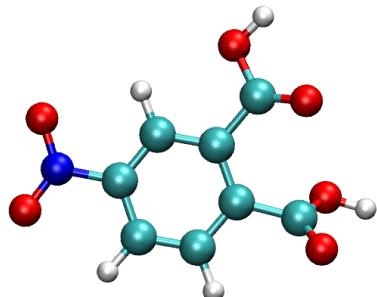


FireTest Número 130

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

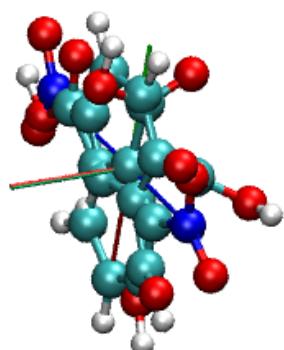
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

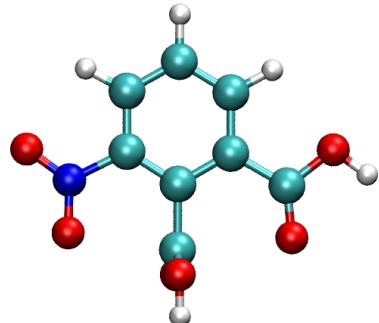
479.308	1242.41	1647.31
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Different

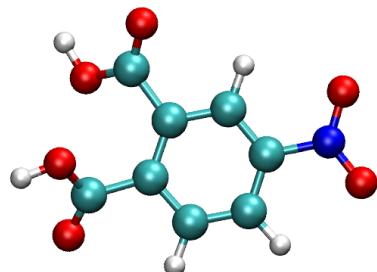


FireTest Número 131

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

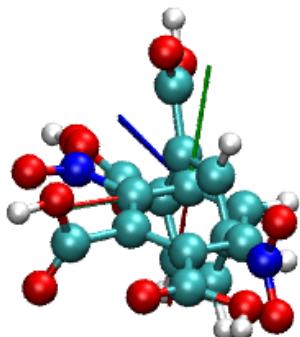
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

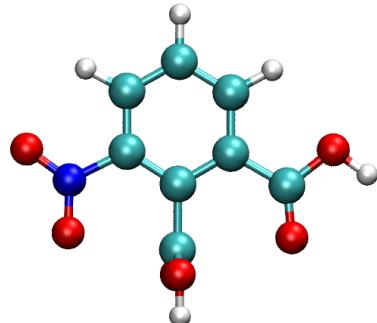
482.027	1240.32	1647.08
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Different

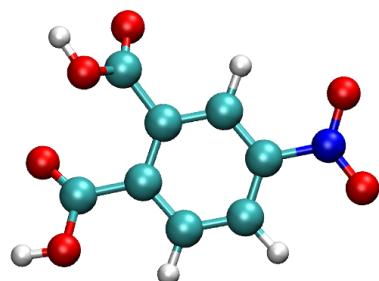


FireTest Número 132

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

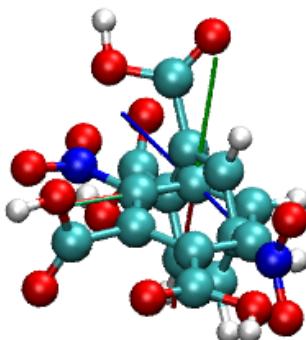
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

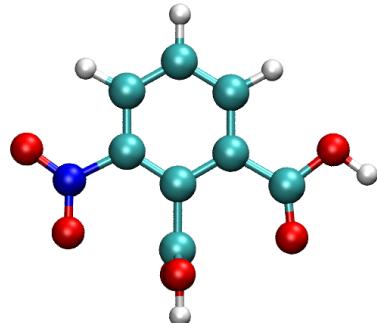
491.663	1231.14	1650.13
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Different

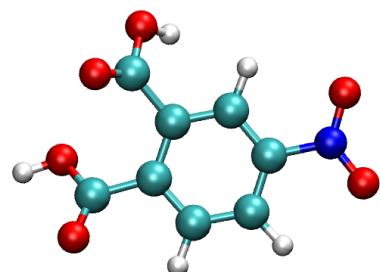


FireTest Número 133

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

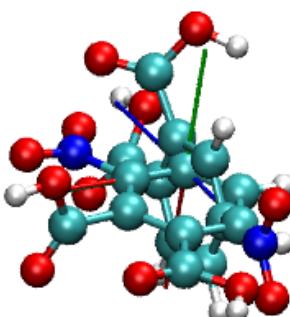
EingenValues - Molecule A

530.045	915.527	1360.79
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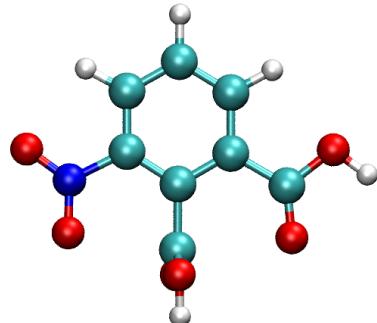
EingenValues - Molecule B

489.011	1233.7	1641.81
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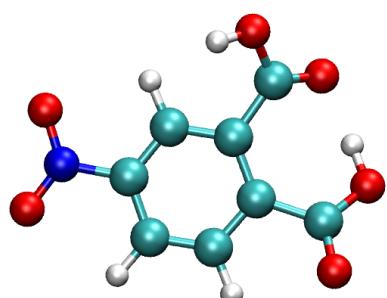
Different



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

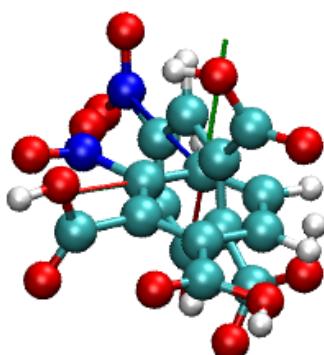
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

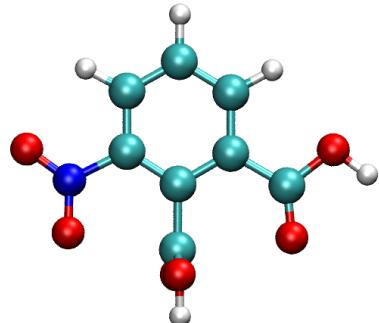
509.668	1219.11	1681.18
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Different

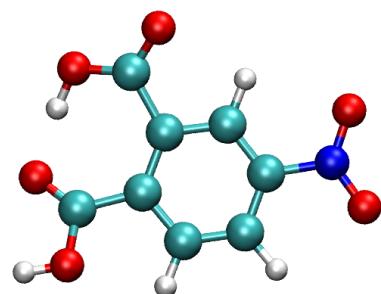


FireTest Número 135

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

EigenVectors - Molecule A

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

EigenVectors - Molecule B

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

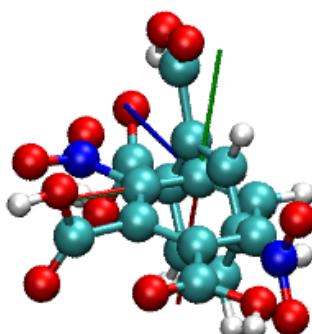
EigenValues - Molecule A

530.045	915.527	1360.79
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EigenValues - Molecule B

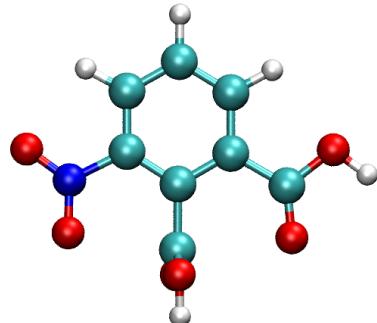
513.751	1208.07	1700.9
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Different

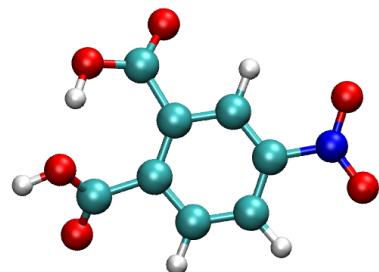


FireTest Número 136

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

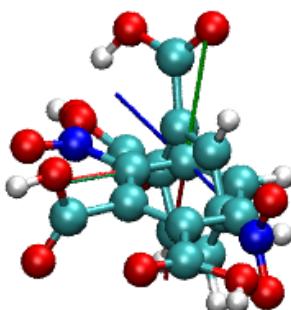
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

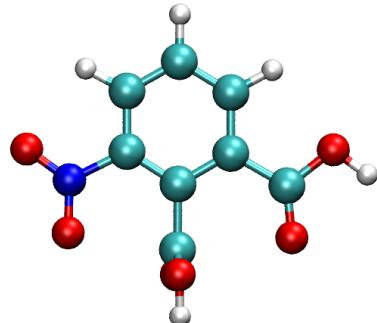
502.409	1232.26	1676.02
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Different

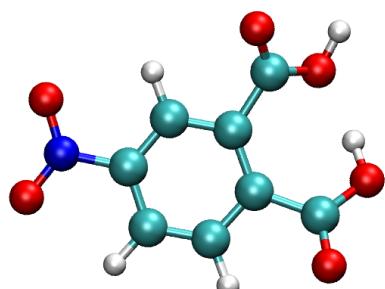


FireTest Número 137

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

EigenVectors - Molecule A

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

EigenVectors - Molecule B

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

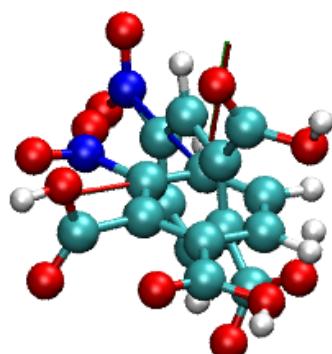
EigenValues - Molecule A

530.045	915.527	1360.79
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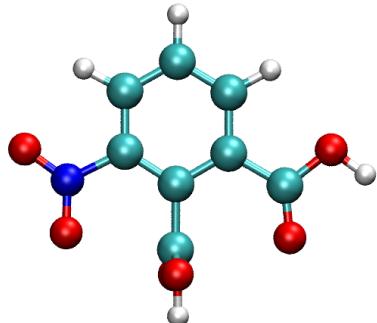
EigenValues - Molecule B

509.897	1225.65	1680.83
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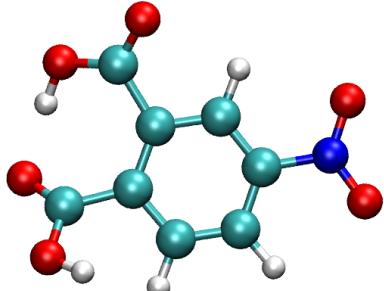
Different



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

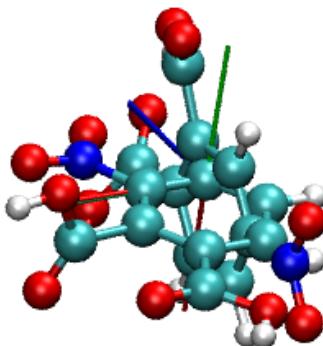
EingenValues - Molecule A

530.045	915.527	1360.79
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EingenValues - Molecule B

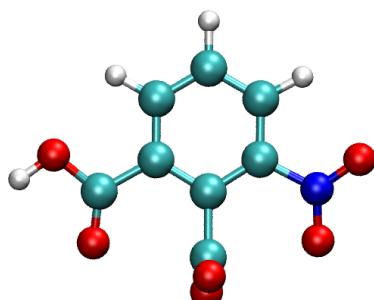
506.607	1222.36	1678.43
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Different

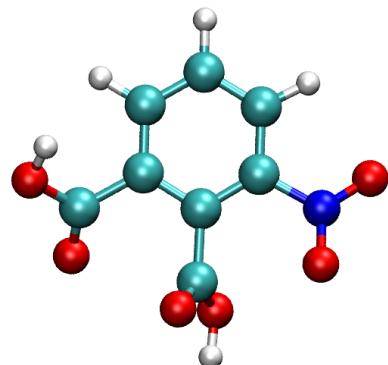


FireTest Número 139

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

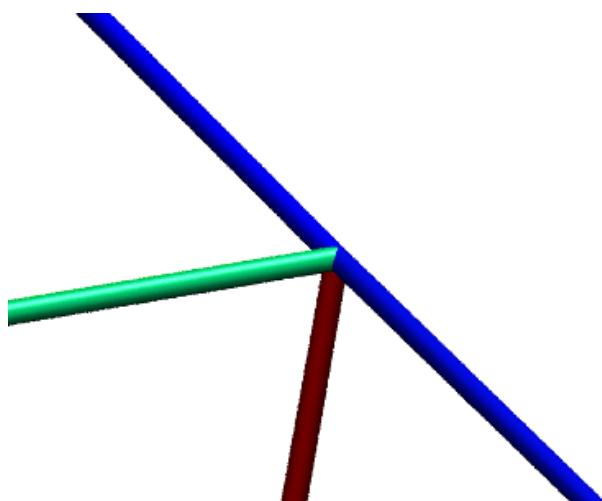
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

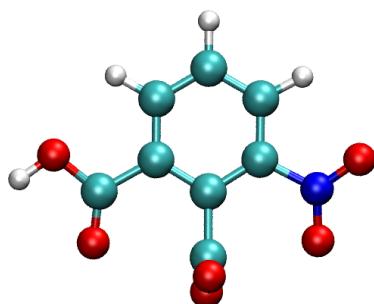
528.663	924.928	1336.12
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Different

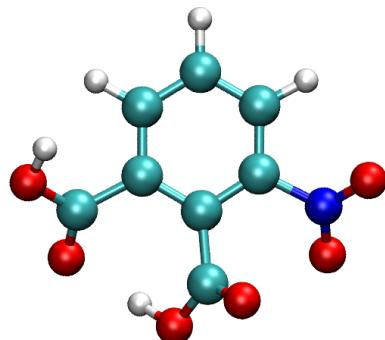


FireTest Número 140

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

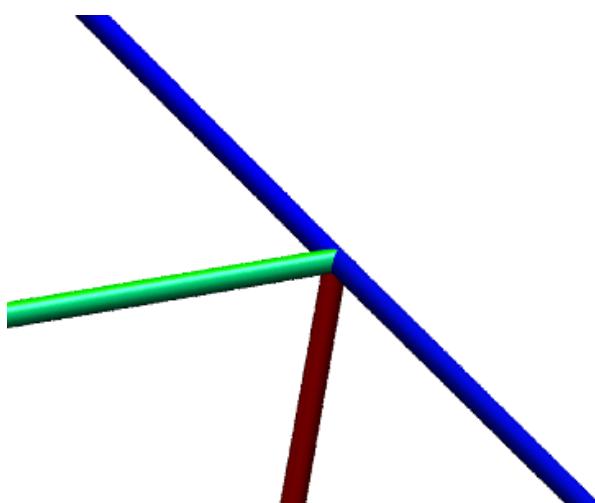
EingenValues - Molecule A

532.89	918.442	1356.93
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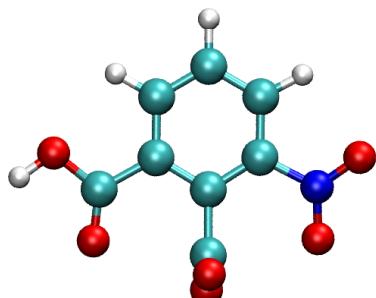
EingenValues - Molecule B

521.475	949.659	1346.18
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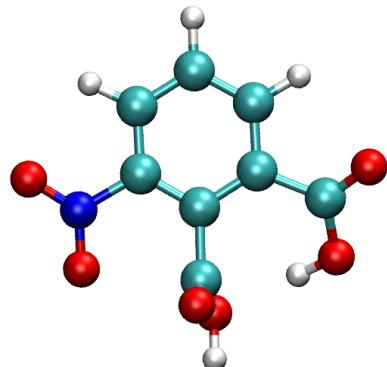
Different



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

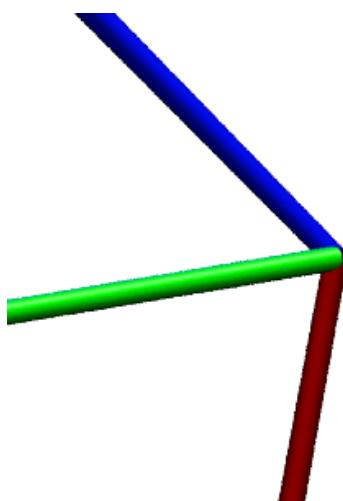
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

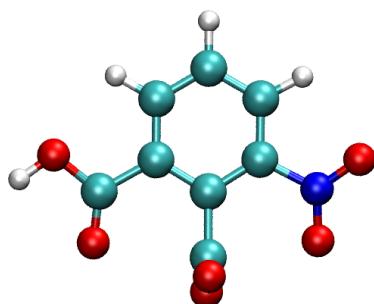
533.726	920.137	1348.3
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Different

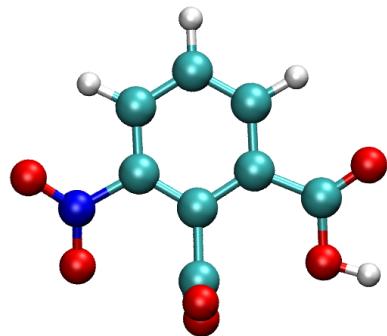


FireTest Número 142

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

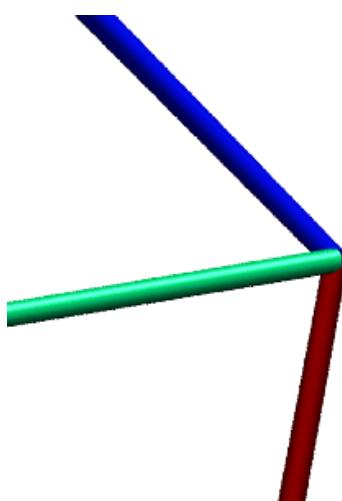
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

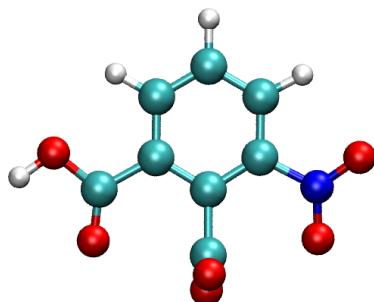
534.81	913.339	1353.78
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Different

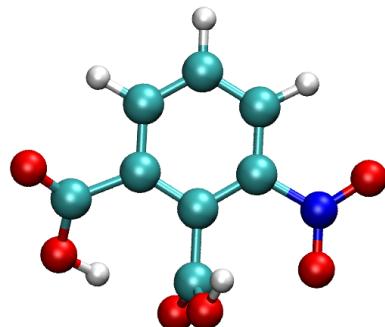


FireTest Número 143

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

EigenVectors - Molecule A

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

EigenVectors - Molecule B

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

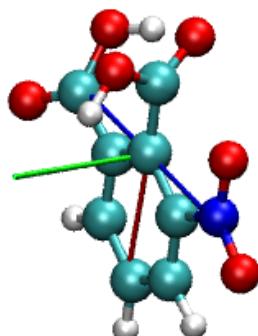
EigenValues - Molecule A

532.89	918.442	1356.93
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EigenValues - Molecule B

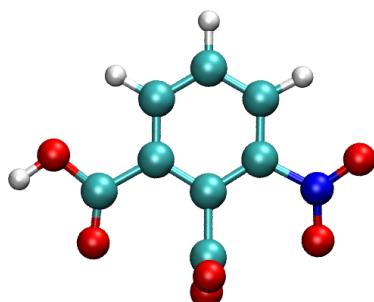
531.691	929.434	1355.4
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Different

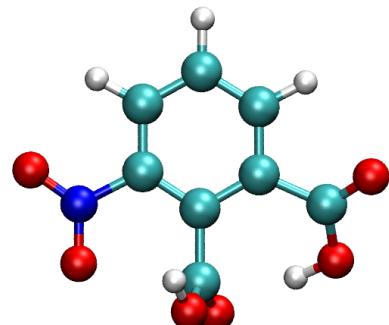


FireTest Número 144

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

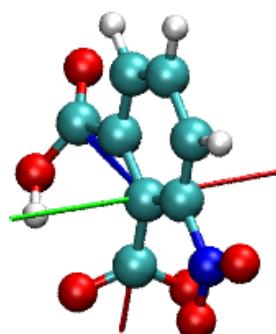
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

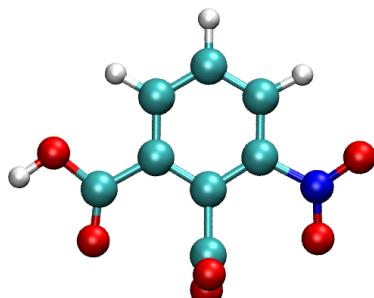
531.698	929.417	1355.4
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Different

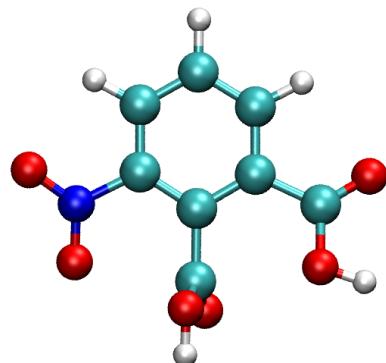


FireTest Número 145

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

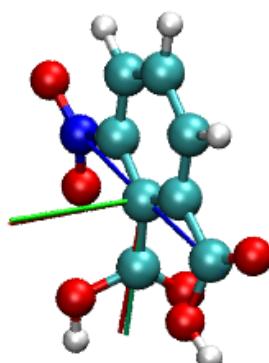
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

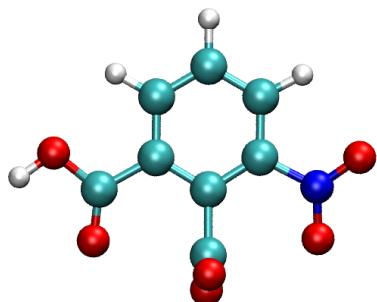
531.43	913.309	1353.35
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Different

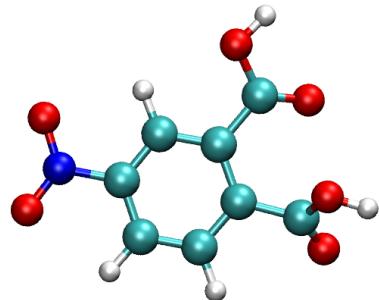


FireTest Número 146

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

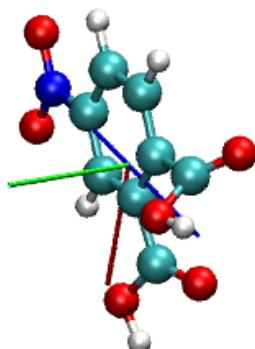
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

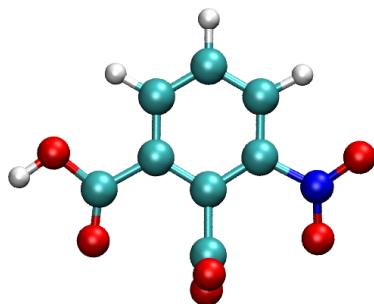
479.363	1242.41	1647.39
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Different

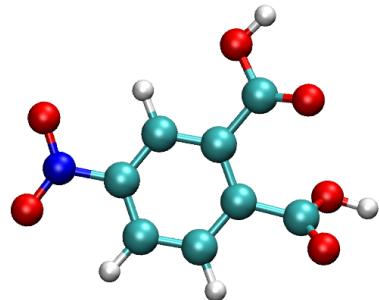


FireTest Número 147

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

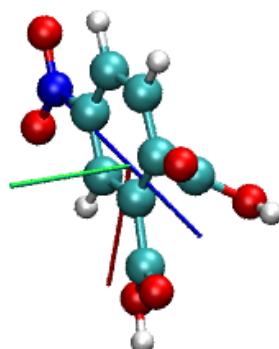
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

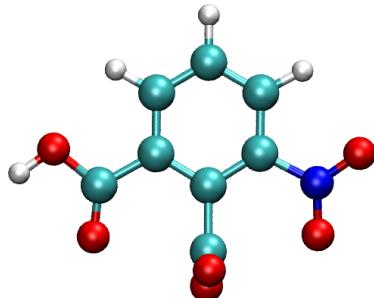
479.308	1242.41	1647.31
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Different

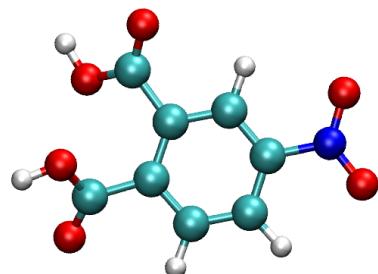


FireTest Número 148

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

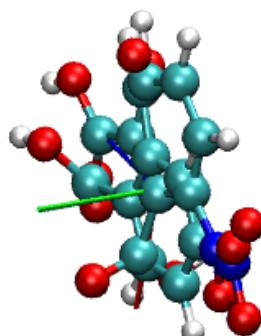
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

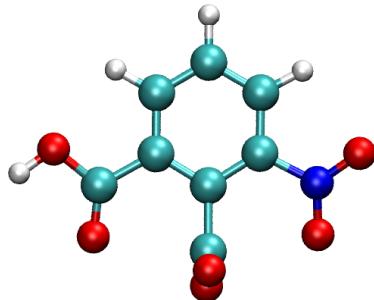
482.027	1240.32	1647.08
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Different

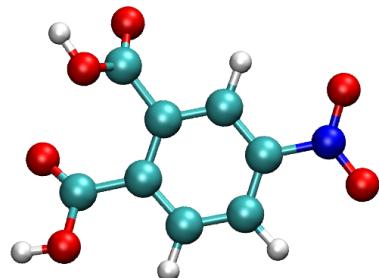


FireTest Número 149

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

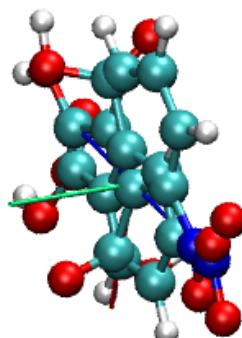
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

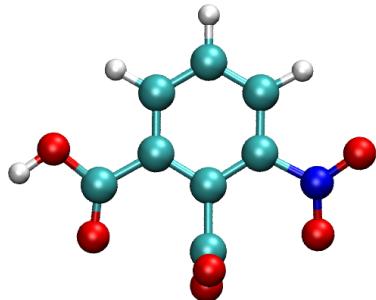
491.663	1231.14	1650.13
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Different

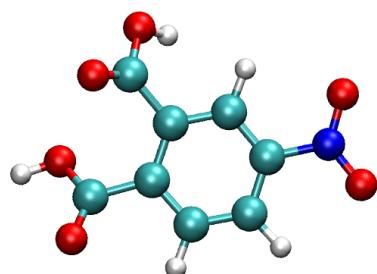


FireTest Número 150

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

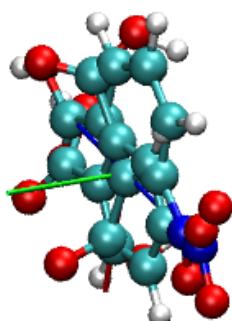
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

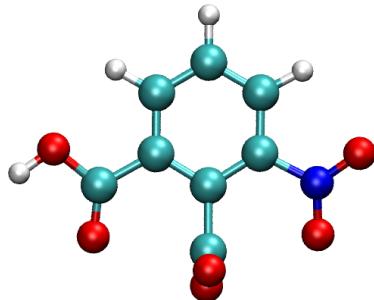
489.011	1233.7	1641.81
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Different

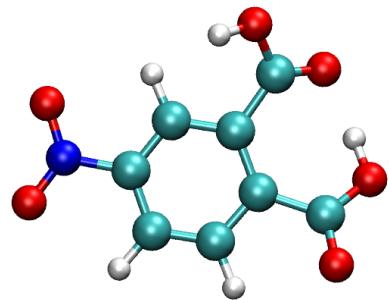


FireTest Número 151

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

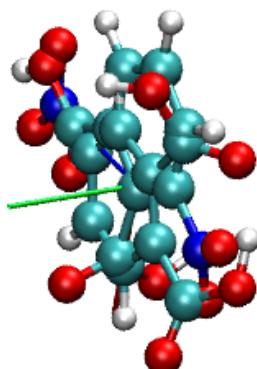
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

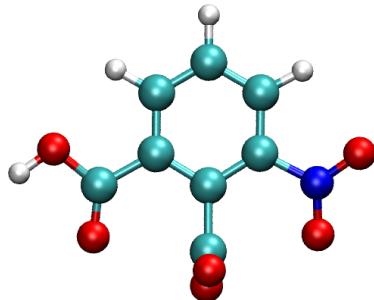
509.668	1219.11	1681.18
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Different

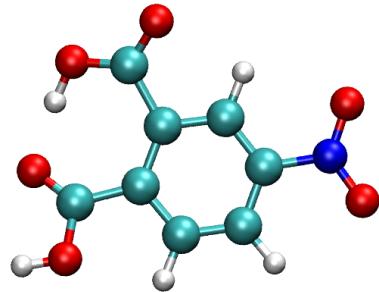


FireTest Número 152

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

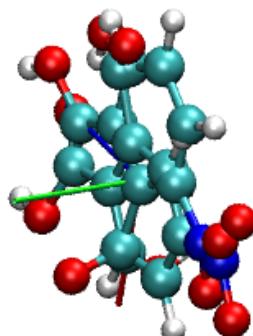
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

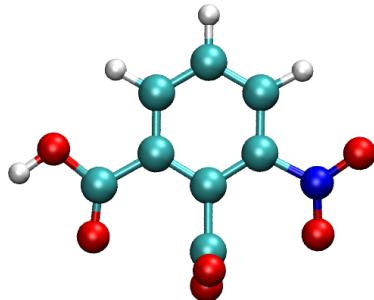
513.751	1208.07	1700.9
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Different

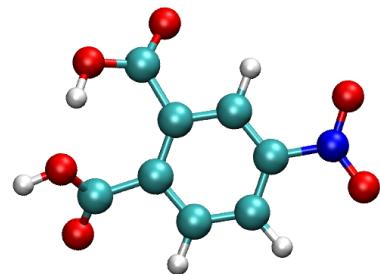


FireTest Número 153

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

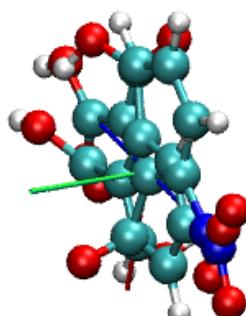
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

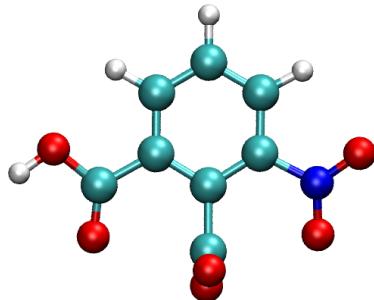
502.409	1232.26	1676.02
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Different

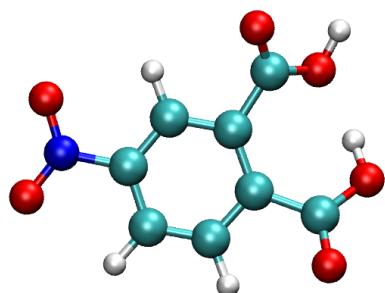


FireTest Número 154

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

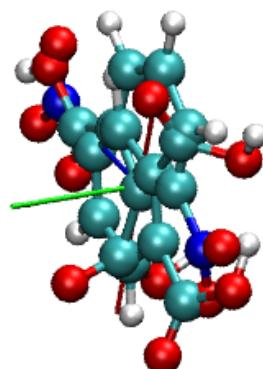
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

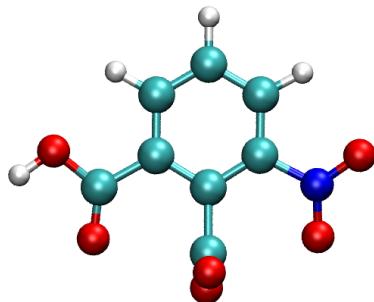
509.897	1225.65	1680.83
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Different

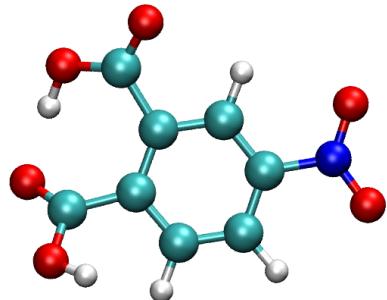


FireTest Número 155

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

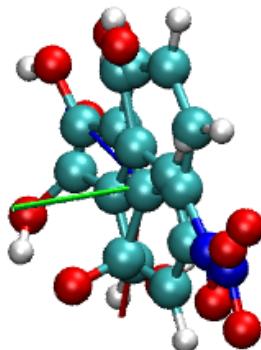
EingenValues - Molecule A

532.89	918.442	1356.93
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EingenValues - Molecule B

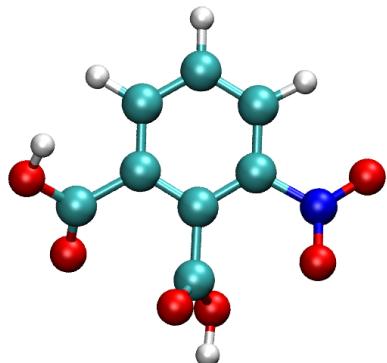
506.607	1222.36	1678.43
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Different

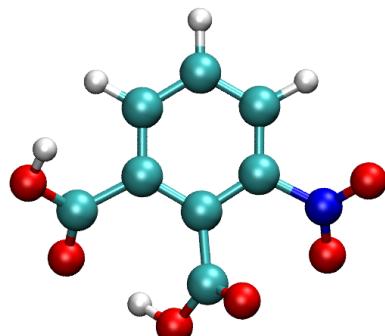


FireTest Número 156

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

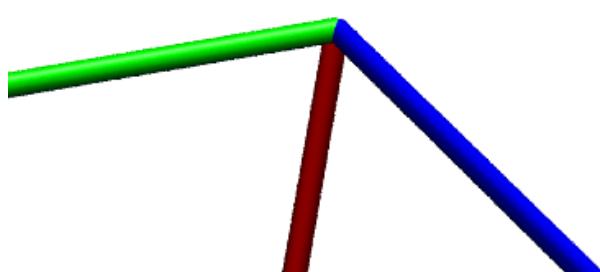
EingenValues - Molecule A

528.663	924.928	1336.12
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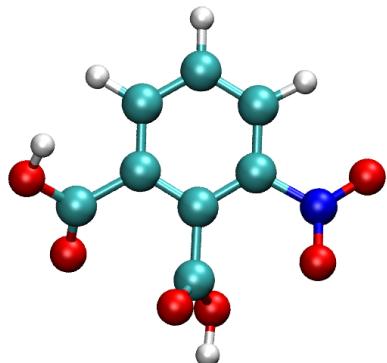
EingenValues - Molecule B

521.475	949.659	1346.18
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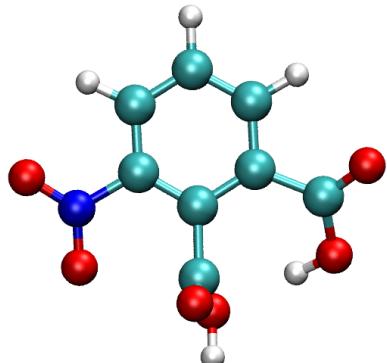
Different



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

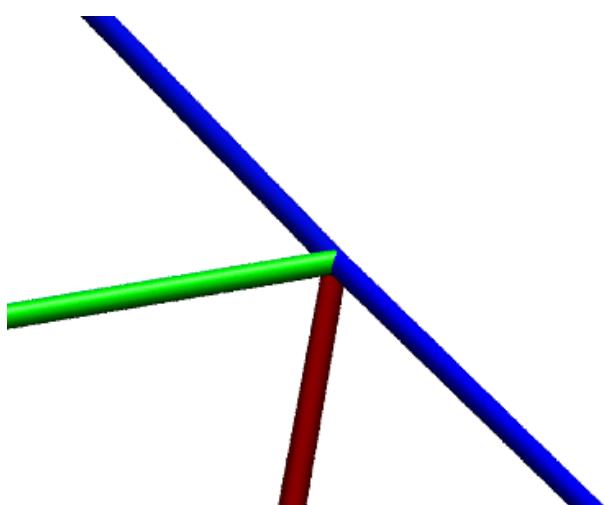
EingenValues - Molecule A

528.663	924.928	1336.12
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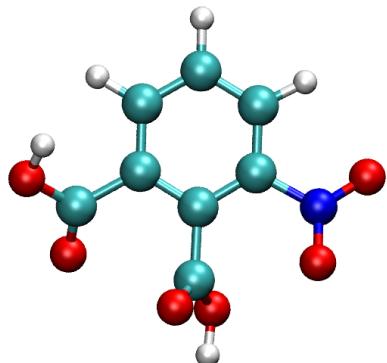
EingenValues - Molecule B

533.726	920.137	1348.3
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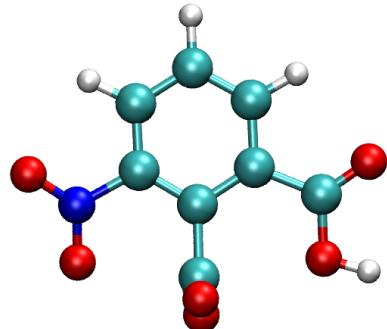
Different



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

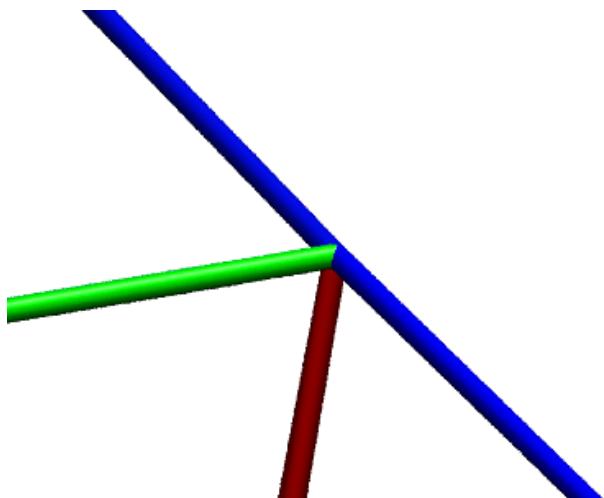
EingenValues - Molecule A

528.663	924.928	1336.12
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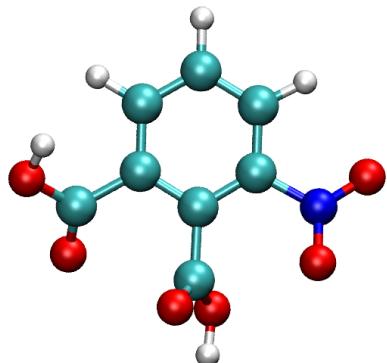
EingenValues - Molecule B

534.81	913.339	1353.78
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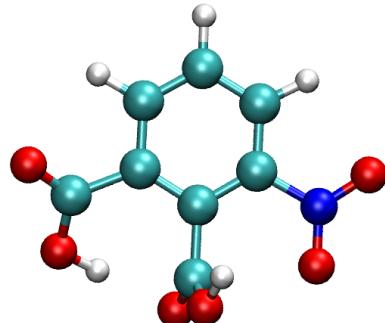
Different



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

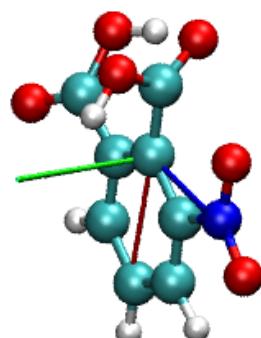
EingenValues - Molecule A

528.663	924.928	1336.12
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EingenValues - Molecule B

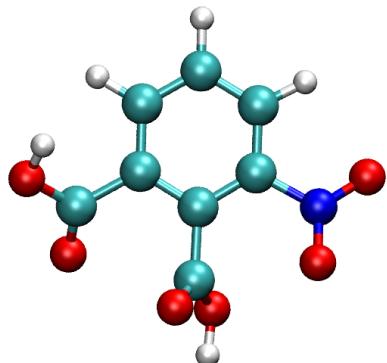
531.691	929.434	1355.4
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Different

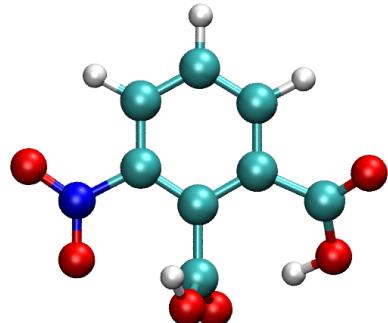


FireTest Número 160

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

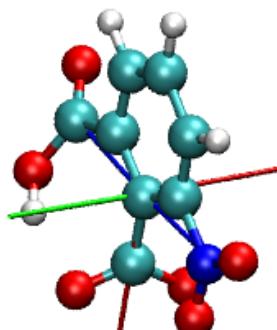
EingenValues - Molecule A

528.663	924.928	1336.12
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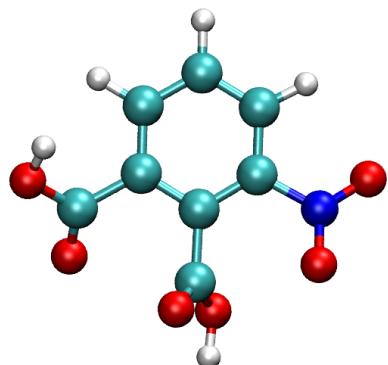
EingenValues - Molecule B

531.698	929.417	1355.4
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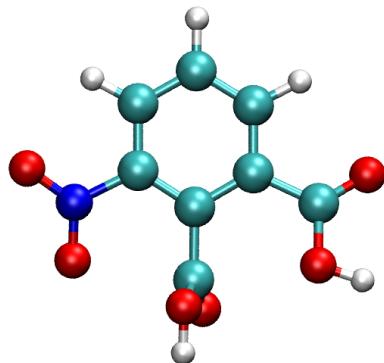
Different



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

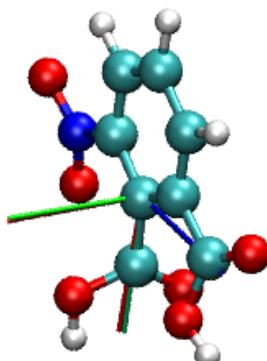
EingenValues - Molecule A

528.663	924.928	1336.12
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EingenValues - Molecule B

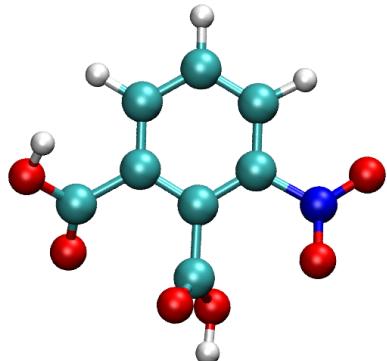
531.43	913.309	1353.35
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Different

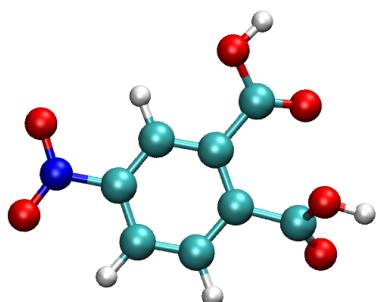


FireTest Número 162

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

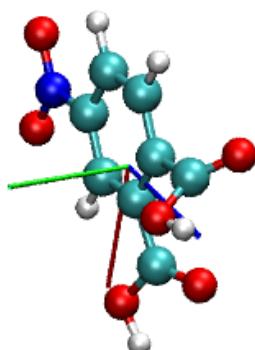
EingenValues - Molecule A

528.663	924.928	1336.12
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EingenValues - Molecule B

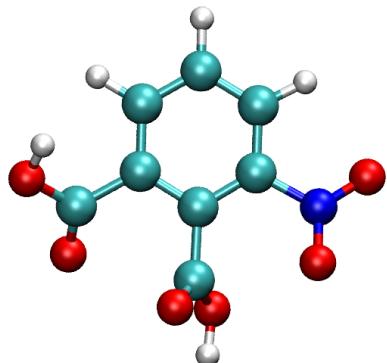
479.363	1242.41	1647.39
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Different

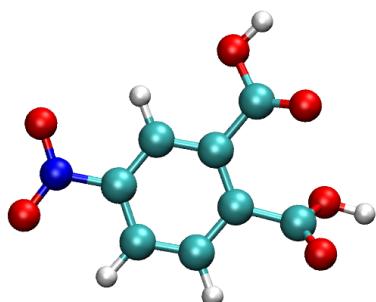


FireTest Número 163

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

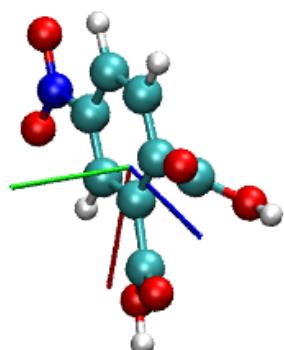
EingenValues - Molecule A

528.663	924.928	1336.12
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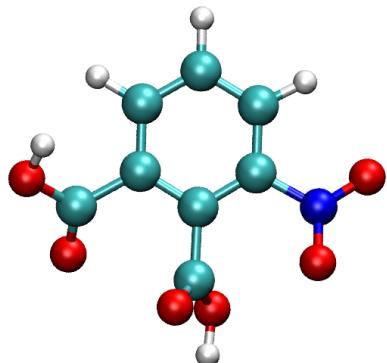
EingenValues - Molecule B

479.308	1242.41	1647.31
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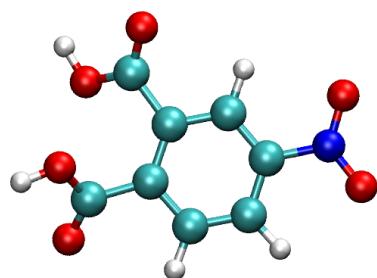
Different



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

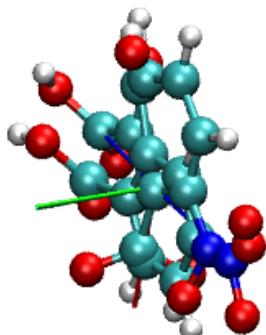
EingenValues - Molecule A

528.663	924.928	1336.12
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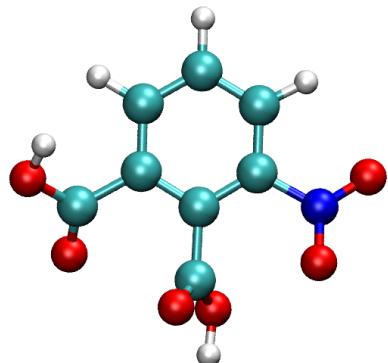
EingenValues - Molecule B

482.027	1240.32	1647.08
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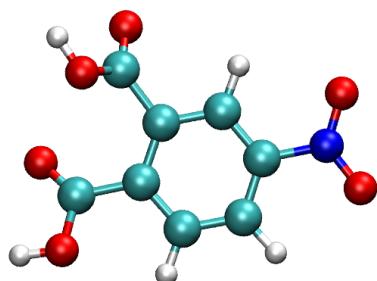
Different



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

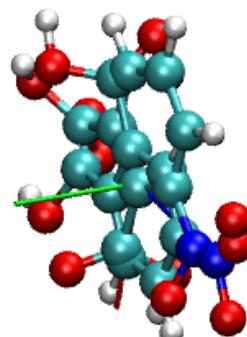
EingenValues - Molecule A

528.663	924.928	1336.12
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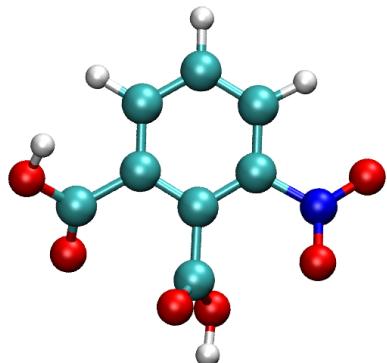
EingenValues - Molecule B

491.663	1231.14	1650.13
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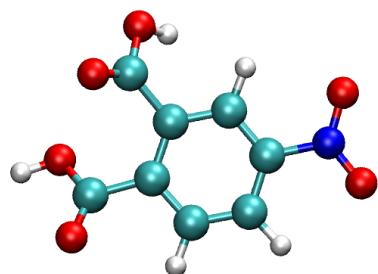
Different



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

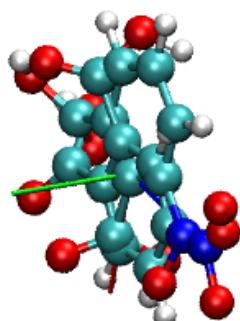
EingenValues - Molecule A

528.663	924.928	1336.12
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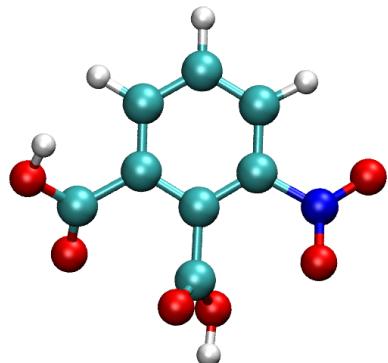
EingenValues - Molecule B

489.011	1233.7	1641.81
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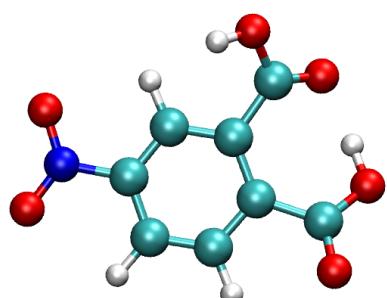
Different



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

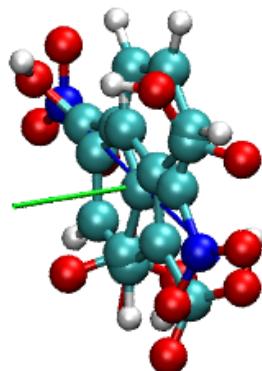
EingenValues - Molecule A

528.663	924.928	1336.12
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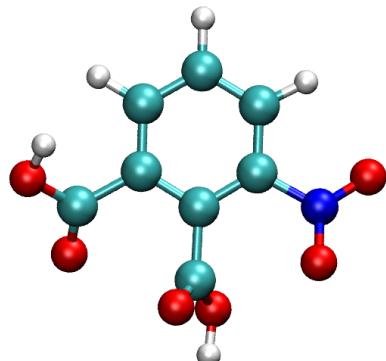
EingenValues - Molecule B

509.668	1219.11	1681.18
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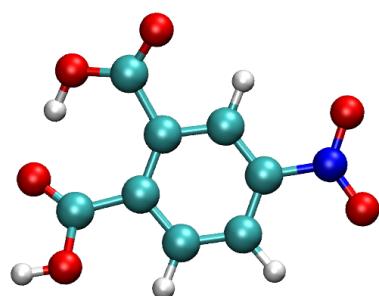
Different



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

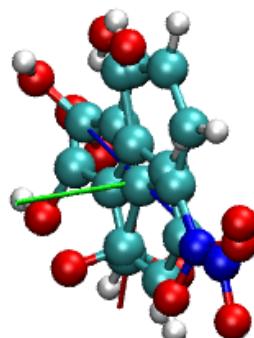
EingenValues - Molecule A

528.663	924.928	1336.12
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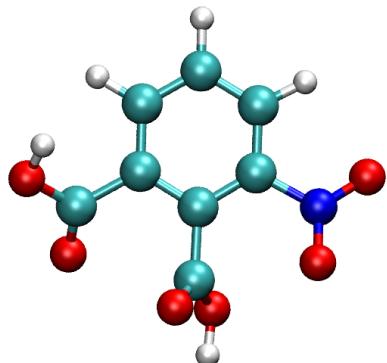
EingenValues - Molecule B

513.751	1208.07	1700.9
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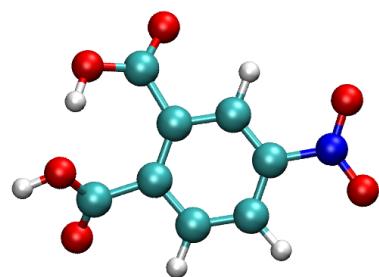
Different



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

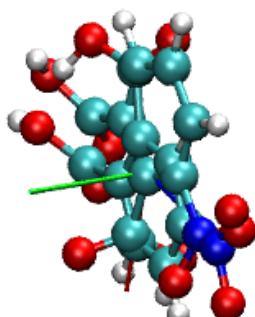
EingenValues - Molecule A

528.663	924.928	1336.12
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EingenValues - Molecule B

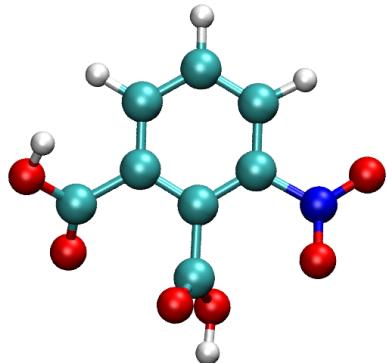
502.409	1232.26	1676.02
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Different

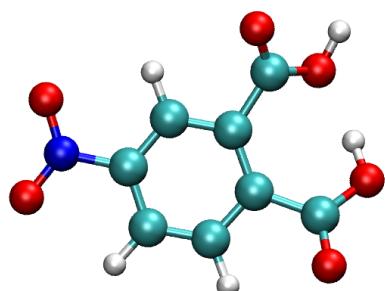


FireTest Número 170

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

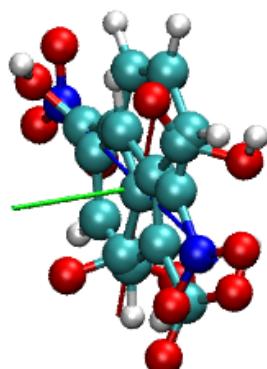
EigenValues - Molecule A

528.663	924.928	1336.12
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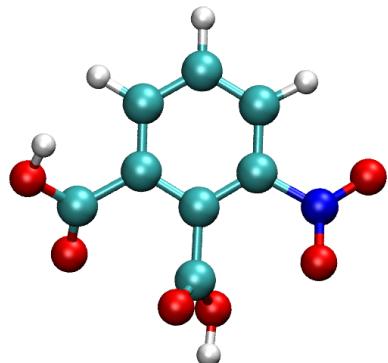
EigenValues - Molecule B

509.897	1225.65	1680.83
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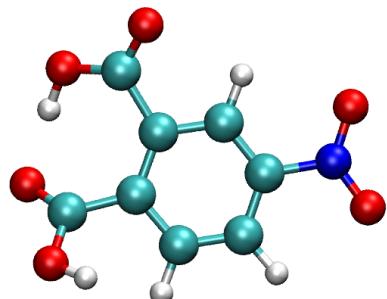
Different



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

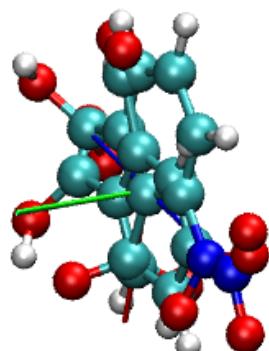
EingenValues - Molecule A

528.663	924.928	1336.12
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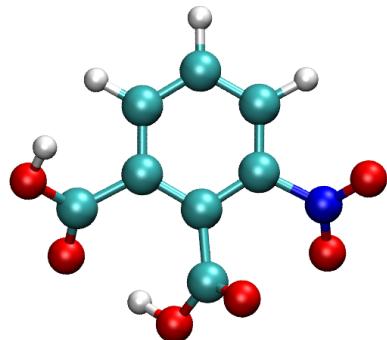
EingenValues - Molecule B

506.607	1222.36	1678.43
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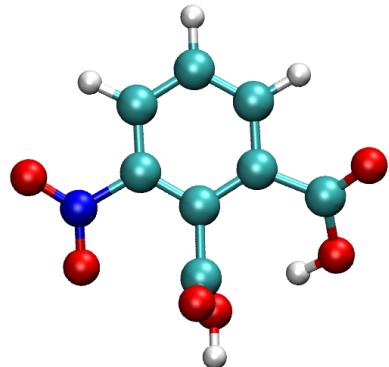
Different



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

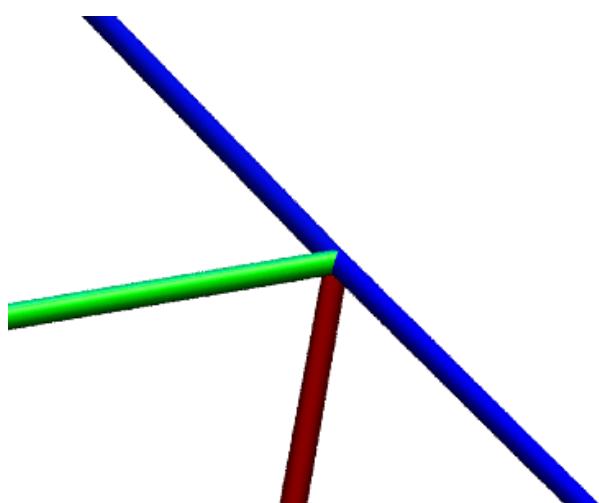
EingenValues - Molecule A

521.475	949.659	1346.18
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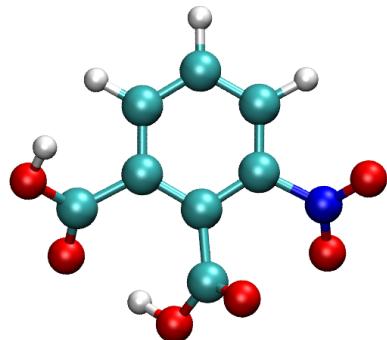
EingenValues - Molecule B

533.726	920.137	1348.3
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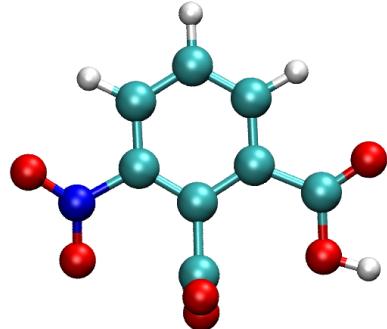
Different



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

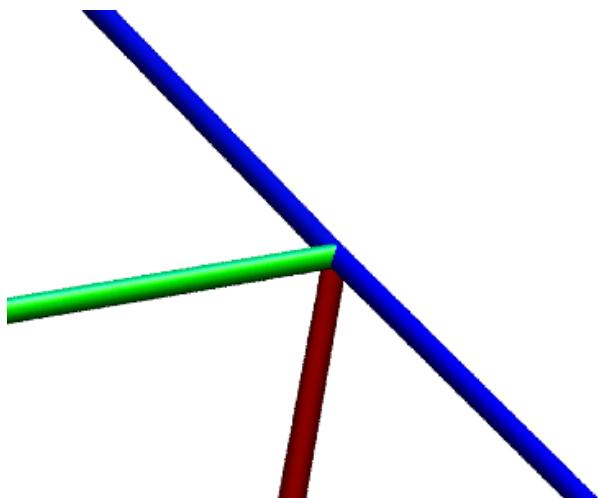
EingenValues - Molecule A

521.475	949.659	1346.18
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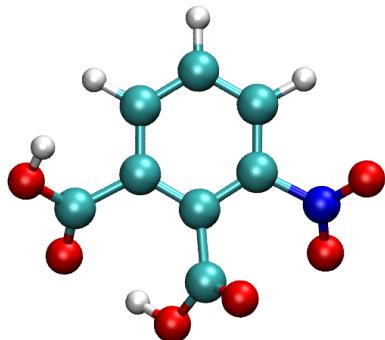
EingenValues - Molecule B

534.81	913.339	1353.78
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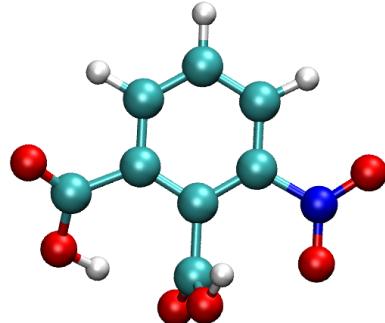
Different



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

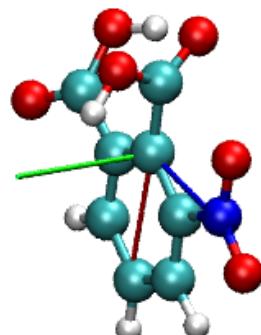
EingenValues - Molecule A

521.475	949.659	1346.18
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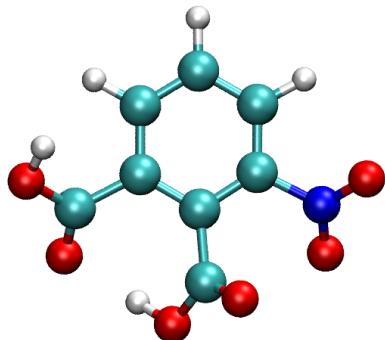
EingenValues - Molecule B

531.691	929.434	1355.4
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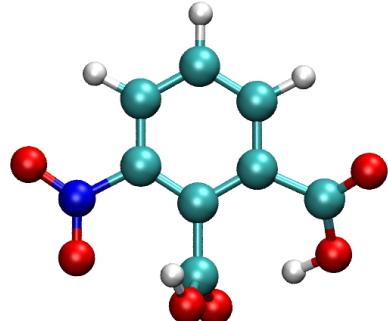
Different



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

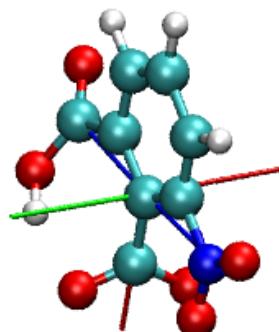
EingenValues - Molecule A

521.475	949.659	1346.18
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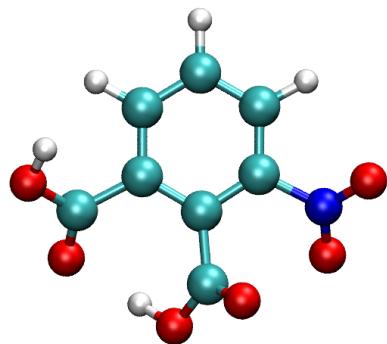
EingenValues - Molecule B

531.698	929.417	1355.4
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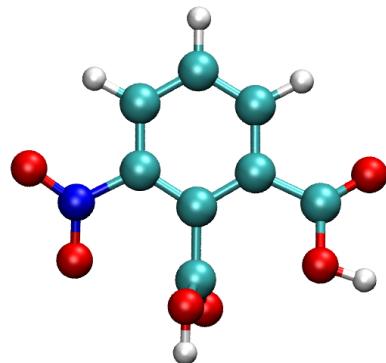
Different



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

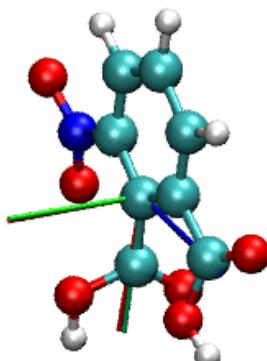
EingenValues - Molecule A

521.475	949.659	1346.18
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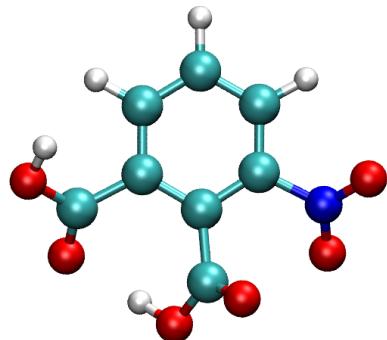
EingenValues - Molecule B

531.43	913.309	1353.35
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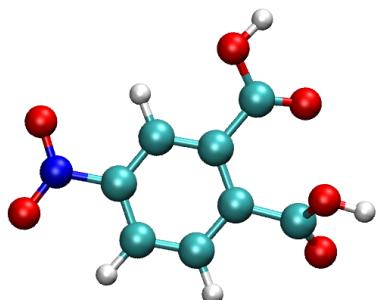
Different



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

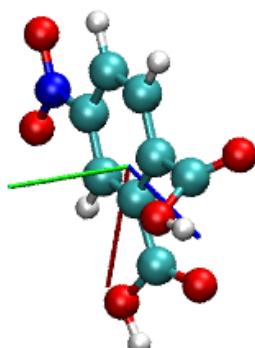
EingenValues - Molecule A

521.475	949.659	1346.18
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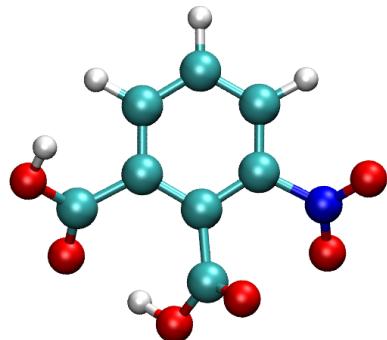
EingenValues - Molecule B

479.363	1242.41	1647.39
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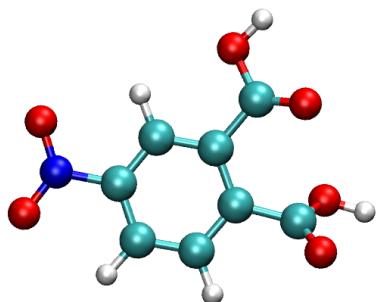
Different



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

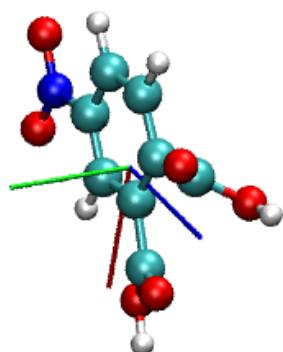
EingenValues - Molecule A

521.475	949.659	1346.18
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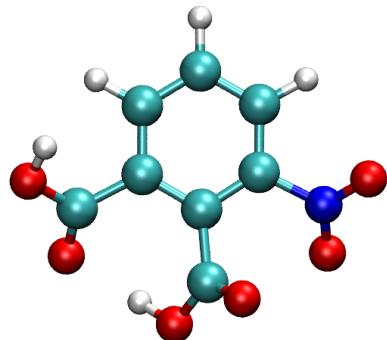
EingenValues - Molecule B

479.308	1242.41	1647.31
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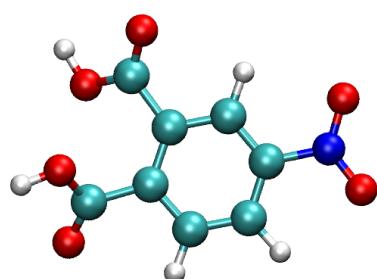
Different



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

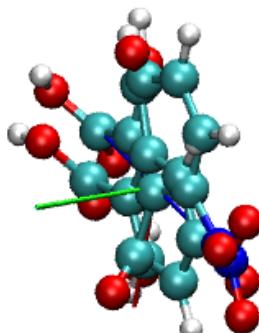
EingenValues - Molecule A

521.475	949.659	1346.18
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EingenValues - Molecule B

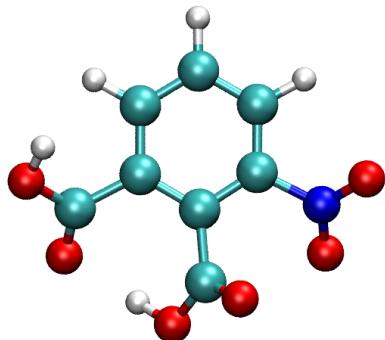
482.027	1240.32	1647.08
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Different

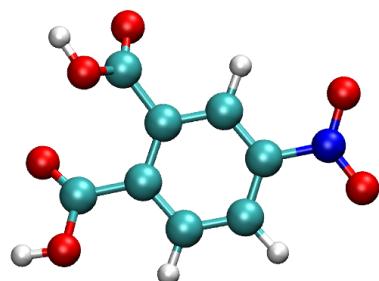


FireTest Número 180

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

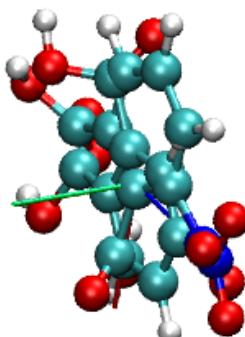
EingenValues - Molecule A

521.475	949.659	1346.18
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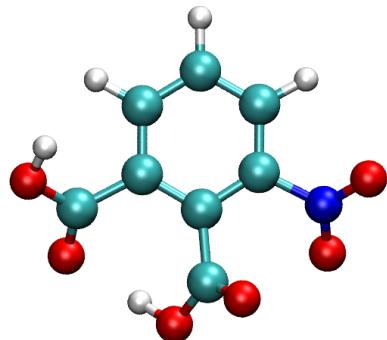
EingenValues - Molecule B

491.663	1231.14	1650.13
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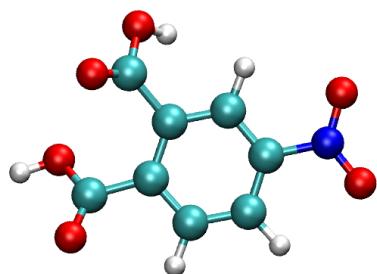
Different



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

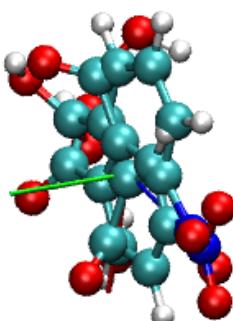
EingenValues - Molecule A

521.475	949.659	1346.18
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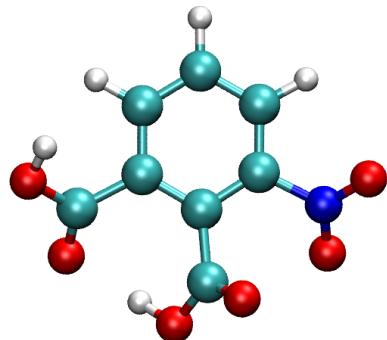
EingenValues - Molecule B

489.011	1233.7	1641.81
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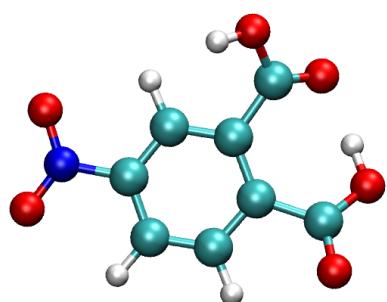
Different



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

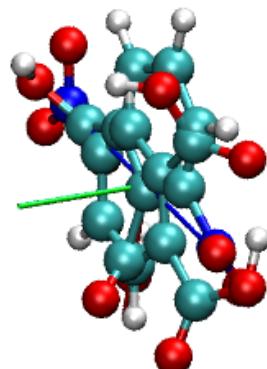
EingenValues - Molecule A

521.475	949.659	1346.18
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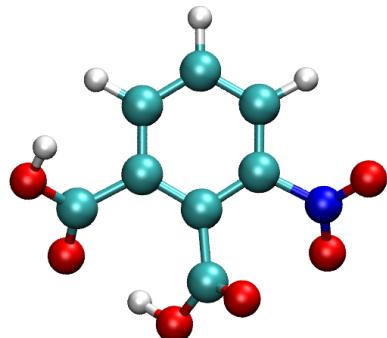
EingenValues - Molecule B

509.668	1219.11	1681.18
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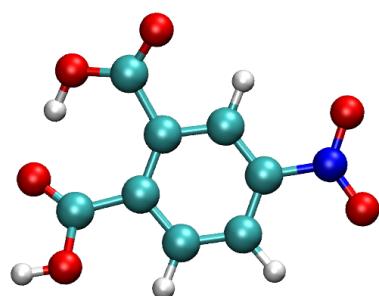
Different



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

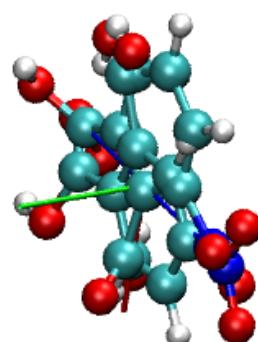
EingenValues - Molecule A

521.475	949.659	1346.18
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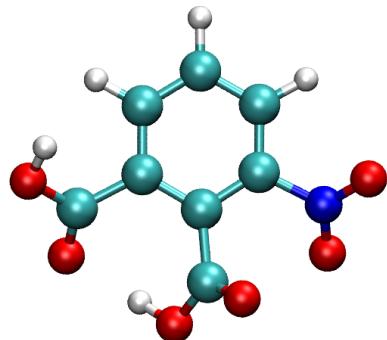
EingenValues - Molecule B

513.751	1208.07	1700.9
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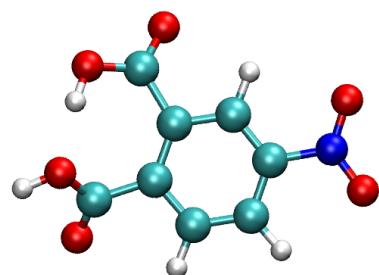
Different



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

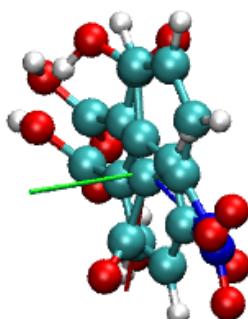
EingenValues - Molecule A

521.475	949.659	1346.18
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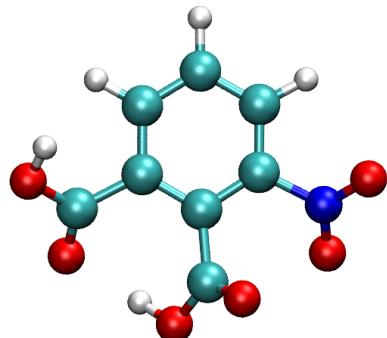
EingenValues - Molecule B

502.409	1232.26	1676.02
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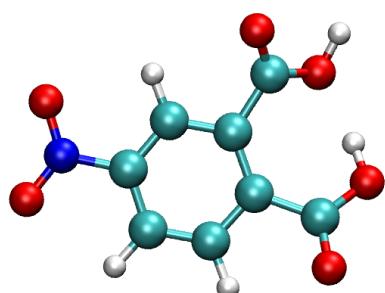
Different



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

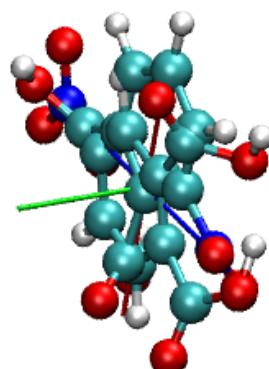
EingenValues - Molecule A

521.475	949.659	1346.18
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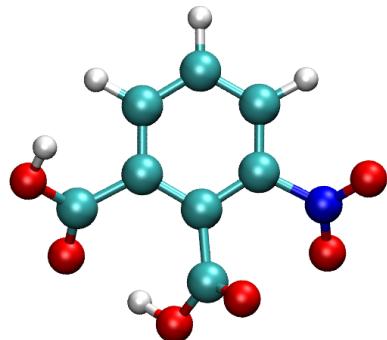
EingenValues - Molecule B

509.897	1225.65	1680.83
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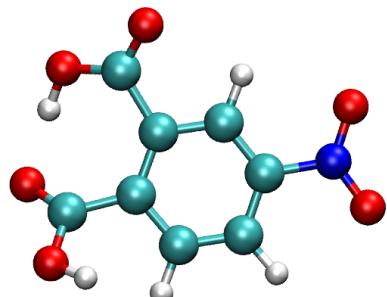
Different



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

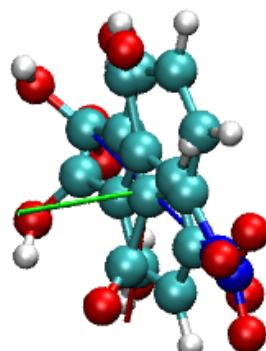
EingenValues - Molecule A

521.475	949.659	1346.18
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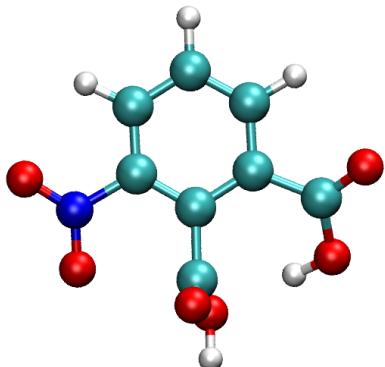
EingenValues - Molecule B

506.607	1222.36	1678.43
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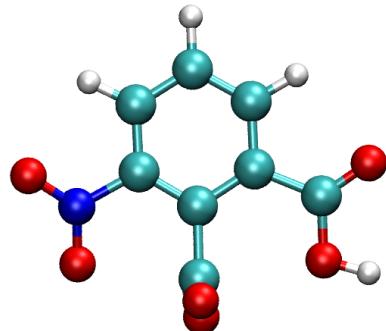
Different



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

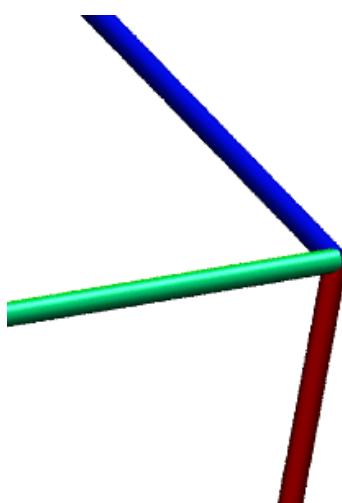
EingenValues - Molecule A

533.726	920.137	1348.3
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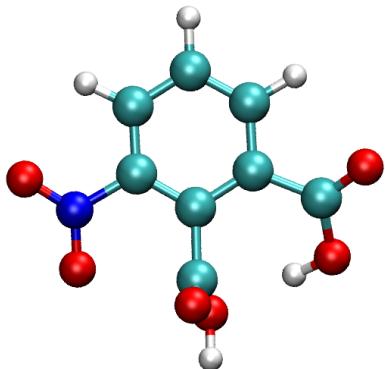
EingenValues - Molecule B

534.81	913.339	1353.78
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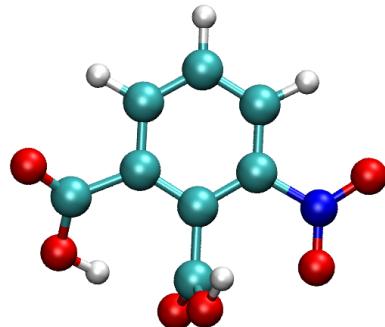
Different



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

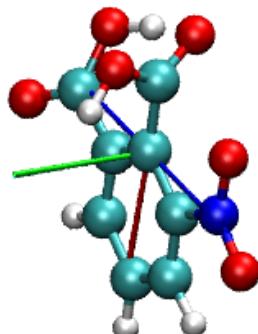
EingenValues - Molecule A

533.726	920.137	1348.3
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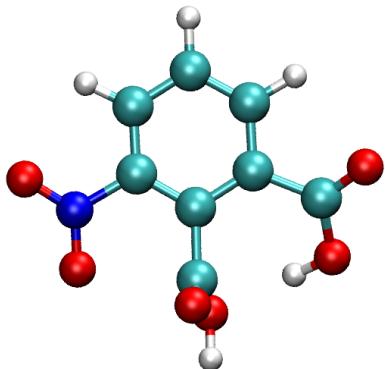
EingenValues - Molecule B

531.691	929.434	1355.4
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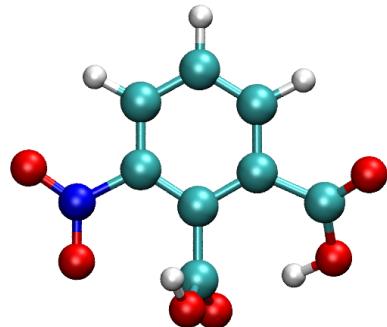
Different



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

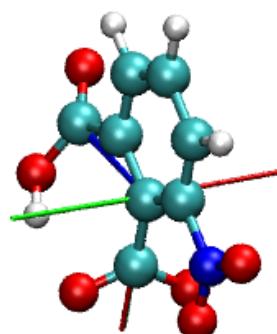
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

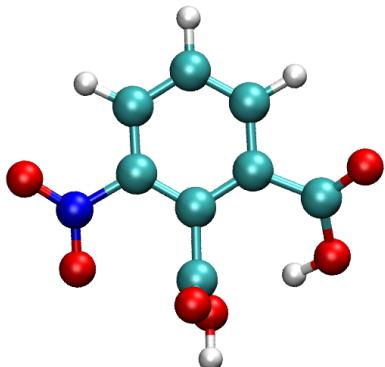
531.698	929.417	1355.4
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Different

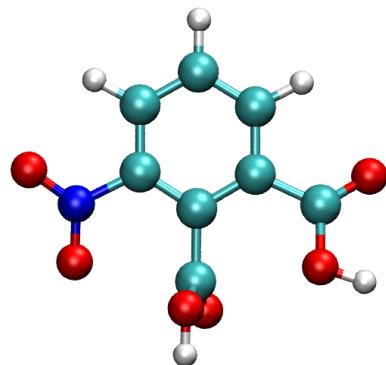


FireTest Número 190

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

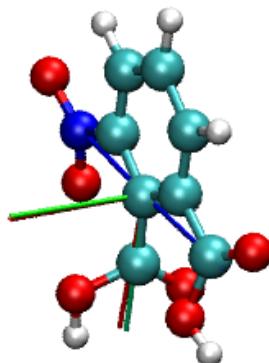
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

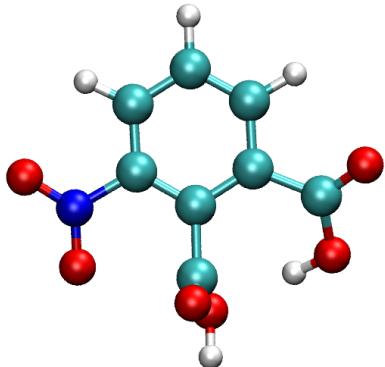
531.43	913.309	1353.35
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Different

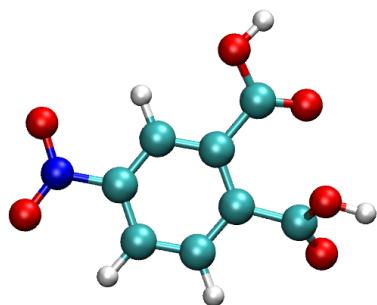


FireTest Número 191

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

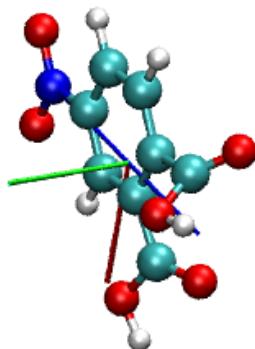
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

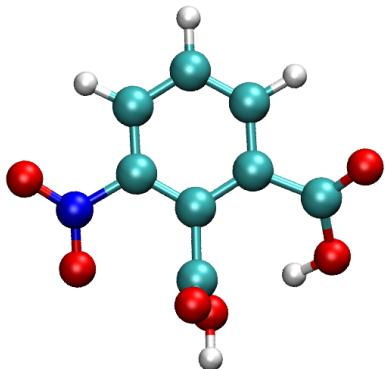
479.363	1242.41	1647.39
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Different

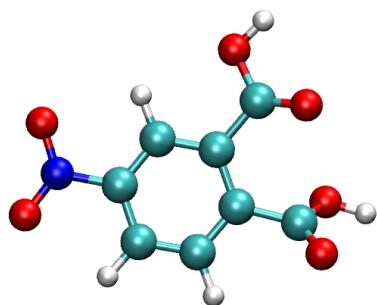


FireTest Número 192

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

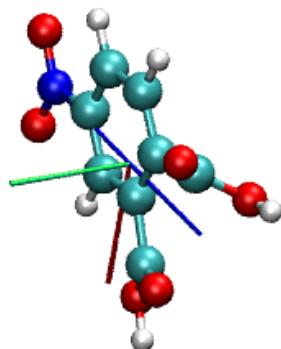
EingenValues - Molecule A

533.726	920.137	1348.3
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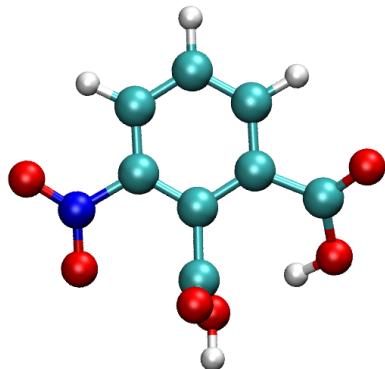
EingenValues - Molecule B

479.308	1242.41	1647.31
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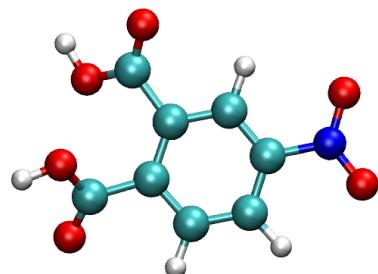
Different



Molecule A 3NFAACj



Molecule B 4NFAACC



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

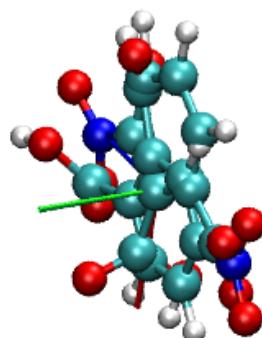
EingenValues - Molecule A

533.726	920.137	1348.3
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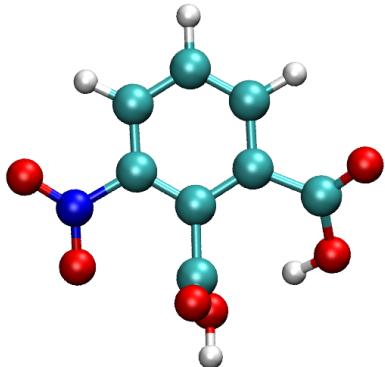
EingenValues - Molecule B

482.027	1240.32	1647.08
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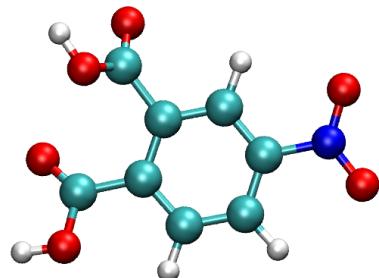
Different



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

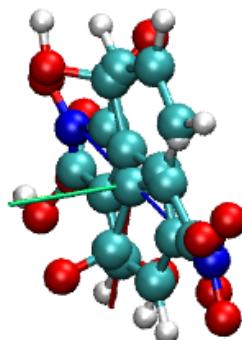
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

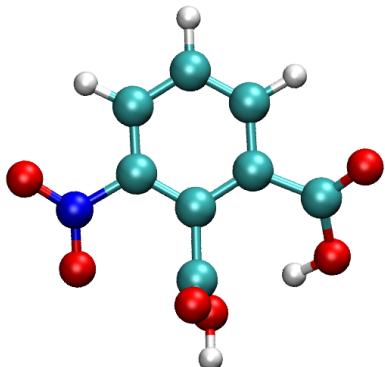
491.663	1231.14	1650.13
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Different

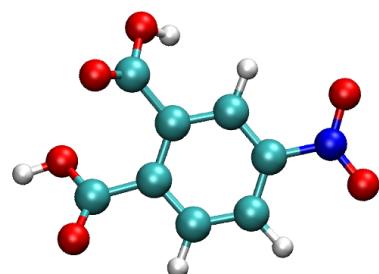


FireTest Número 195

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

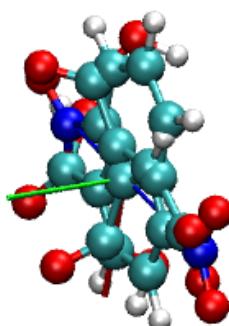
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

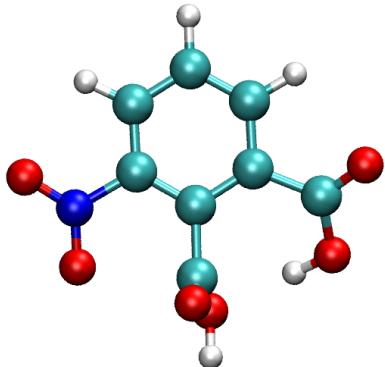
489.011	1233.7	1641.81
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Different

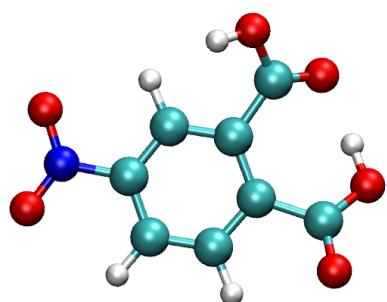


FireTest Número 196

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

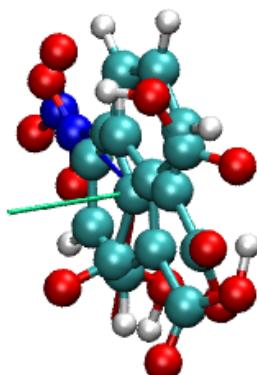
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

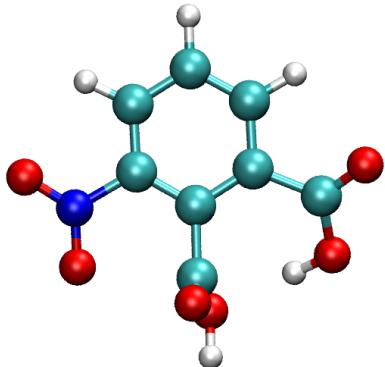
509.668	1219.11	1681.18
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Different

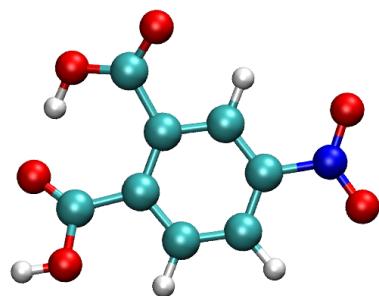


FireTest Número 197

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

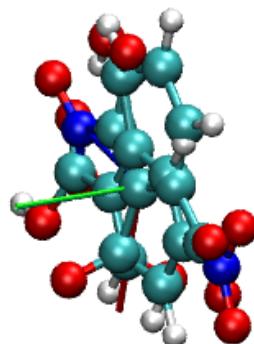
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

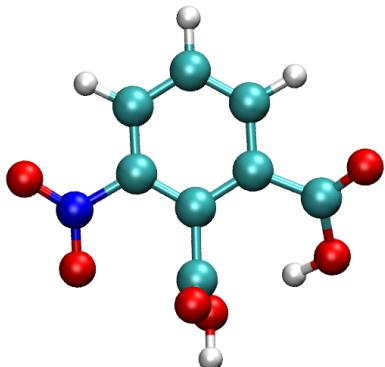
513.751	1208.07	1700.9
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Different

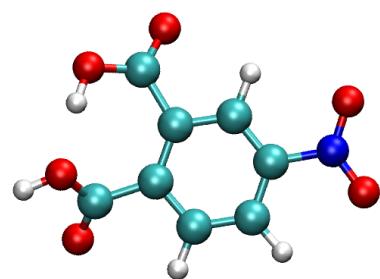


FireTest Número 198

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

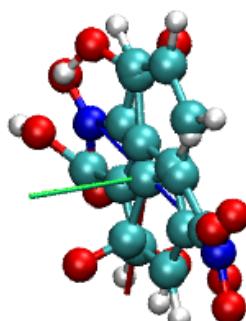
EingenValues - Molecule A

533.726	920.137	1348.3
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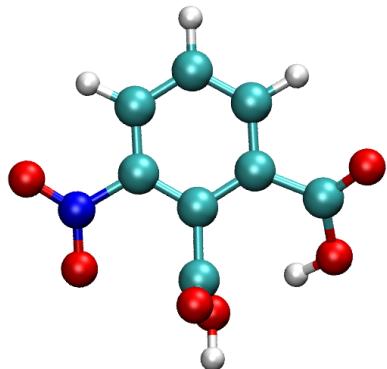
EingenValues - Molecule B

502.409	1232.26	1676.02
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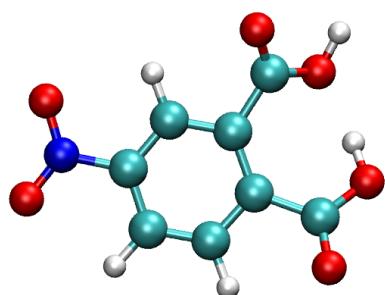
Different



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

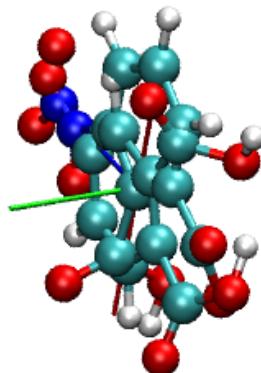
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

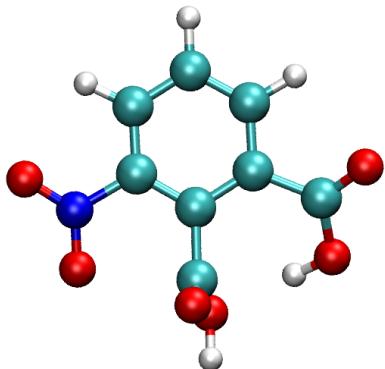
509.897	1225.65	1680.83
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Different

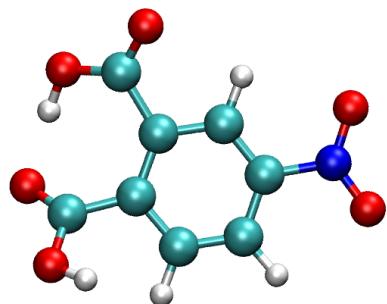


FireTest Número 200

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

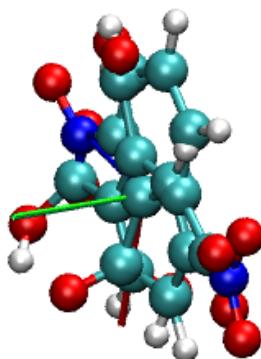
EingenValues - Molecule A

533.726	920.137	1348.3
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EingenValues - Molecule B

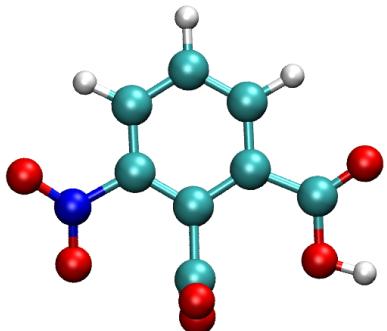
506.607	1222.36	1678.43
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Different

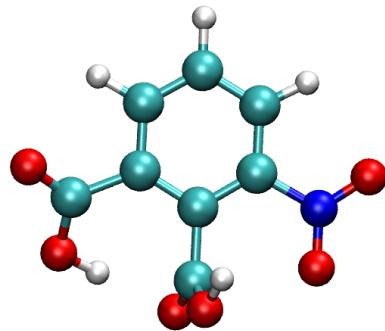


FireTest Número 201

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

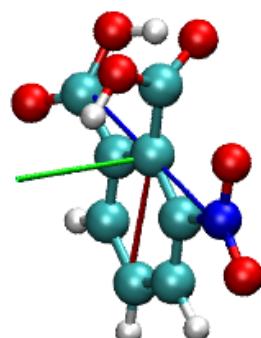
EingenValues - Molecule A

534.81	913.339	1353.78
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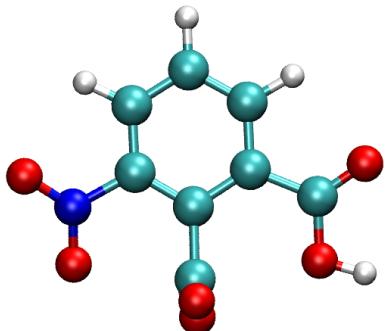
EingenValues - Molecule B

531.691	929.434	1355.4
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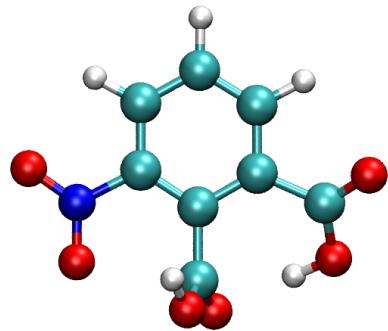
Different



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

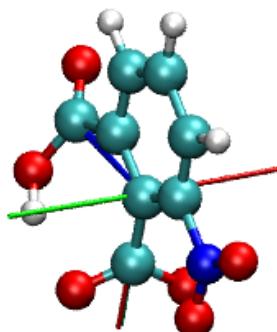
EingenValues - Molecule A

534.81	913.339	1353.78
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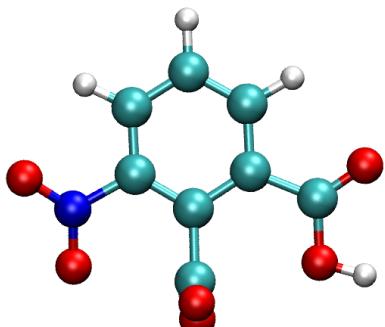
EingenValues - Molecule B

531.698	929.417	1355.4
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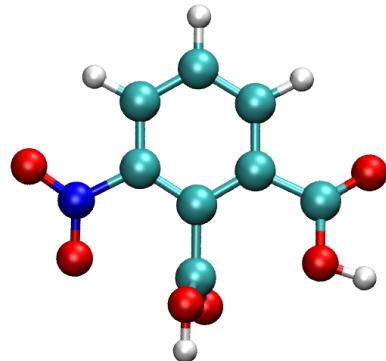
Different



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

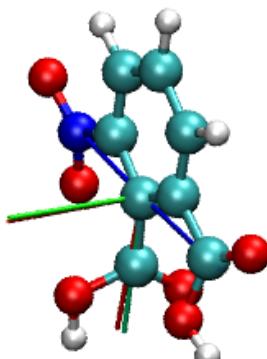
EingenValues - Molecule A

534.81	913.339	1353.78
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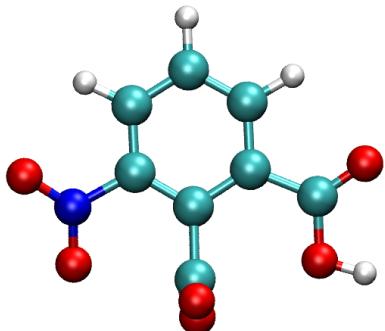
EingenValues - Molecule B

531.43	913.309	1353.35
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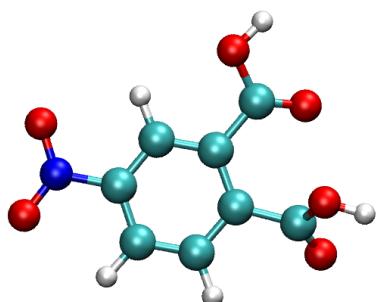
Different



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

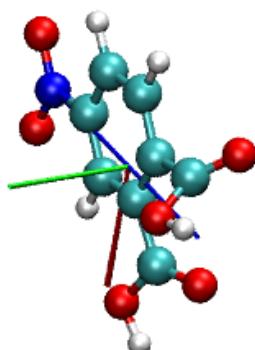
EingenValues - Molecule A

534.81	913.339	1353.78
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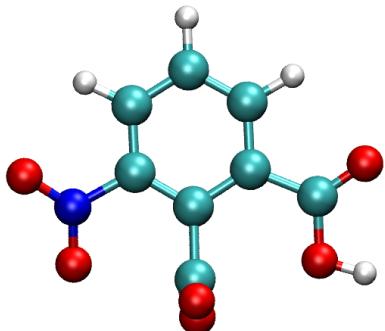
EingenValues - Molecule B

479.363	1242.41	1647.39
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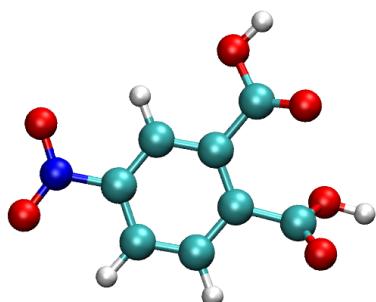
Different



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

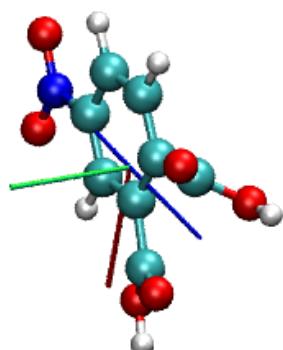
EingenValues - Molecule A

534.81	913.339	1353.78
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EingenValues - Molecule B

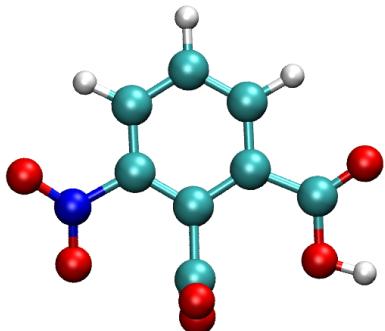
479.308	1242.41	1647.31
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Different

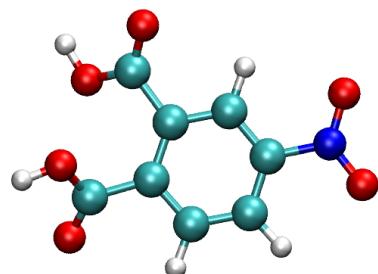


FireTest Número 206

Molecule A 3NFAACk



Molecule B 4NFAACCc



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

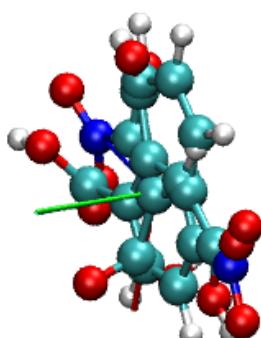
EingenValues - Molecule A

534.81	913.339	1353.78
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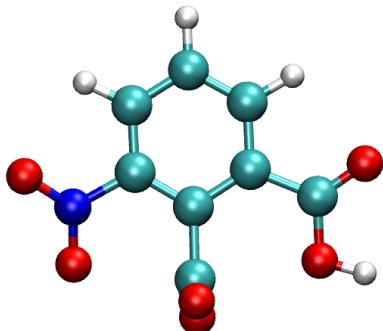
EingenValues - Molecule B

482.027	1240.32	1647.08
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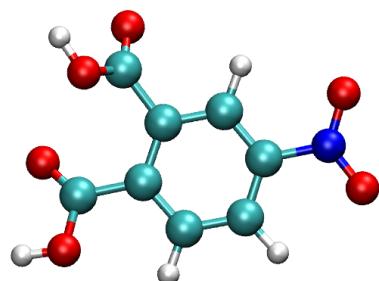
Different



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

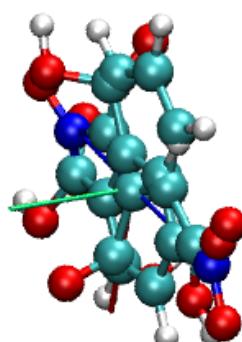
EingenValues - Molecule A

534.81	913.339	1353.78
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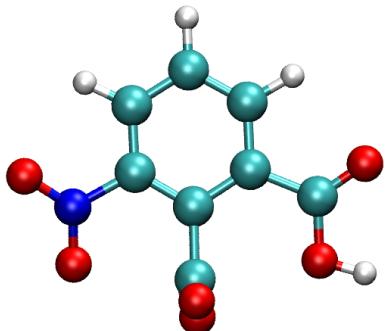
EingenValues - Molecule B

491.663	1231.14	1650.13
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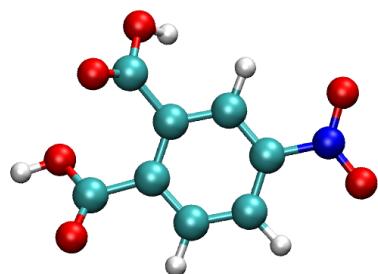
Different



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

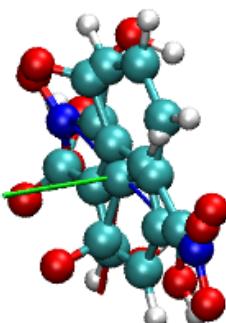
EingenValues - Molecule A

534.81	913.339	1353.78
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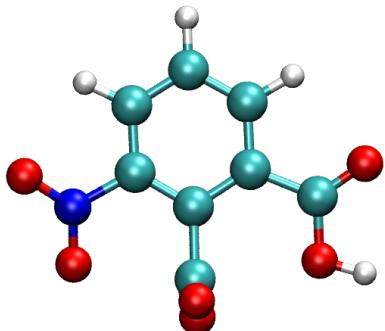
EingenValues - Molecule B

489.011	1233.7	1641.81
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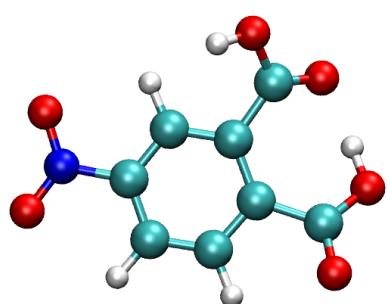
Different



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

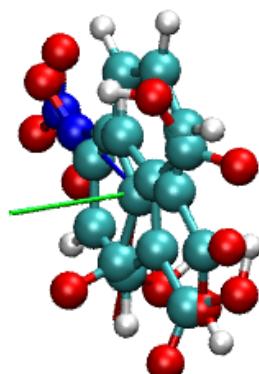
EingenValues - Molecule A

534.81	913.339	1353.78
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EingenValues - Molecule B

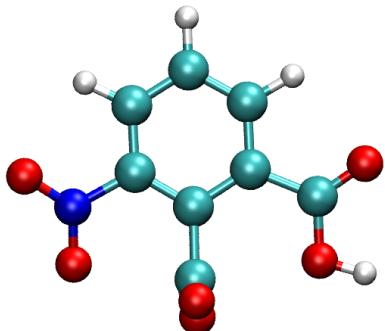
509.668	1219.11	1681.18
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Different

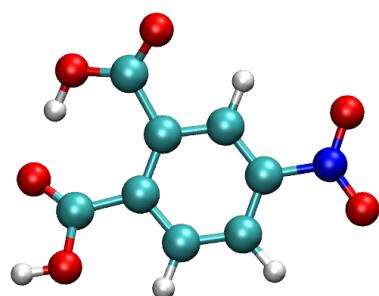


FireTest Número 210

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

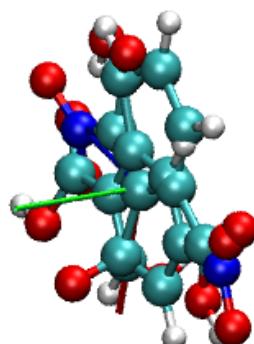
EingenValues - Molecule A

534.81	913.339	1353.78
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EingenValues - Molecule B

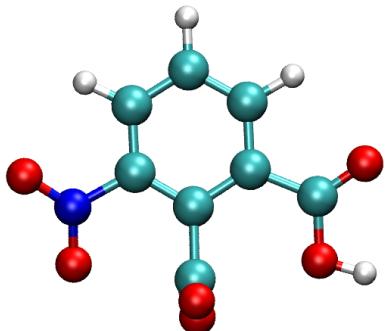
513.751	1208.07	1700.9
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Different

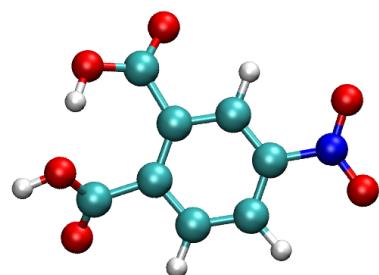


FireTest Número 211

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

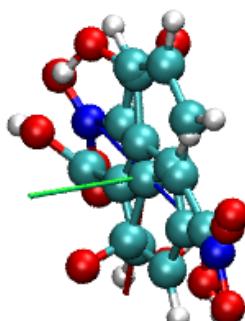
EingenValues - Molecule A

534.81	913.339	1353.78
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EingenValues - Molecule B

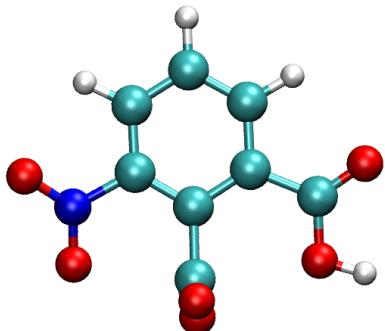
502.409	1232.26	1676.02
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Different

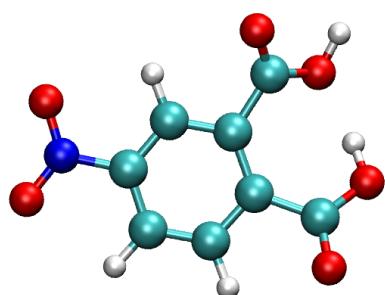


FireTest Número 212

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

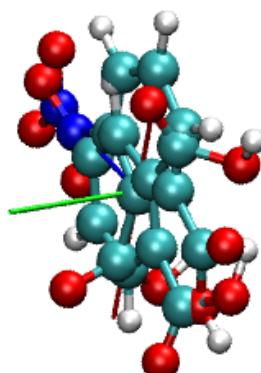
EingenValues - Molecule A

534.81	913.339	1353.78
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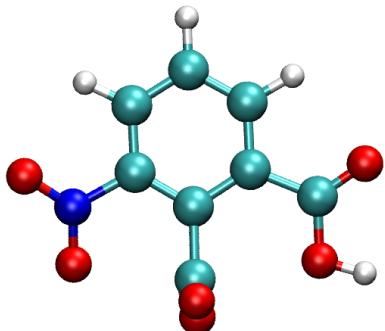
EingenValues - Molecule B

509.897	1225.65	1680.83
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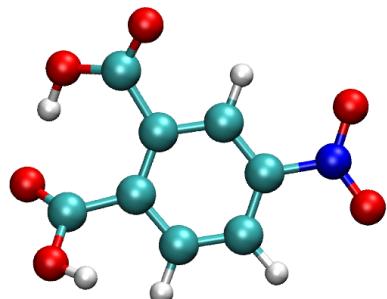
Different



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

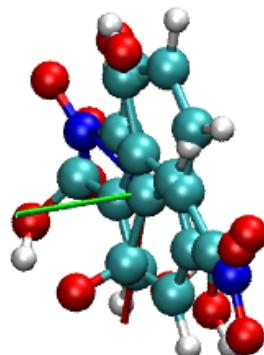
EingenValues - Molecule A

534.81	913.339	1353.78
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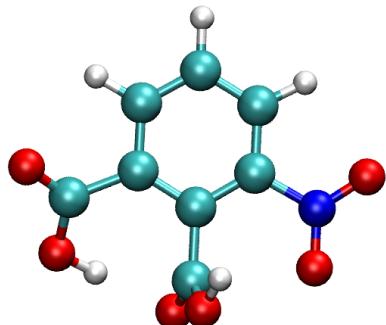
EingenValues - Molecule B

506.607	1222.36	1678.43
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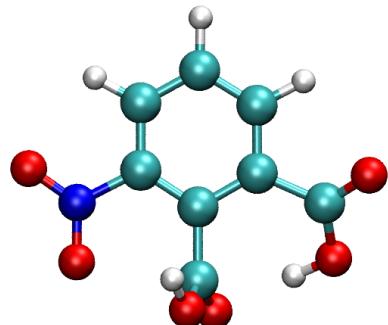
Different



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

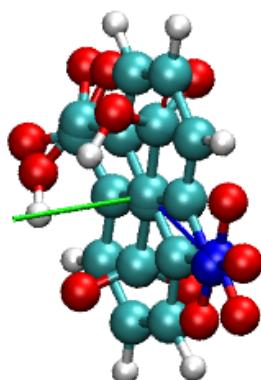
EingenValues - Molecule A

531.691	929.434	1355.4
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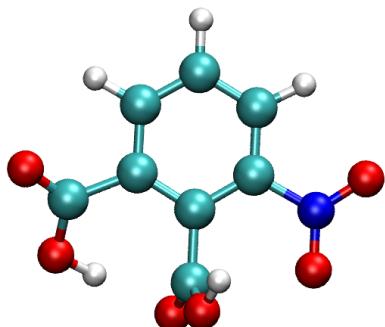
EingenValues - Molecule B

531.698	929.417	1355.4
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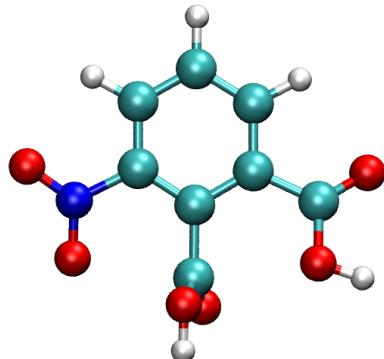
Equal



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

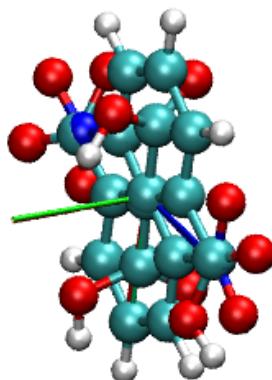
EingenValues - Molecule A

531.691	929.434	1355.4
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EingenValues - Molecule B

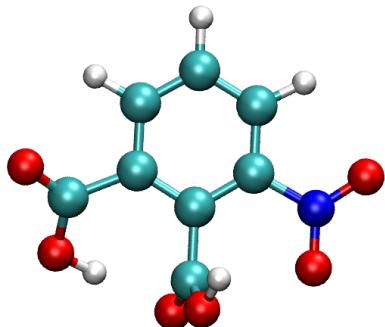
531.43	913.309	1353.35
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Different

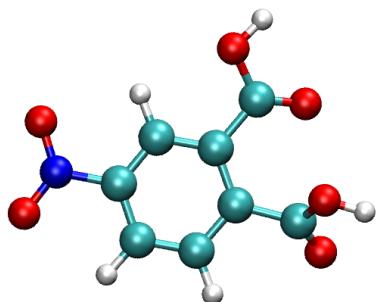


FireTest Número 216

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

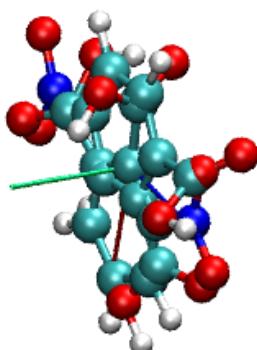
EingenValues - Molecule A

531.691	929.434	1355.4
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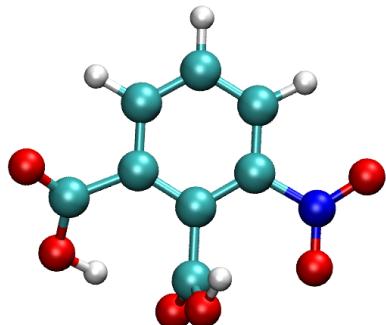
EingenValues - Molecule B

479.363	1242.41	1647.39
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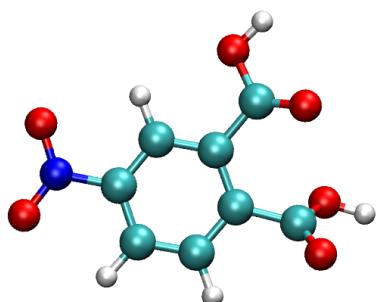
Different



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

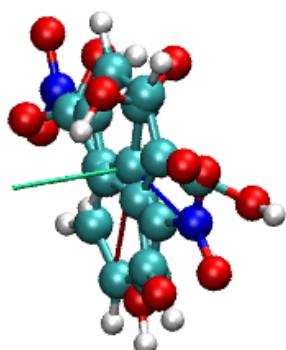
EingenValues - Molecule A

531.691	929.434	1355.4
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EingenValues - Molecule B

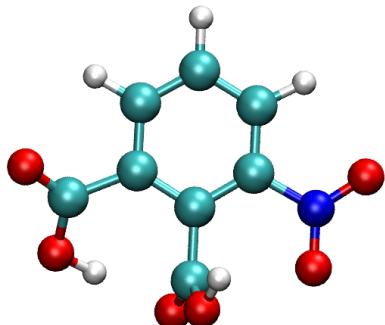
479.308	1242.41	1647.31
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Different

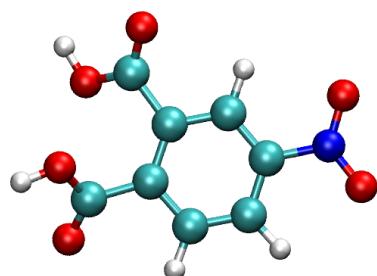


FireTest Número 218

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

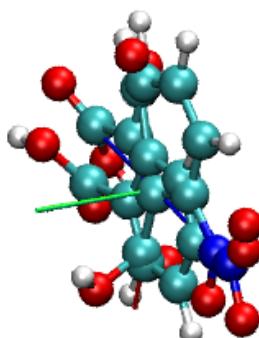
EingenValues - Molecule A

531.691	929.434	1355.4
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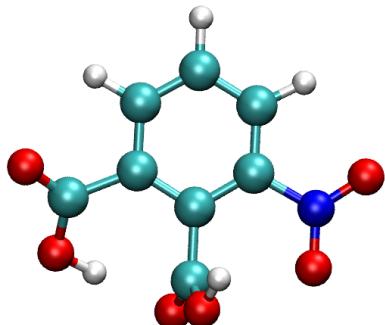
EingenValues - Molecule B

482.027	1240.32	1647.08
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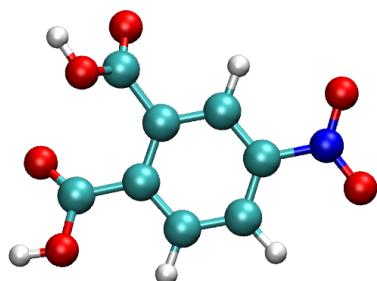
Different



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

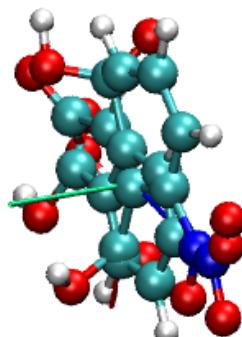
EingenValues - Molecule A

531.691	929.434	1355.4
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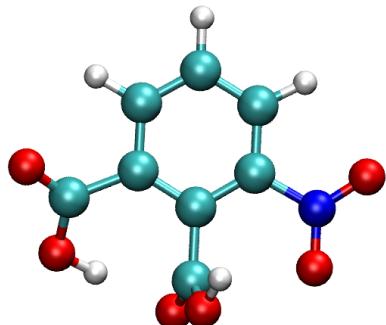
EingenValues - Molecule B

491.663	1231.14	1650.13
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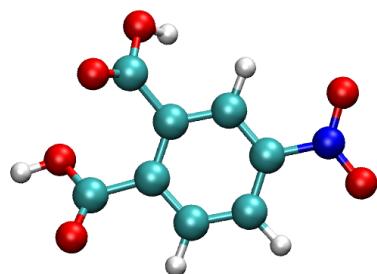
Different



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

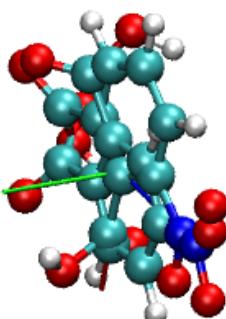
EingenValues - Molecule A

531.691	929.434	1355.4
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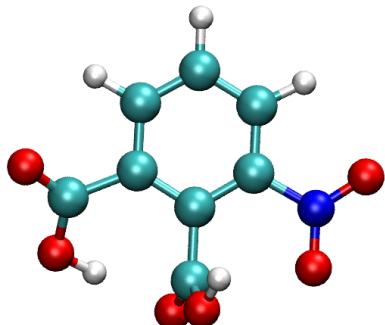
EingenValues - Molecule B

489.011	1233.7	1641.81
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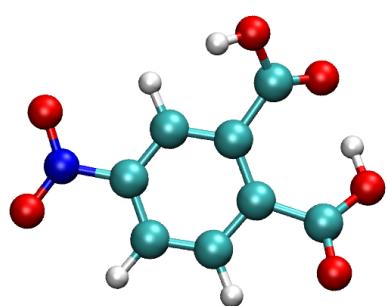
Different



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

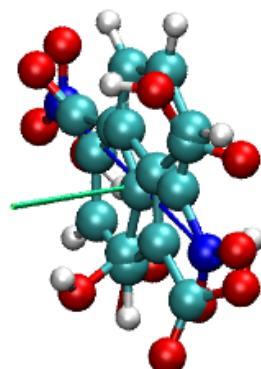
EingenValues - Molecule A

531.691	929.434	1355.4
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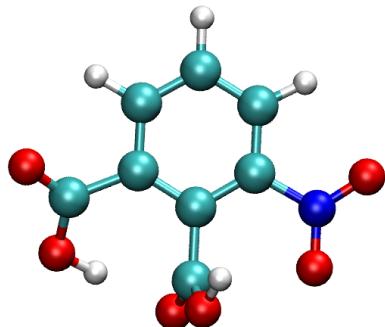
EingenValues - Molecule B

509.668	1219.11	1681.18
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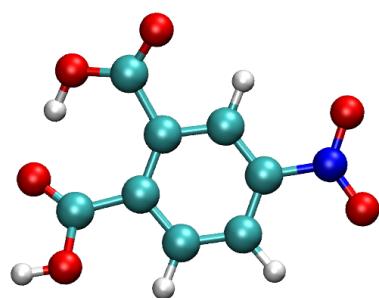
Different



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

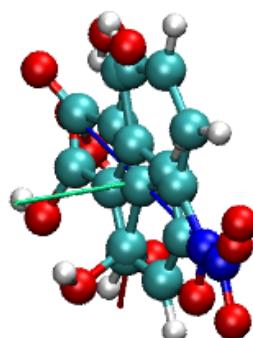
EingenValues - Molecule A

531.691	929.434	1355.4
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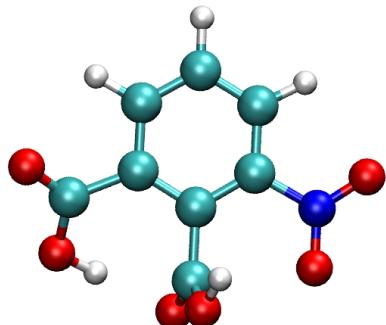
EingenValues - Molecule B

513.751	1208.07	1700.9
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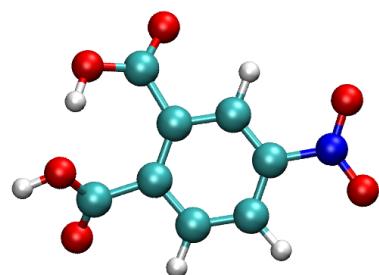
Different



Molecule A 3NFAACl



Molecule B 4NFAACi



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

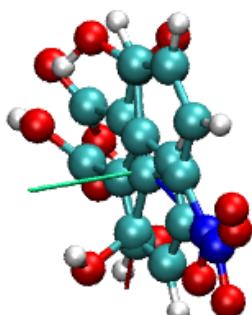
EingenValues - Molecule A

531.691	929.434	1355.4
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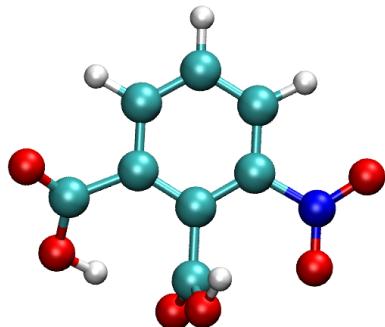
EingenValues - Molecule B

502.409	1232.26	1676.02
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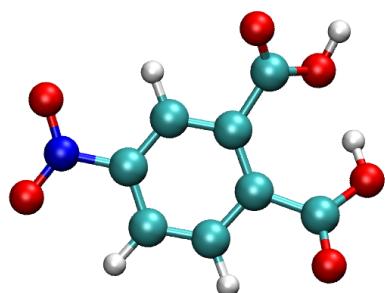
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

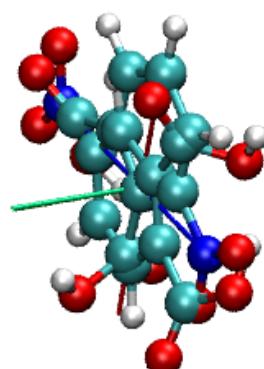
EingenValues - Molecule A

531.691	929.434	1355.4
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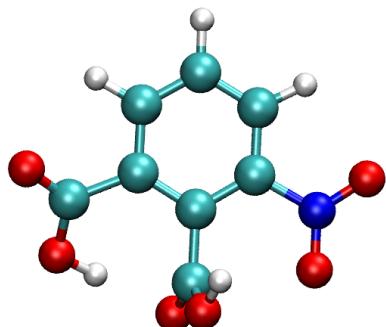
EingenValues - Molecule B

509.897	1225.65	1680.83
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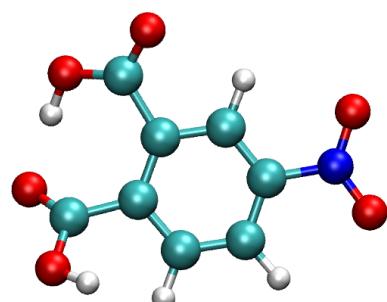
Different



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

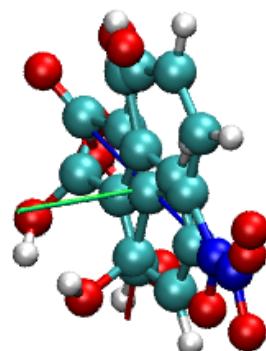
EingenValues - Molecule A

531.691	929.434	1355.4
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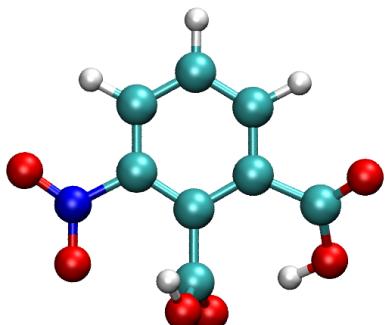
EingenValues - Molecule B

506.607	1222.36	1678.43
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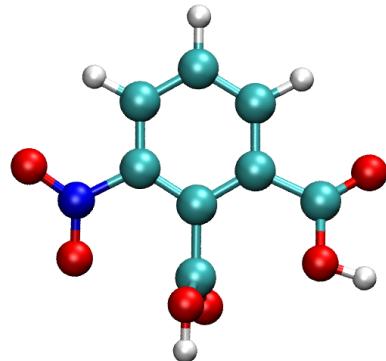
Different



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

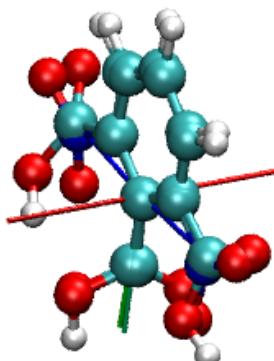
EingenValues - Molecule A

531.698	929.417	1355.4
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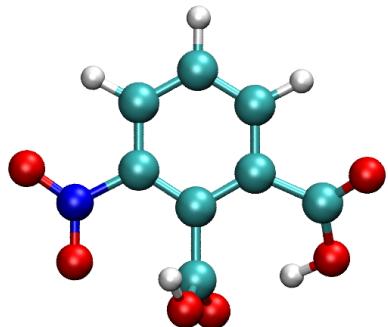
EingenValues - Molecule B

531.43	913.309	1353.35
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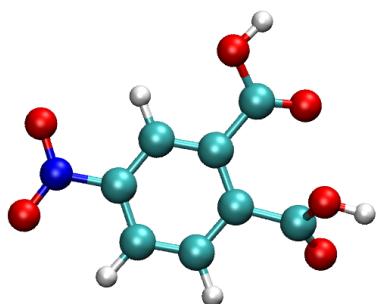
Different



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

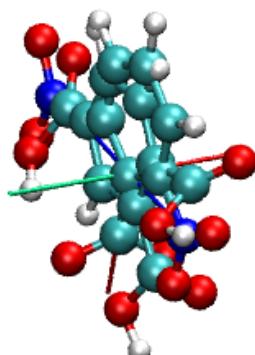
EingenValues - Molecule A

531.698	929.417	1355.4
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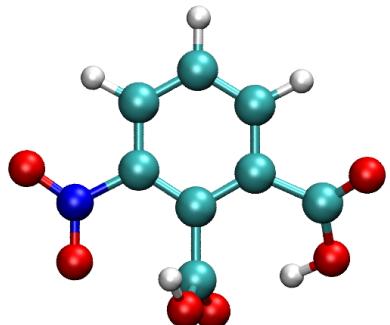
EingenValues - Molecule B

479.363	1242.41	1647.39
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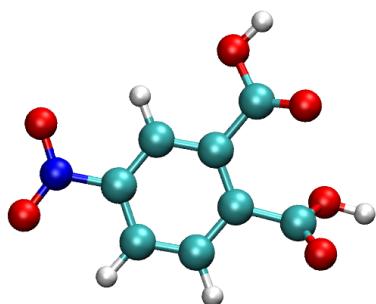
Different



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

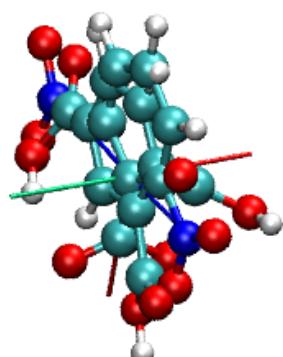
EingenValues - Molecule A

531.698	929.417	1355.4
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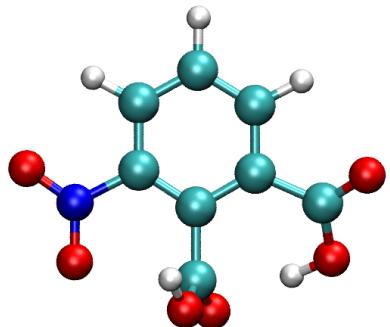
EingenValues - Molecule B

479.308	1242.41	1647.31
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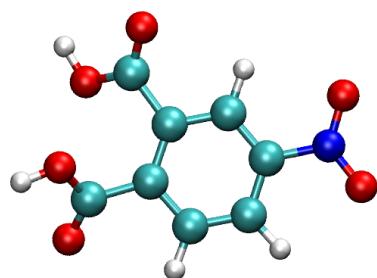
Different



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

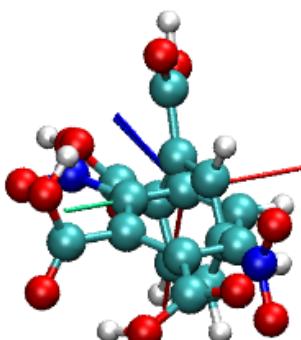
EingenValues - Molecule A

531.698	929.417	1355.4
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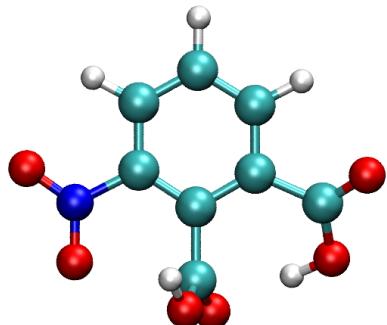
EingenValues - Molecule B

482.027	1240.32	1647.08
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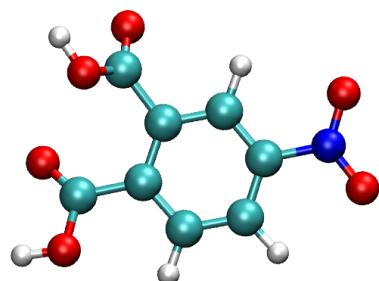
Different



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

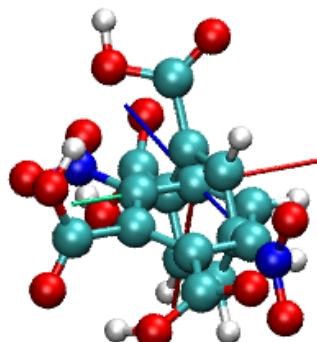
EingenValues - Molecule A

531.698	929.417	1355.4
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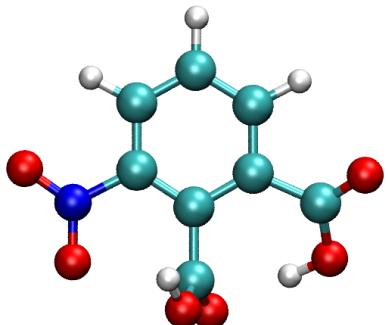
EingenValues - Molecule B

491.663	1231.14	1650.13
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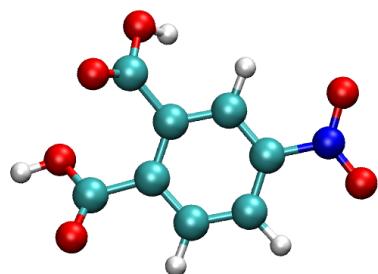
Different



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

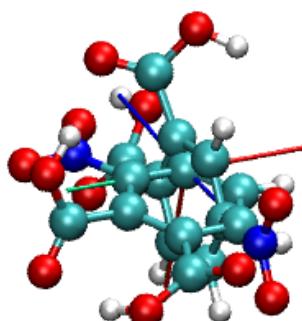
EingenValues - Molecule A

531.698	929.417	1355.4
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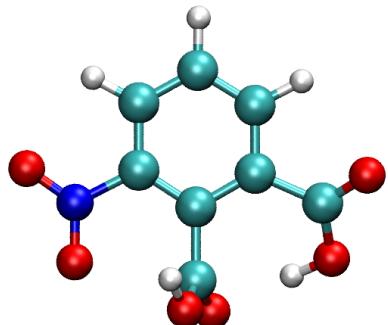
EingenValues - Molecule B

489.011	1233.7	1641.81
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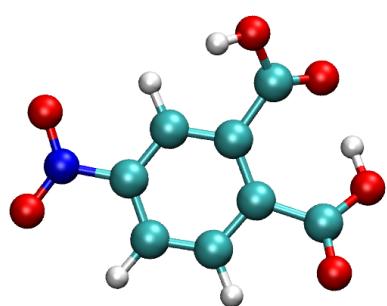
Different



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

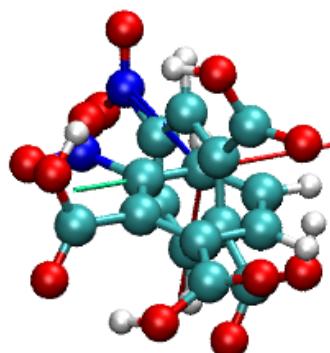
EingenValues - Molecule A

531.698	929.417	1355.4
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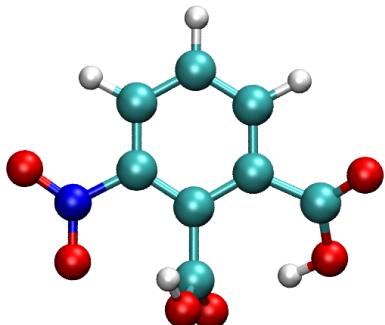
EingenValues - Molecule B

509.668	1219.11	1681.18
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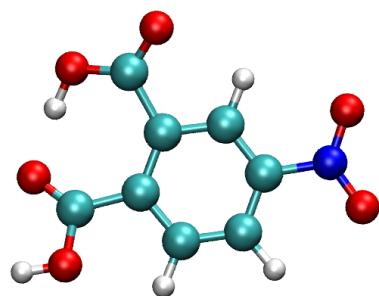
Different



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

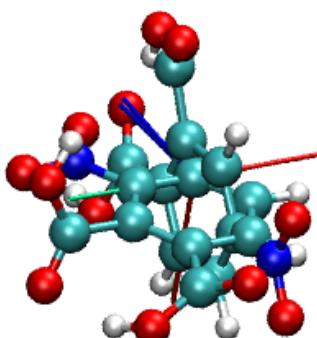
EingenValues - Molecule A

531.698	929.417	1355.4
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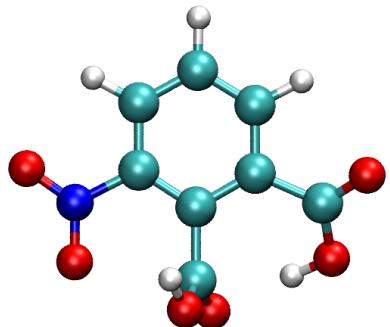
EingenValues - Molecule B

513.751	1208.07	1700.9
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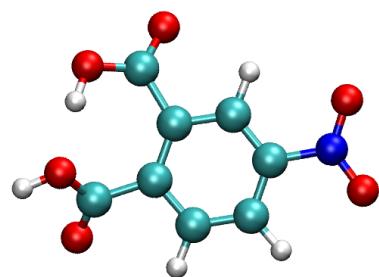
Different



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

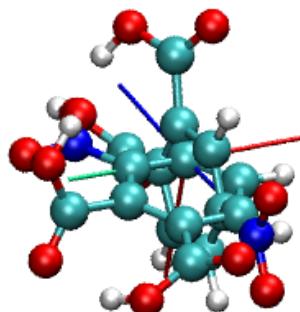
EingenValues - Molecule A

531.698	929.417	1355.4
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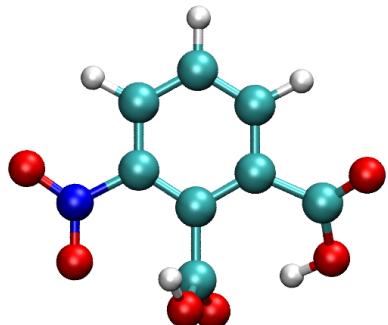
EingenValues - Molecule B

502.409	1232.26	1676.02
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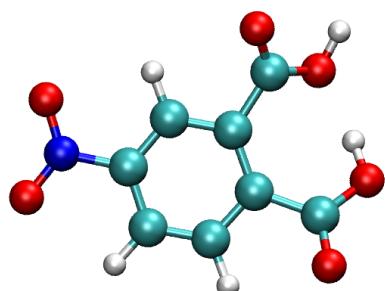
Different



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

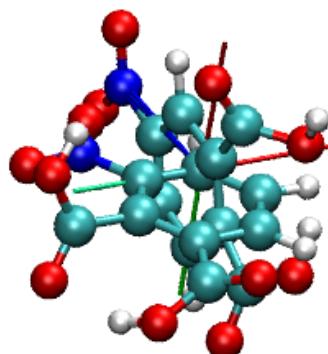
EingenValues - Molecule A

531.698	929.417	1355.4
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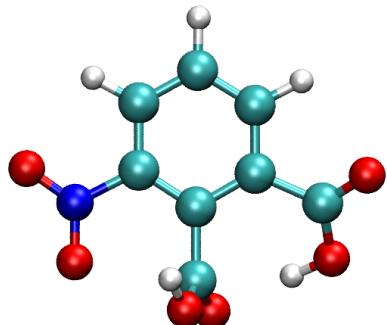
EingenValues - Molecule B

509.897	1225.65	1680.83
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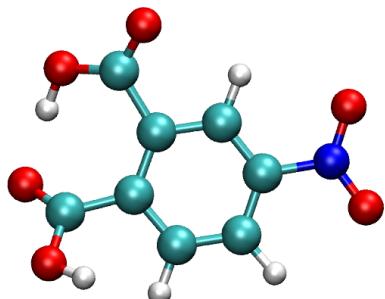
Different



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

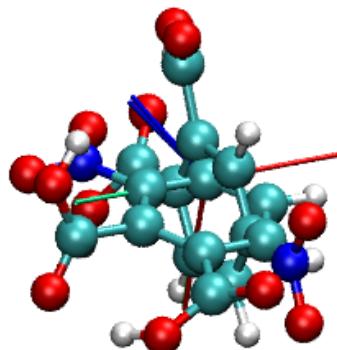
EingenValues - Molecule A

531.698	929.417	1355.4
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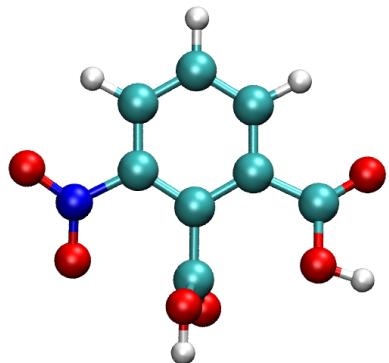
EingenValues - Molecule B

506.607	1222.36	1678.43
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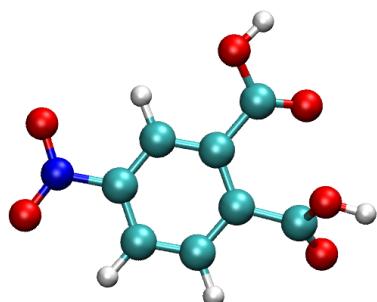
Different



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

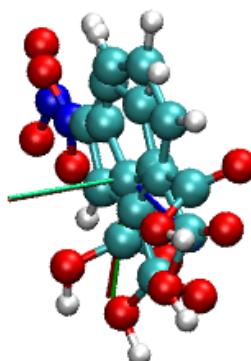
EingenValues - Molecule A

531.43	913.309	1353.35
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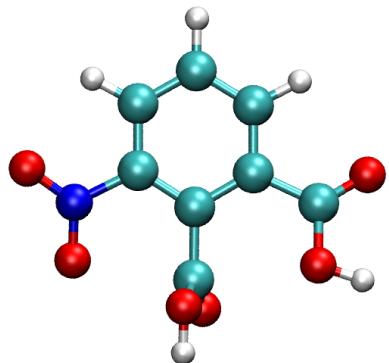
EingenValues - Molecule B

479.363	1242.41	1647.39
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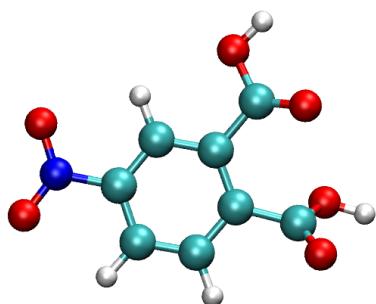
Different



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

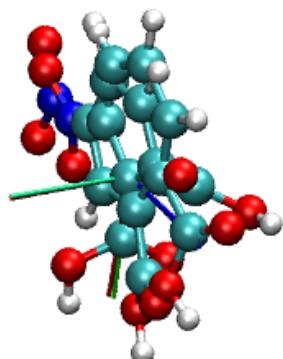
EingenValues - Molecule A

531.43	913.309	1353.35
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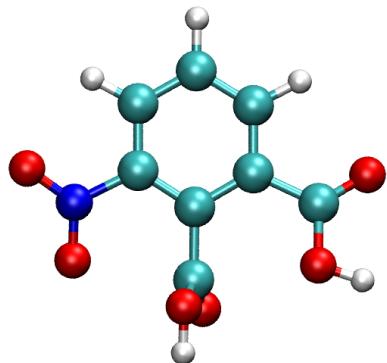
EingenValues - Molecule B

479.308	1242.41	1647.31
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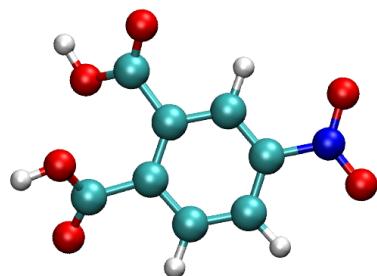
Different



Molecule A 3NFAACn



Molecule B 4NFAACCc



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

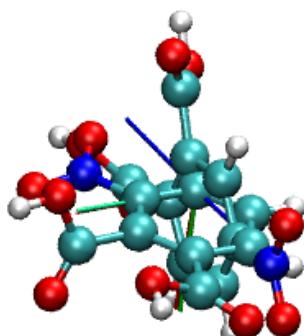
EingenValues - Molecule A

531.43	913.309	1353.35
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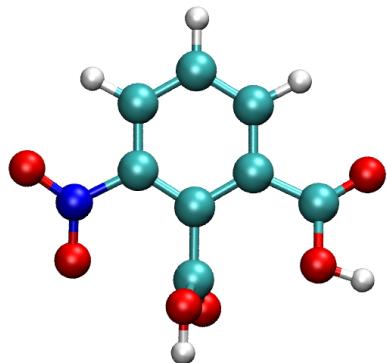
EingenValues - Molecule B

482.027	1240.32	1647.08
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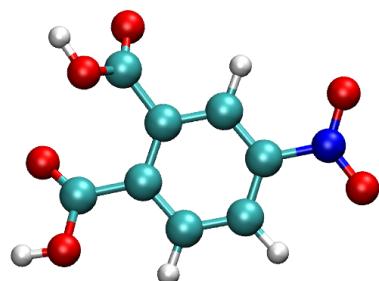
Different



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

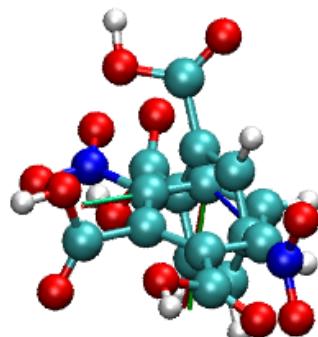
EingenValues - Molecule A

531.43	913.309	1353.35
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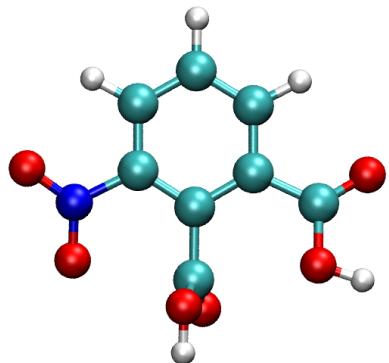
EingenValues - Molecule B

491.663	1231.14	1650.13
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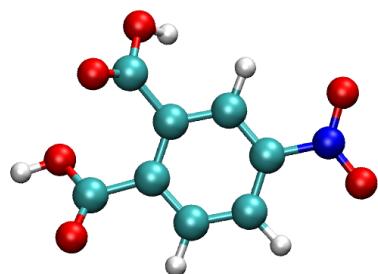
Different



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

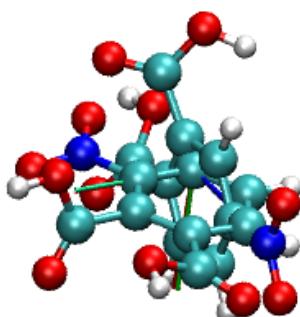
EingenValues - Molecule A

531.43	913.309	1353.35
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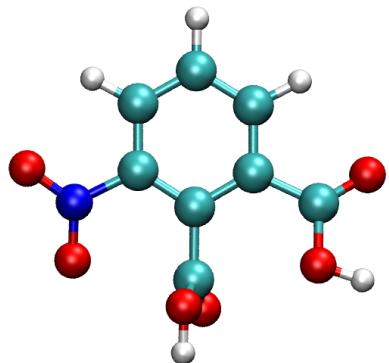
EingenValues - Molecule B

489.011	1233.7	1641.81
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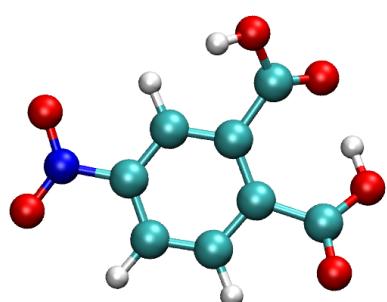
Different



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

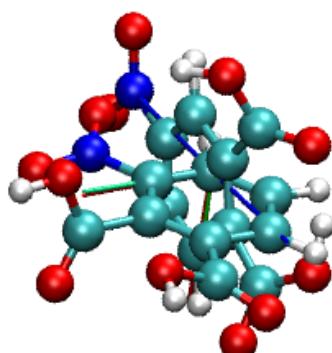
EingenValues - Molecule A

531.43	913.309	1353.35
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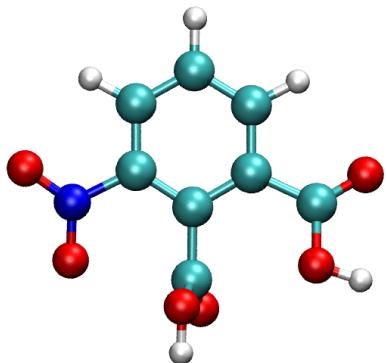
EingenValues - Molecule B

509.668	1219.11	1681.18
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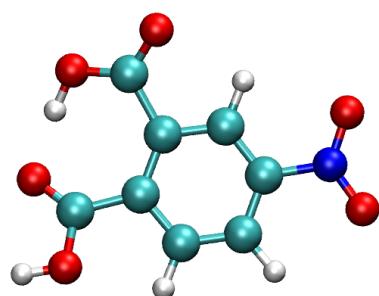
Different



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

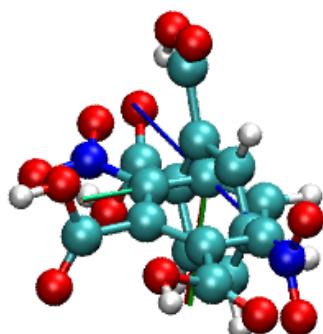
EingenValues - Molecule A

531.43	913.309	1353.35
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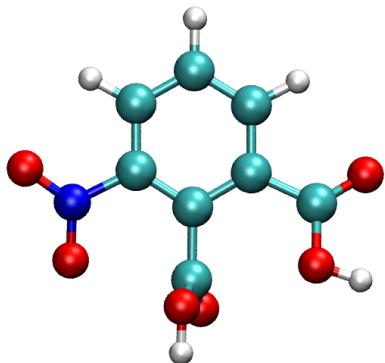
EingenValues - Molecule B

513.751	1208.07	1700.9
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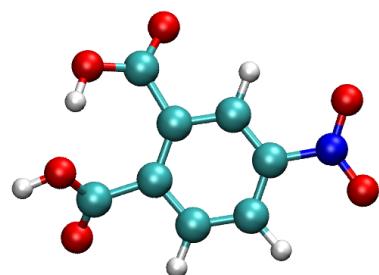
Different



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

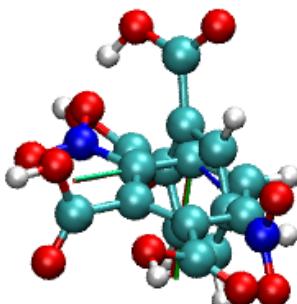
EingenValues - Molecule A

531.43	913.309	1353.35
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EingenValues - Molecule B

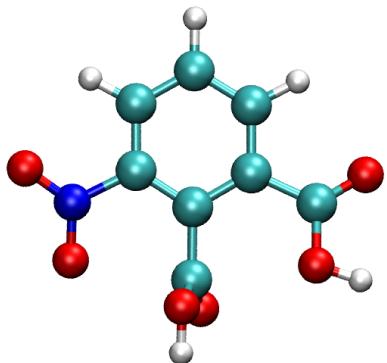
502.409	1232.26	1676.02
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Different

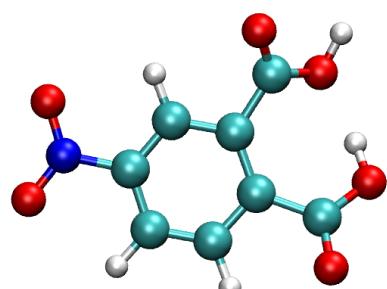


FireTest Número 245

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

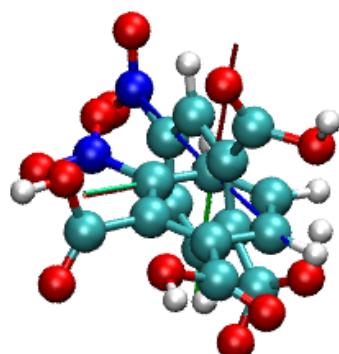
EingenValues - Molecule A

531.43	913.309	1353.35
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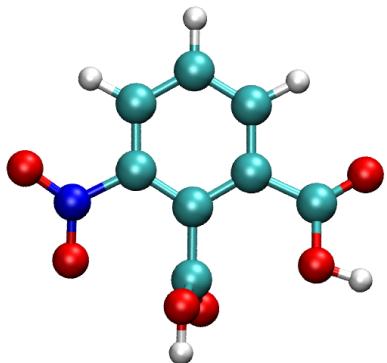
EingenValues - Molecule B

509.897	1225.65	1680.83
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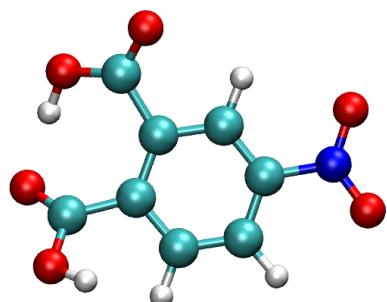
Different



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

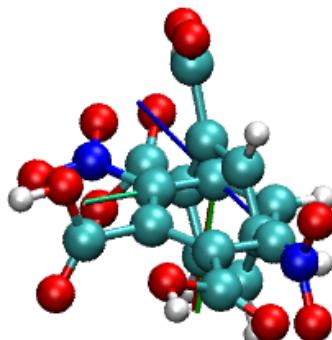
EingenValues - Molecule A

531.43	913.309	1353.35
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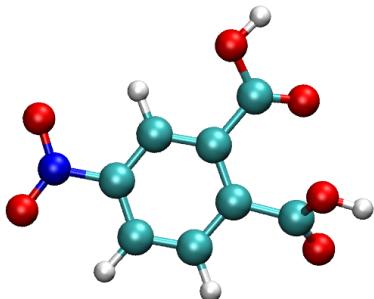
EingenValues - Molecule B

506.607	1222.36	1678.43
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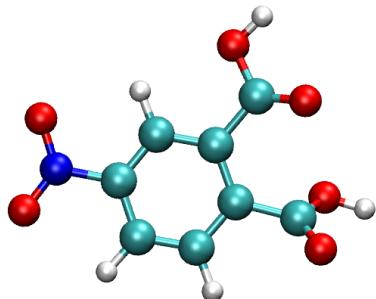
Different



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

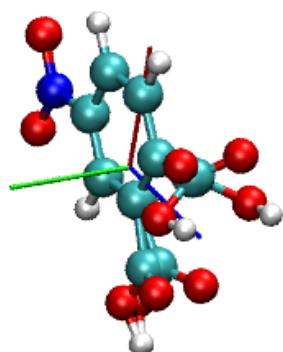
EingenValues - Molecule A

479.363	1242.41	1647.39
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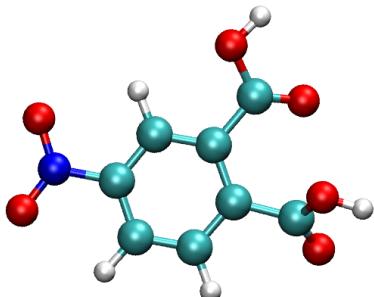
EingenValues - Molecule B

479.308	1242.41	1647.31
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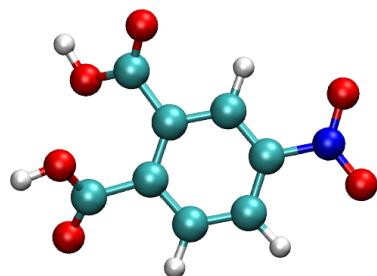
Enantiomers



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

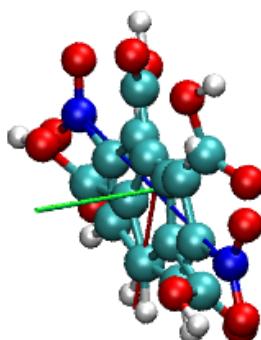
EingenValues - Molecule A

479.363	1242.41	1647.39
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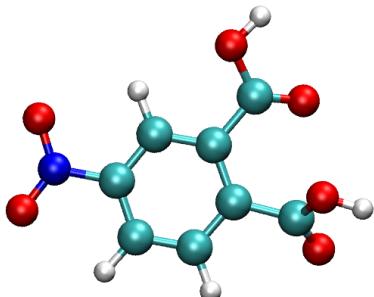
EingenValues - Molecule B

482.027	1240.32	1647.08
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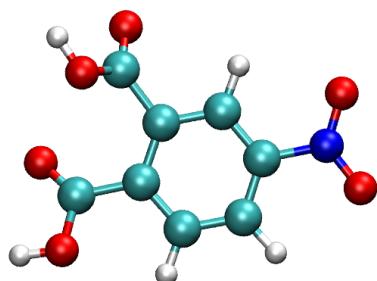
Different



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

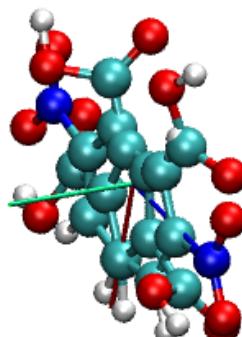
EingenValues - Molecule A

479.363	1242.41	1647.39
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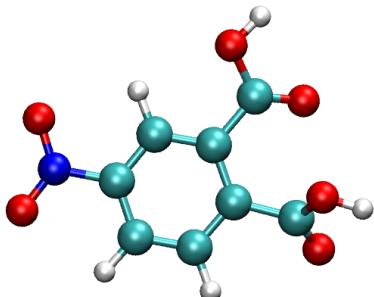
EingenValues - Molecule B

491.663	1231.14	1650.13
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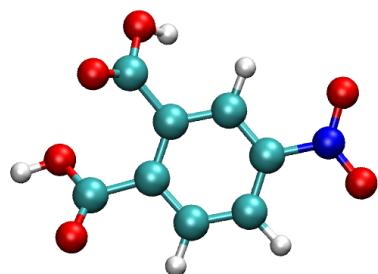
Different



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

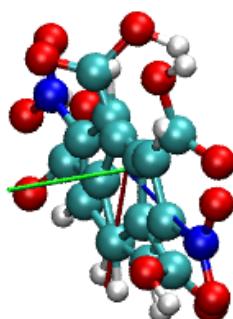
EingenValues - Molecule A

479.363	1242.41	1647.39
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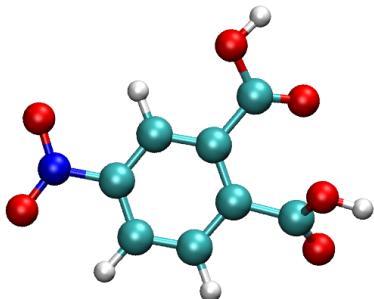
EingenValues - Molecule B

489.011	1233.7	1641.81
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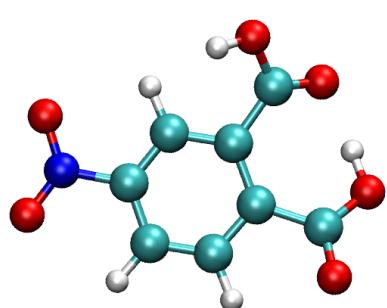
Different



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

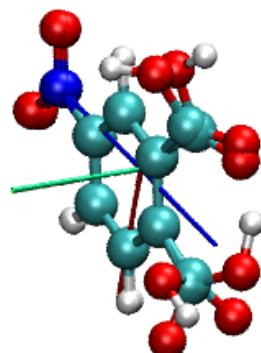
EingenValues - Molecule A

479.363	1242.41	1647.39
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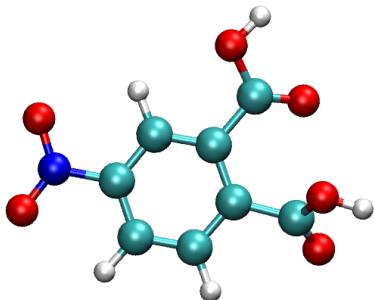
EingenValues - Molecule B

509.668	1219.11	1681.18
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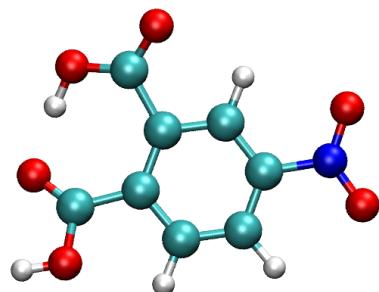
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

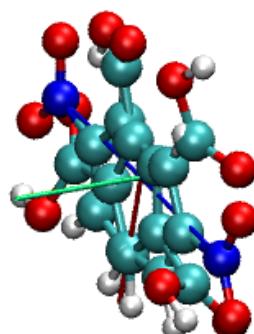
EingenValues - Molecule A

479.363	1242.41	1647.39
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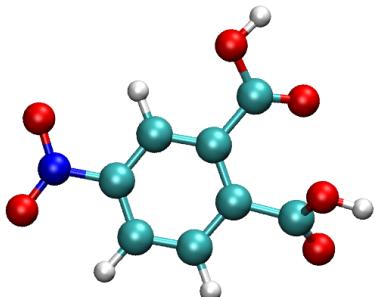
EingenValues - Molecule B

513.751	1208.07	1700.9
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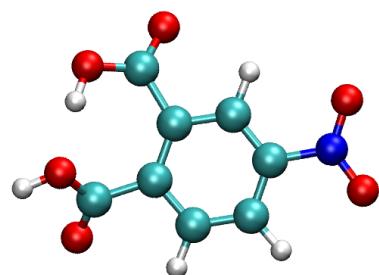
Different



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

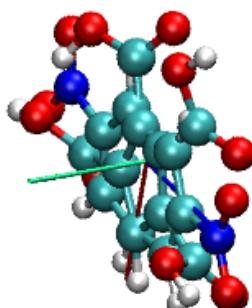
EingenValues - Molecule A

479.363	1242.41	1647.39
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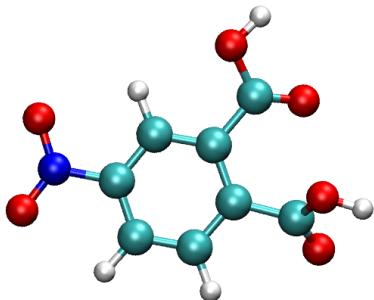
EingenValues - Molecule B

502.409	1232.26	1676.02
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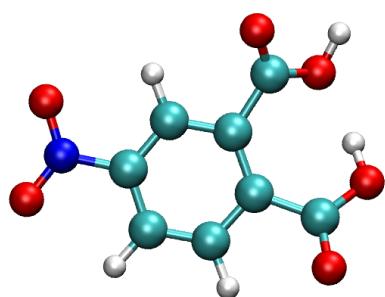
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

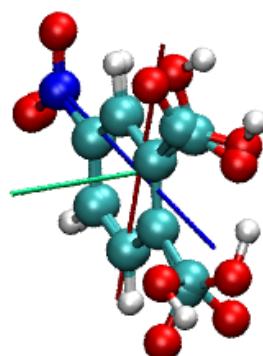
EingenValues - Molecule A

479.363	1242.41	1647.39
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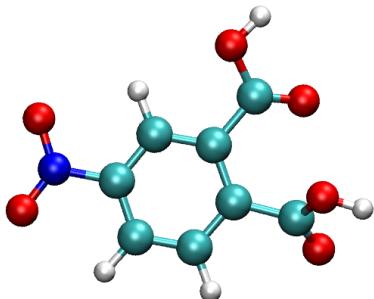
EingenValues - Molecule B

509.897	1225.65	1680.83
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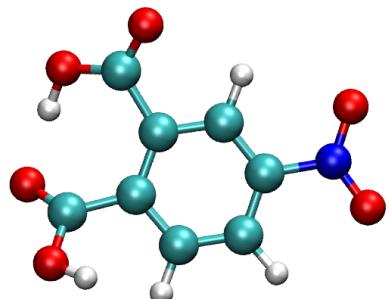
Different



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

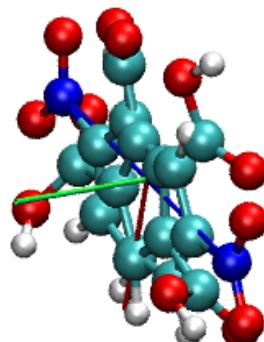
EingenValues - Molecule A

479.363	1242.41	1647.39
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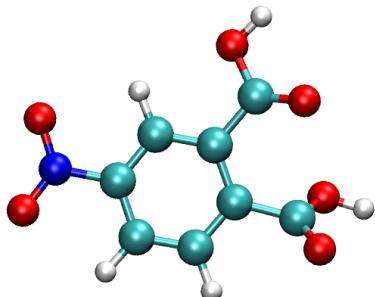
EingenValues - Molecule B

506.607	1222.36	1678.43
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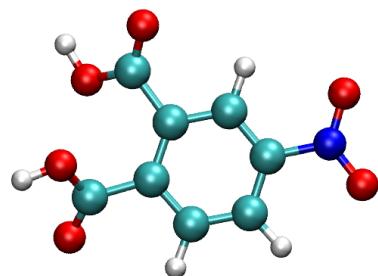
Different



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

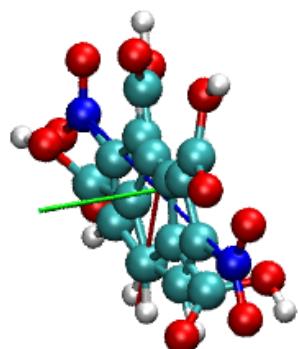
EingenValues - Molecule A

479.308	1242.41	1647.31
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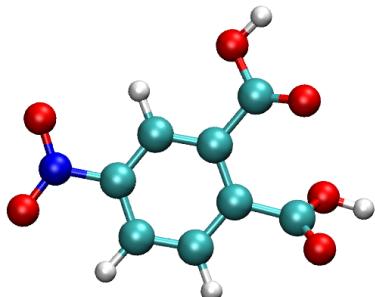
EingenValues - Molecule B

482.027	1240.32	1647.08
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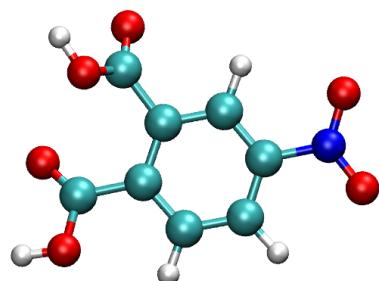
Different



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

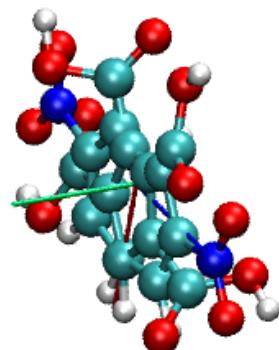
EingenValues - Molecule A

479.308	1242.41	1647.31
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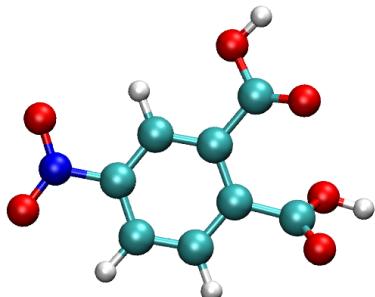
EingenValues - Molecule B

491.663	1231.14	1650.13
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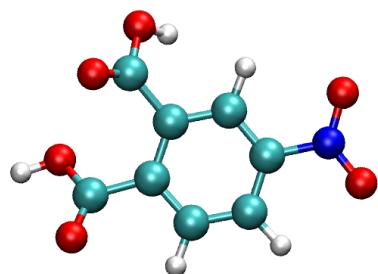
Different



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

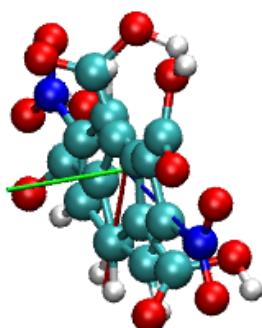
EingenValues - Molecule A

479.308	1242.41	1647.31
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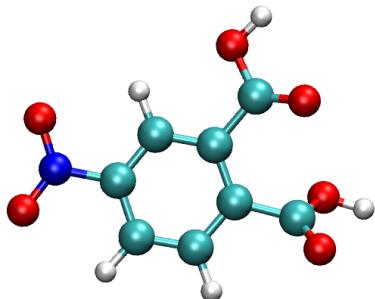
EingenValues - Molecule B

489.011	1233.7	1641.81
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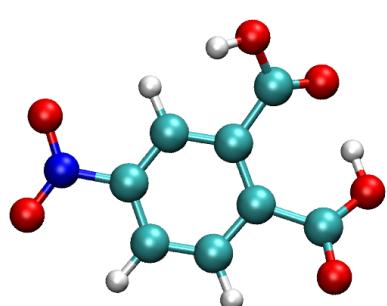
Different



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

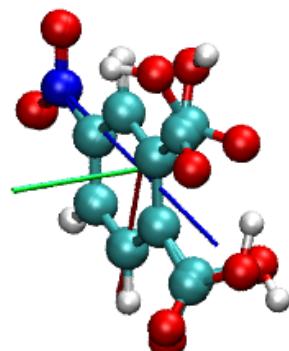
EingenValues - Molecule A

479.308	1242.41	1647.31
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EingenValues - Molecule B

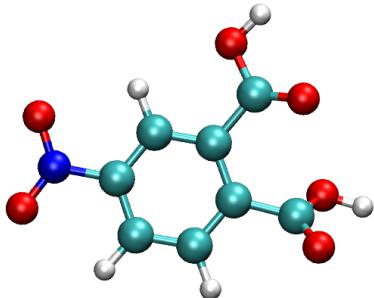
509.668	1219.11	1681.18
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Different

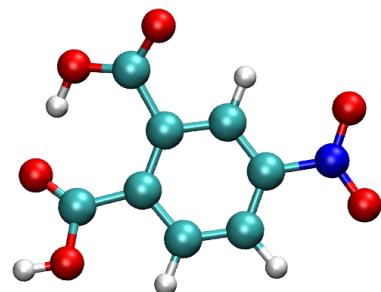


FireTest Número 260

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

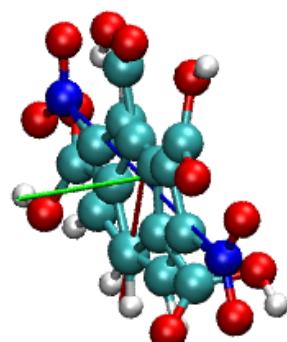
EigenValues - Molecule A

479.308	1242.41	1647.31
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EigenValues - Molecule B

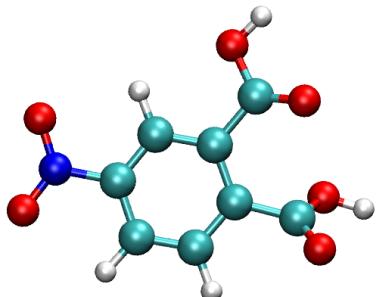
513.751	1208.07	1700.9
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Different

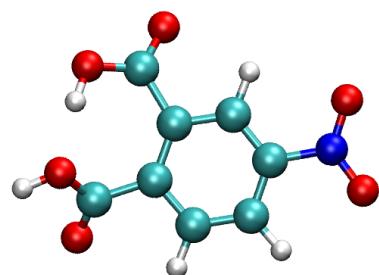


FireTest Número 261

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

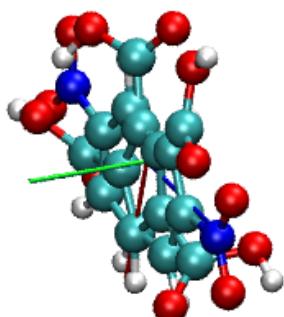
EingenValues - Molecule A

479.308	1242.41	1647.31
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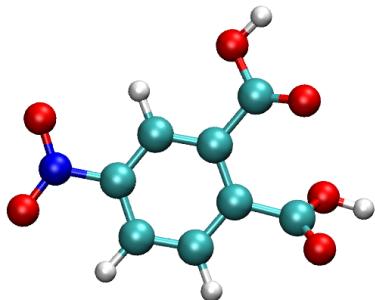
EingenValues - Molecule B

502.409	1232.26	1676.02
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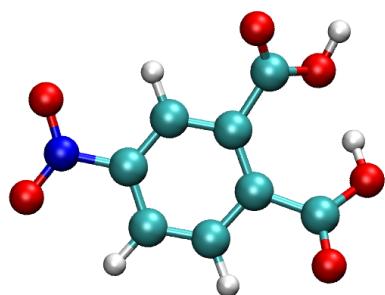
Different



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

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

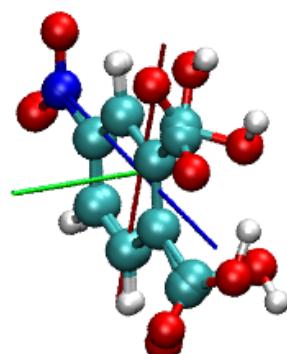
EingenValues - Molecule A

479.308	1242.41	1647.31
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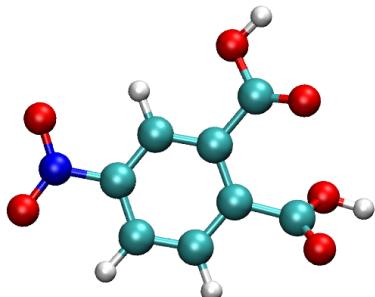
EingenValues - Molecule B

509.897	1225.65	1680.83
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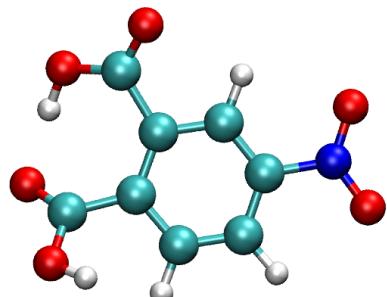
Different



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

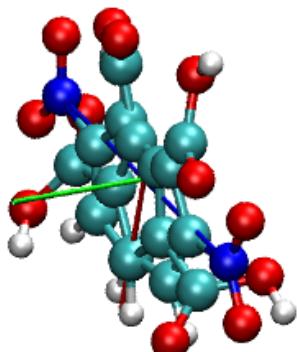
EingenValues - Molecule A

479.308	1242.41	1647.31
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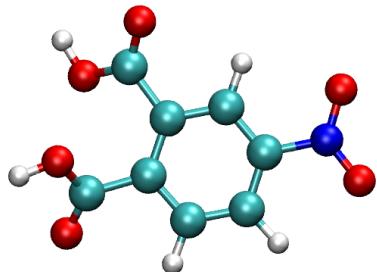
EingenValues - Molecule B

506.607	1222.36	1678.43
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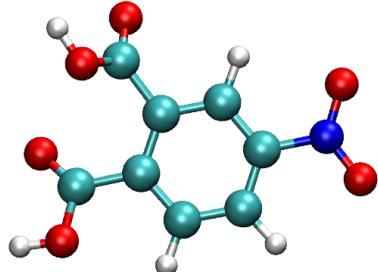
Different



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

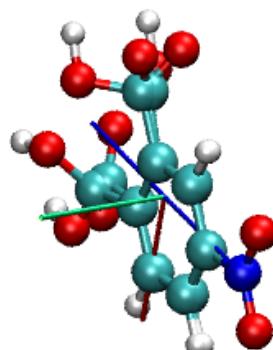
EingenValues - Molecule A

482.027	1240.32	1647.08
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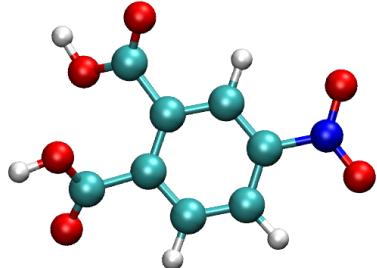
EingenValues - Molecule B

491.663	1231.14	1650.13
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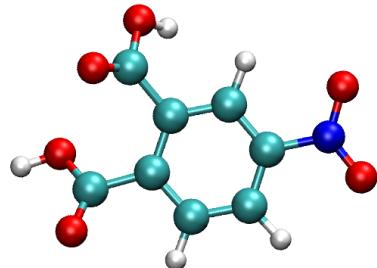
Different



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

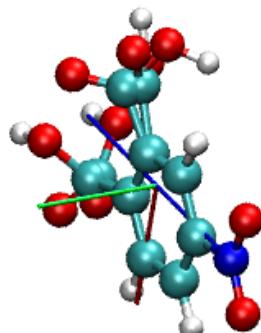
EingenValues - Molecule A

482.027	1240.32	1647.08
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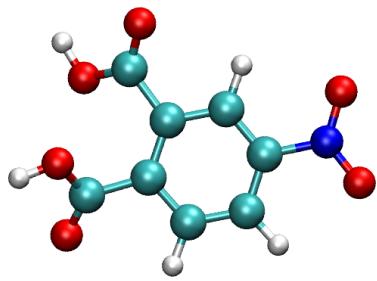
EingenValues - Molecule B

489.011	1233.7	1641.81
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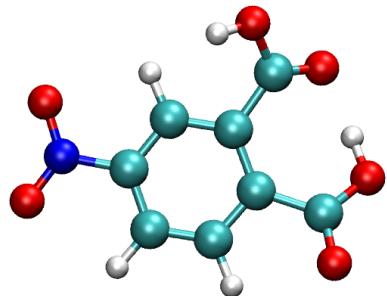
Different



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

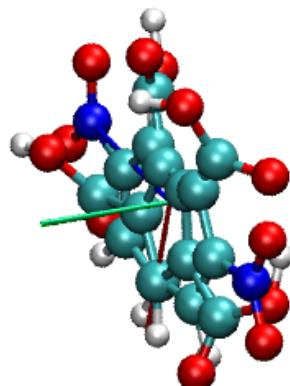
EingenValues - Molecule A

482.027	1240.32	1647.08
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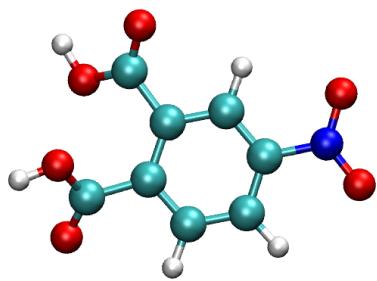
EingenValues - Molecule B

509.668	1219.11	1681.18
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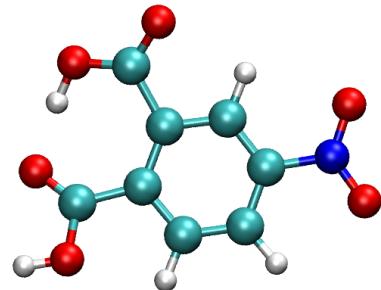
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

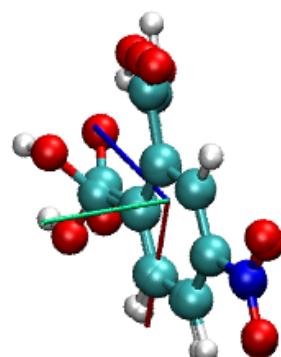
EingenValues - Molecule A

482.027	1240.32	1647.08
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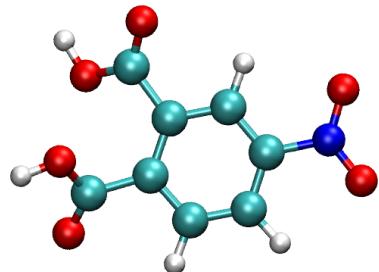
EingenValues - Molecule B

513.751	1208.07	1700.9
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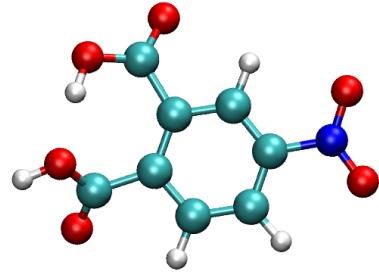
Different



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

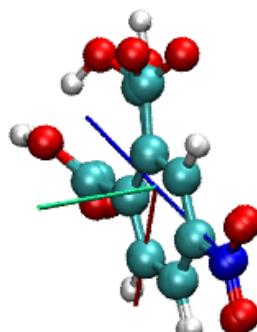
EingenValues - Molecule A

482.027	1240.32	1647.08
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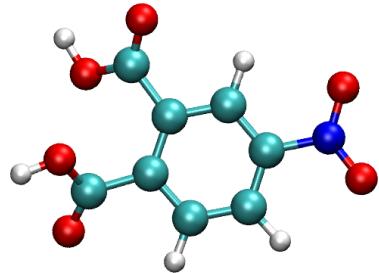
EingenValues - Molecule B

502.409	1232.26	1676.02
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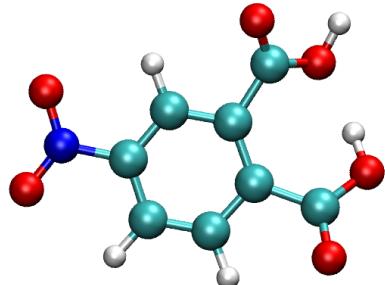
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

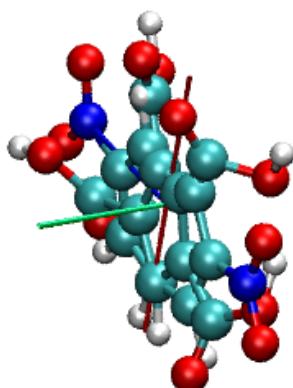
EingenValues - Molecule A

482.027	1240.32	1647.08
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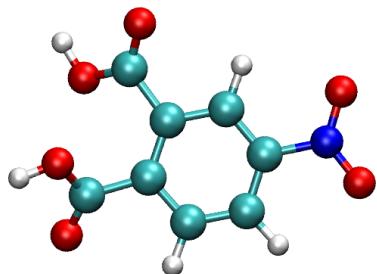
EingenValues - Molecule B

509.897	1225.65	1680.83
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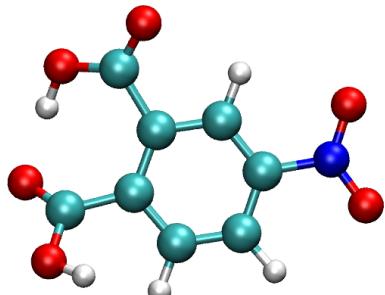
Different



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

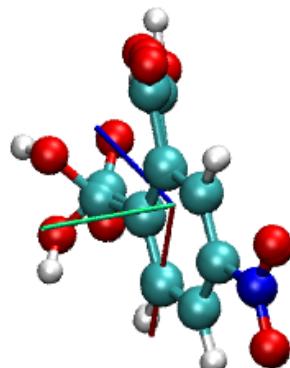
EingenValues - Molecule A

482.027	1240.32	1647.08
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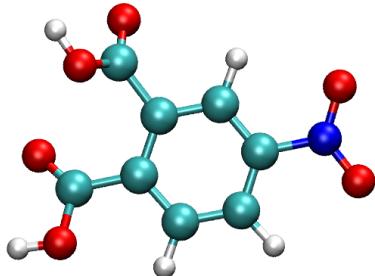
EingenValues - Molecule B

506.607	1222.36	1678.43
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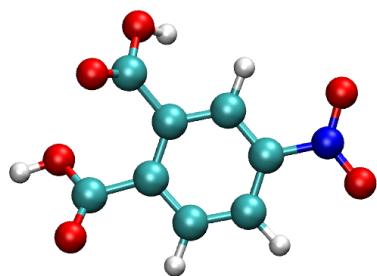
Different



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

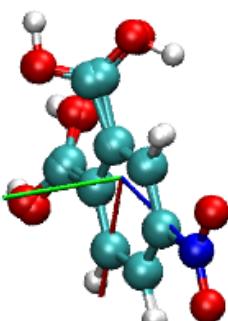
EingenValues - Molecule A

491.663	1231.14	1650.13
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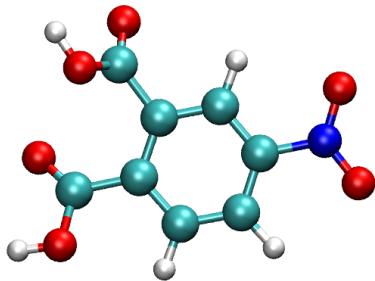
EingenValues - Molecule B

489.011	1233.7	1641.81
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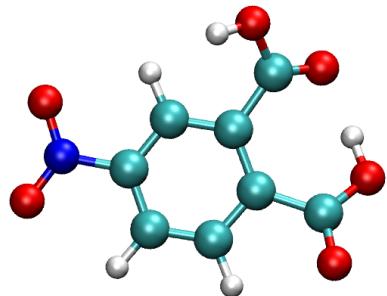
Different



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

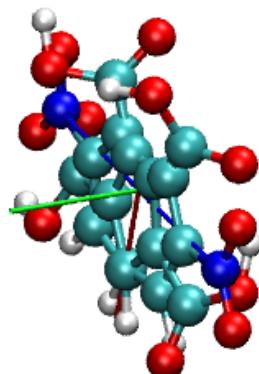
EingenValues - Molecule A

491.663	1231.14	1650.13
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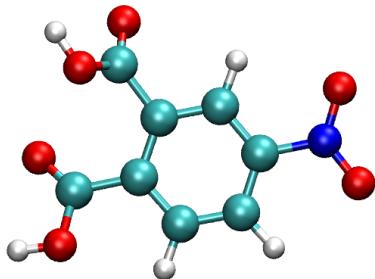
EingenValues - Molecule B

509.668	1219.11	1681.18
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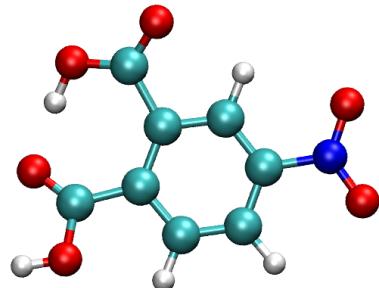
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

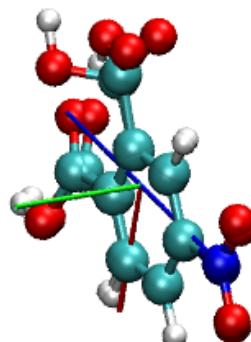
EingenValues - Molecule A

491.663	1231.14	1650.13
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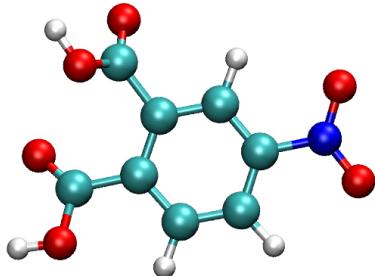
EingenValues - Molecule B

513.751	1208.07	1700.9
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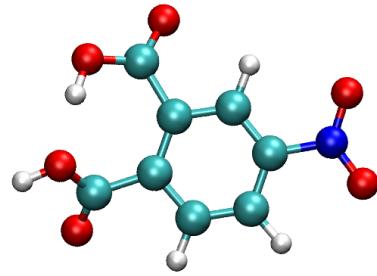
Different



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

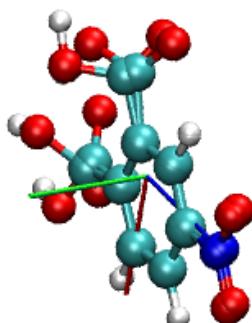
EingenValues - Molecule A

491.663	1231.14	1650.13
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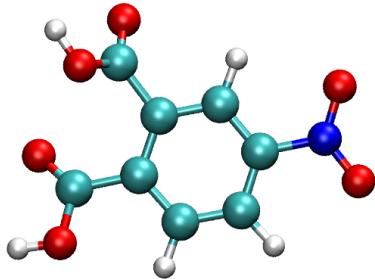
EingenValues - Molecule B

502.409	1232.26	1676.02
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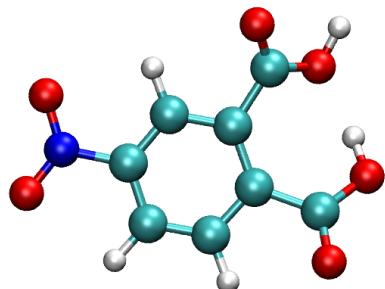
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

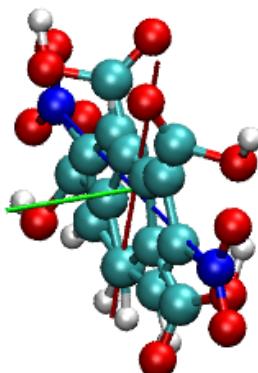
EingenValues - Molecule A

491.663	1231.14	1650.13
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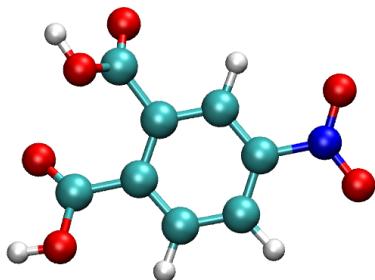
EingenValues - Molecule B

509.897	1225.65	1680.83
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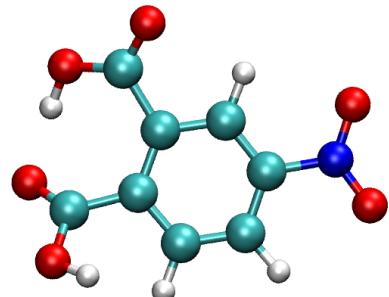
Different



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

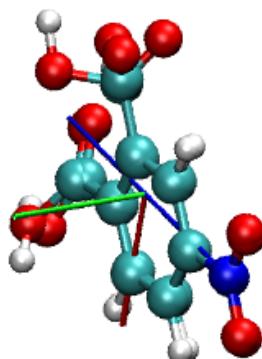
EingenValues - Molecule A

491.663	1231.14	1650.13
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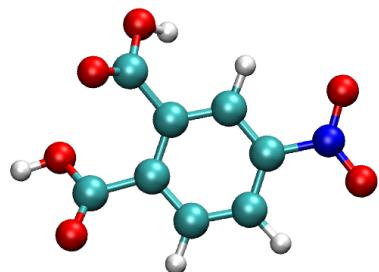
EingenValues - Molecule B

506.607	1222.36	1678.43
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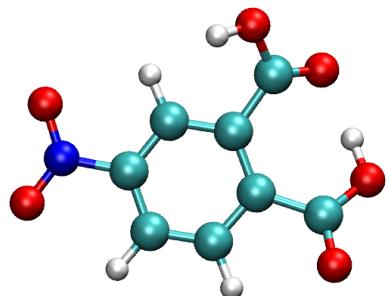
Different



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

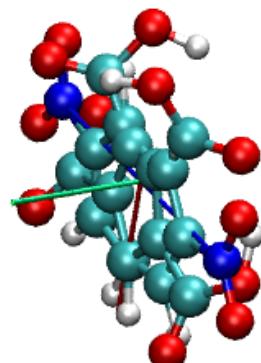
EingenValues - Molecule A

489.011	1233.7	1641.81
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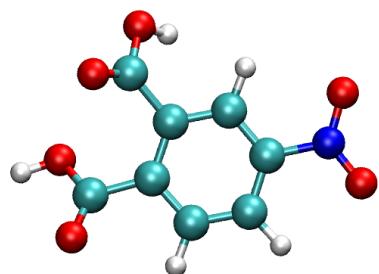
EingenValues - Molecule B

509.668	1219.11	1681.18
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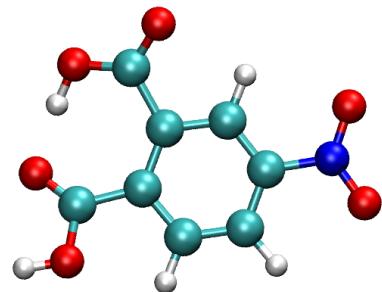
Different



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

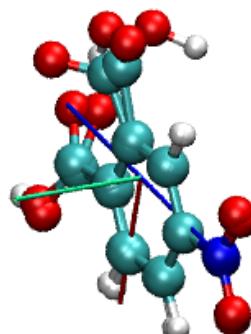
EingenValues - Molecule A

489.011	1233.7	1641.81
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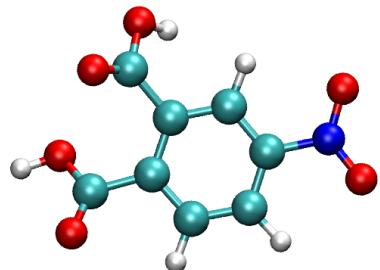
EingenValues - Molecule B

513.751	1208.07	1700.9
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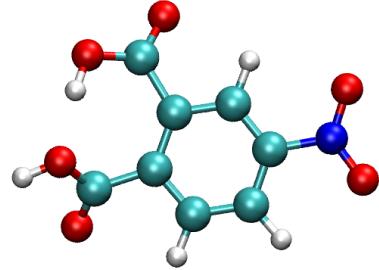
Different



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

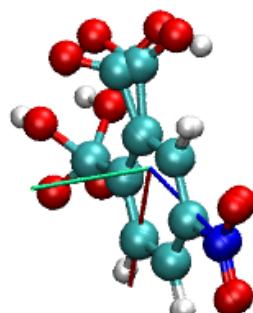
EingenValues - Molecule A

489.011	1233.7	1641.81
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EingenValues - Molecule B

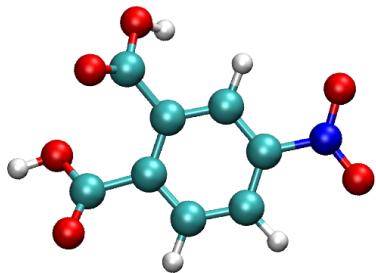
502.409	1232.26	1676.02
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Different

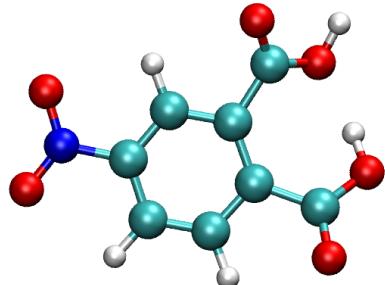


FireTest Número 280

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

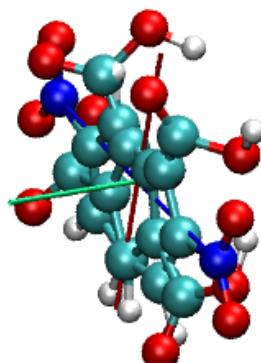
EigenValues - Molecule A

489.011	1233.7	1641.81
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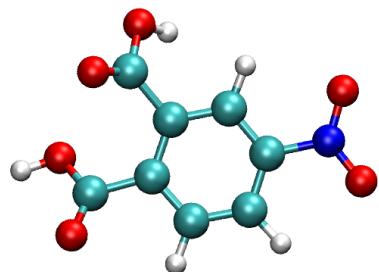
EigenValues - Molecule B

509.897	1225.65	1680.83
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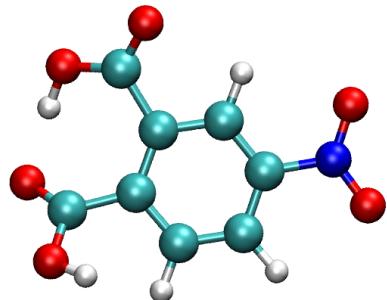
Different



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

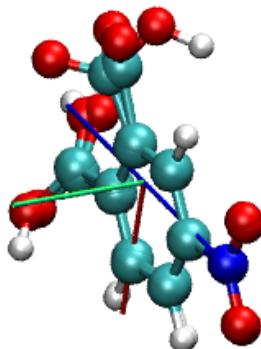
EingenValues - Molecule A

489.011	1233.7	1641.81
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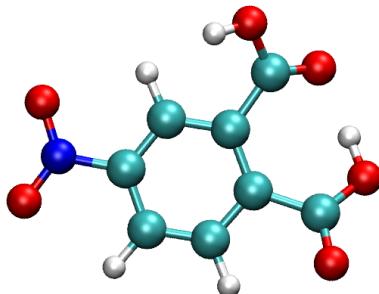
EingenValues - Molecule B

506.607	1222.36	1678.43
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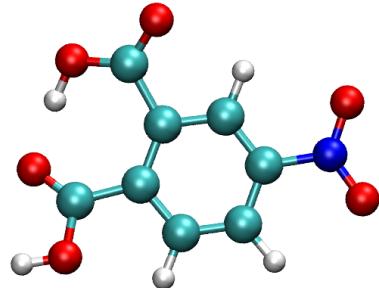
Different



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

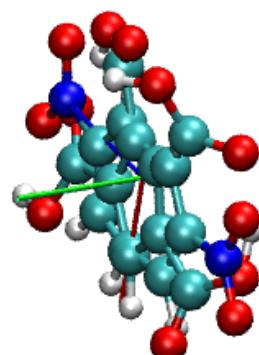
EingenValues - Molecule A

509.668	1219.11	1681.18
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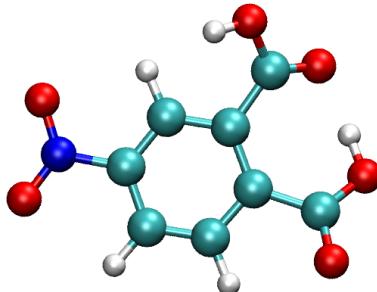
EingenValues - Molecule B

513.751	1208.07	1700.9
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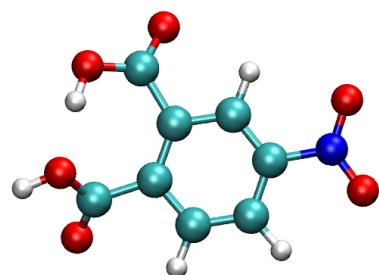
Different



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

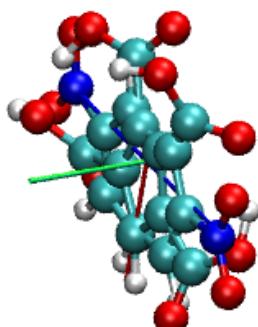
EingenValues - Molecule A

509.668	1219.11	1681.18
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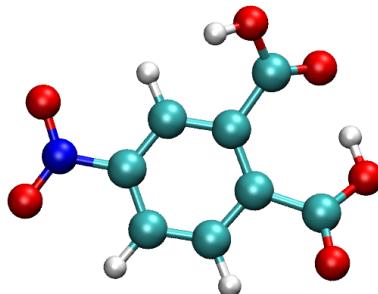
EingenValues - Molecule B

502.409	1232.26	1676.02
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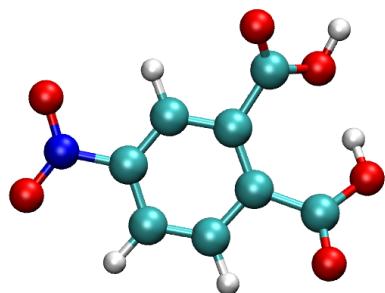
Different



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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

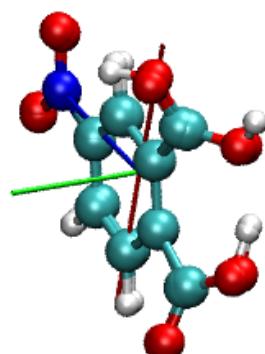
EingenValues - Molecule A

509.668	1219.11	1681.18
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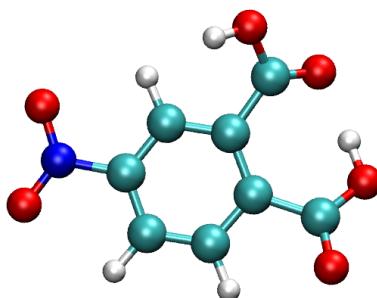
EingenValues - Molecule B

509.897	1225.65	1680.83
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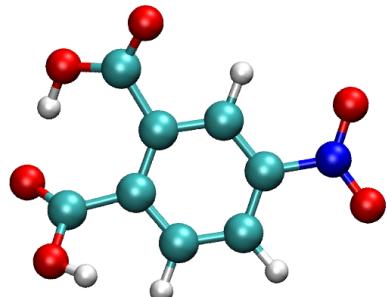
Different



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

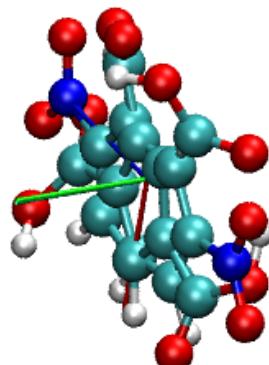
EingenValues - Molecule A

509.668	1219.11	1681.18
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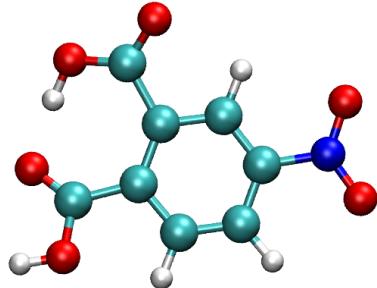
EingenValues - Molecule B

506.607	1222.36	1678.43
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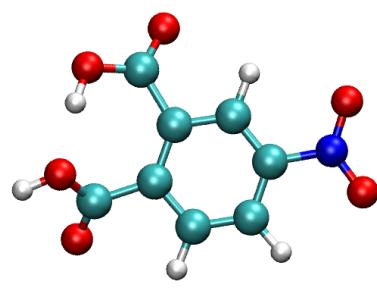
Different



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

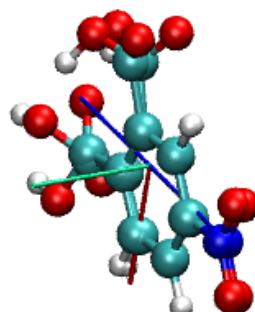
EingenValues - Molecule A

513.751	1208.07	1700.9
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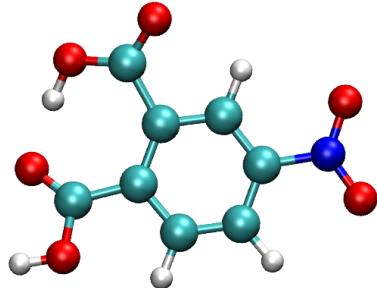
EingenValues - Molecule B

502.409	1232.26	1676.02
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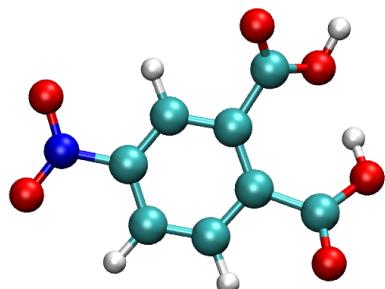
Different



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

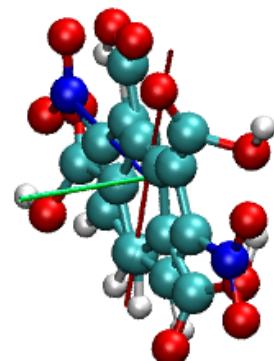
EingenValues - Molecule A

513.751	1208.07	1700.9
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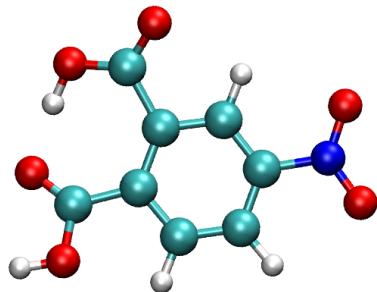
EingenValues - Molecule B

509.897	1225.65	1680.83
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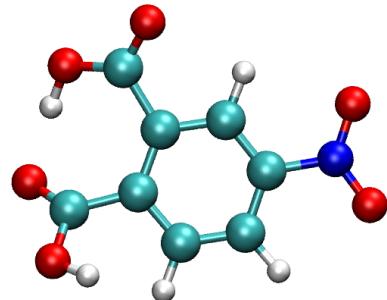
Different



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

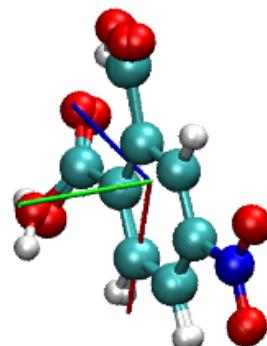
EingenValues - Molecule A

513.751	1208.07	1700.9
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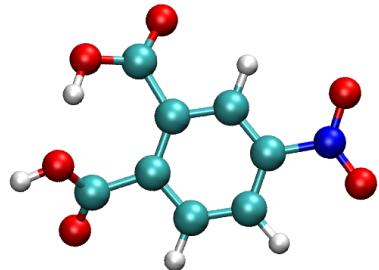
EingenValues - Molecule B

506.607	1222.36	1678.43
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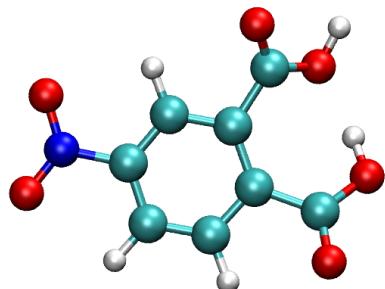
Different



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

EingenVectors - Molecule A

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

EingenVectors - Molecule B

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

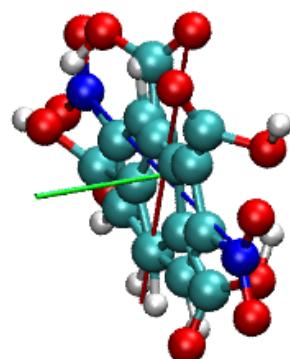
EingenValues - Molecule A

502.409	1232.26	1676.02
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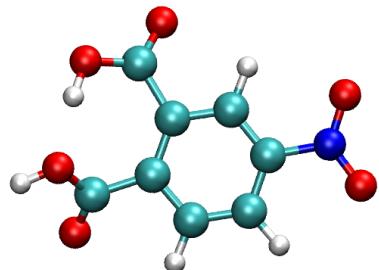
EingenValues - Molecule B

509.897	1225.65	1680.83
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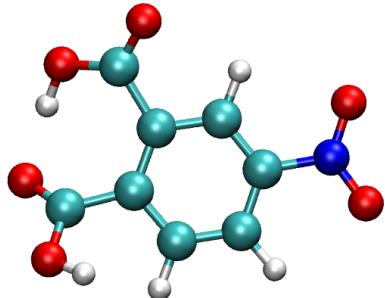
Different



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

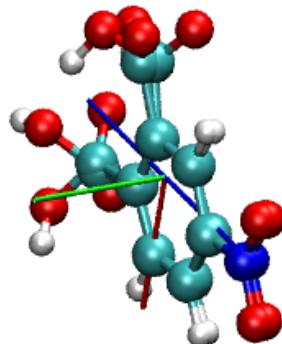
EingenValues - Molecule A

502.409	1232.26	1676.02
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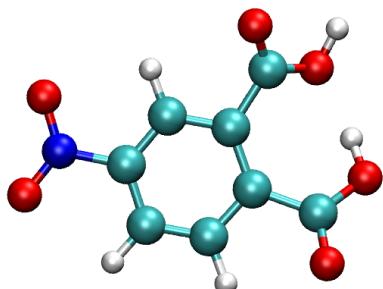
EingenValues - Molecule B

506.607	1222.36	1678.43
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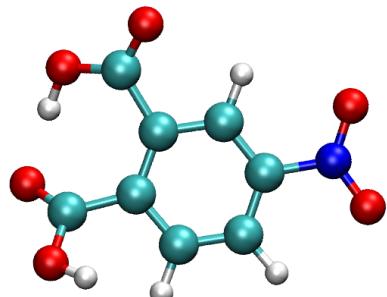
Different



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

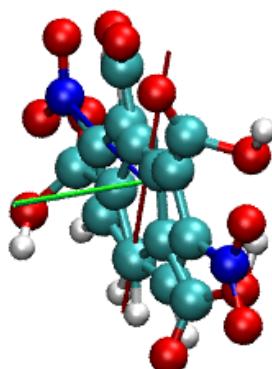
EingenValues - Molecule A

509.897	1225.65	1680.83
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EingenValues - Molecule B

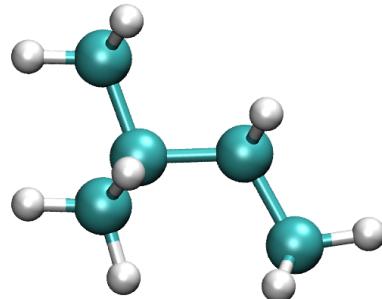
506.607	1222.36	1678.43
---------	---------	---------

Different



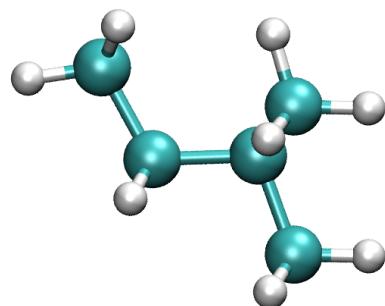
IsomerC6H14 Número 292

Molecule A 2,2-dimethyl-butane.out.G09



Molecule B

2,2-dimethyl-butane.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

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869274 & 0.494331 & 0 \\ 0.494331 & 0.869274 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.869273 & 0.494332 & 0 \\ 0.494332 & 0.869273 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

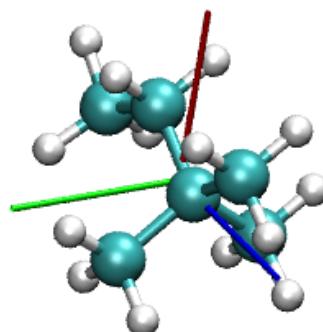
EingenValues - Molecule A

$$\begin{vmatrix} 118.683 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

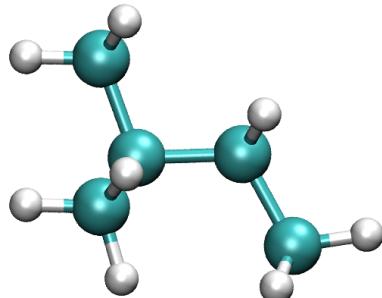
$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

Equal

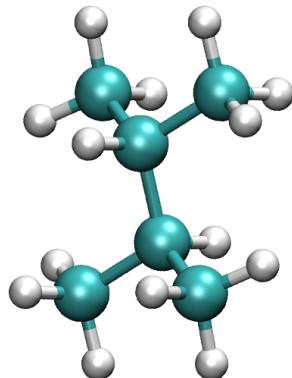


IsomerC6H14 Número 293

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

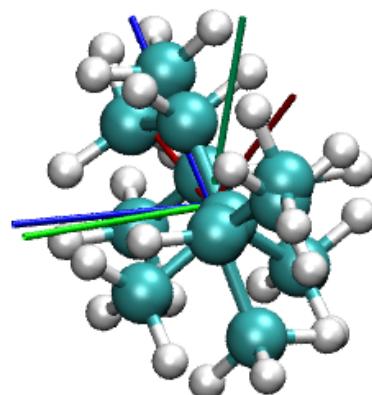
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

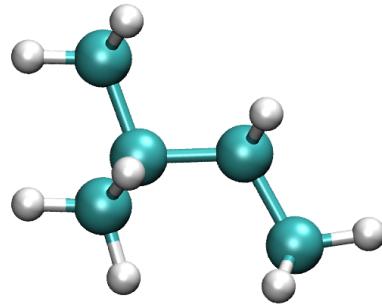
120.611	177.08	272.075
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Different



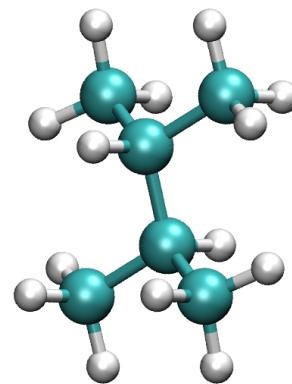
IsomerC6H14 Número 294

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

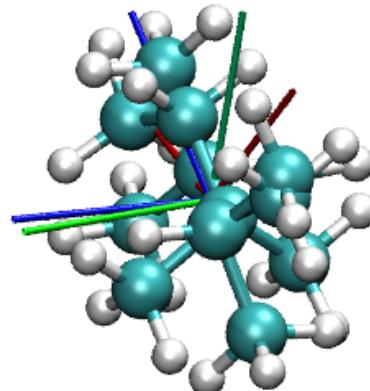
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

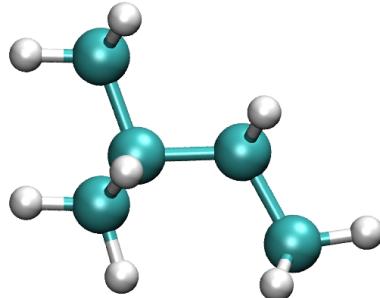
120.611	177.08	272.076
---------	--------	---------

Different

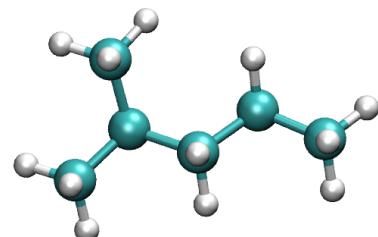


IsomerC6H14 Número 295

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

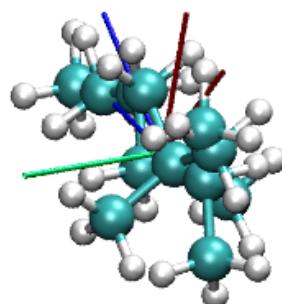
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

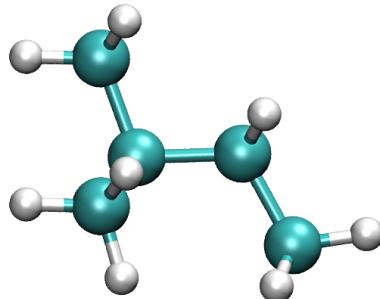
76.7698	299.061	347.558
---------	---------	---------

Different



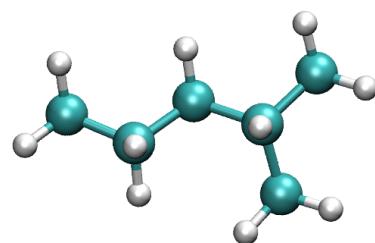
IsomerC6H14 Número 296

Molecule A 2,2-dimethyl-butane_out_G09



Molecule B

2-methyl-pentane_out_G09_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

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

$$\begin{vmatrix} -0.869274 & 0.494331 & 0 \\ 0.494331 & 0.869274 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999999 & -0.00105562 & -0.000587505 \\ -0.00105685 & 0.999997 & 0.00210312 \\ -0.000585284 & -0.00210374 & 0.999998 \end{vmatrix}$$

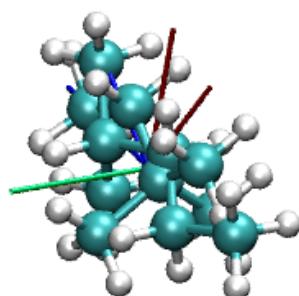
EingenValues - Molecule A

$$\begin{vmatrix} 118.683 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

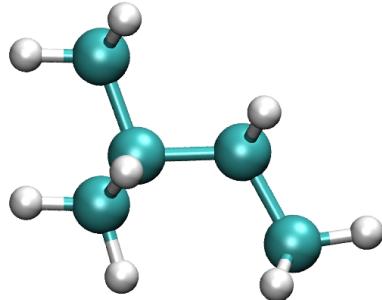
$$\begin{vmatrix} 76.7699 & 299.061 & 347.558 \end{vmatrix}$$

Different

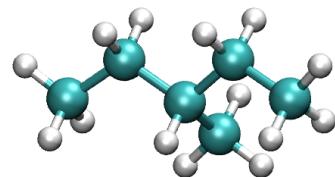


IsomerC6H14 Número 297

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

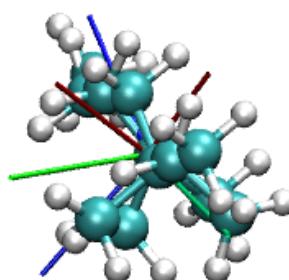
EingenValues - Molecule A

118.683	204.724	205.419
---------	---------	---------

EingenValues - Molecule B

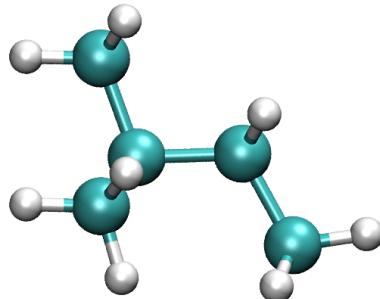
77.8079	276.009	320.597
---------	---------	---------

Different



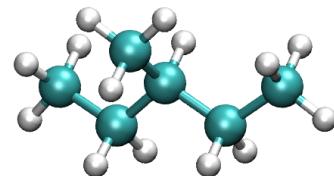
IsomerC6H14 Número 298

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

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

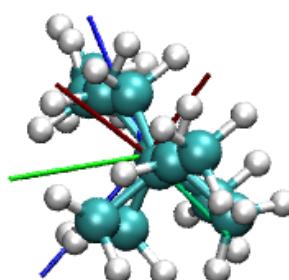
EingenValues - Molecule A

$$\begin{vmatrix} 118.683 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

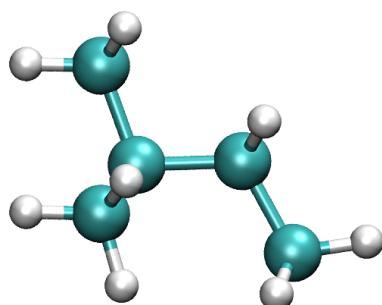
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Different

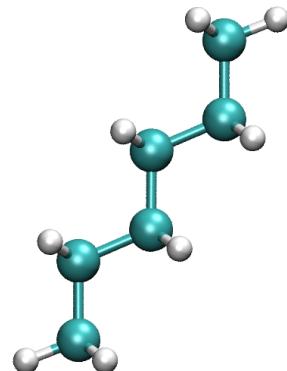


IsomerC6H14 Número 299

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

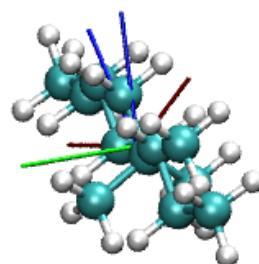
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

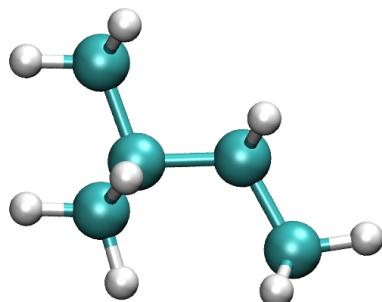
34.6869	449.234	465.177
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Different

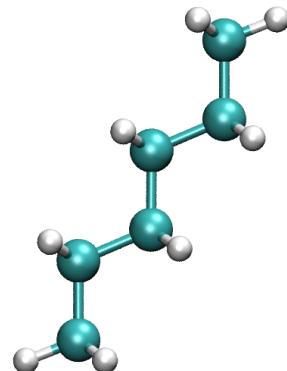


IsomerC6H14 Número 300

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

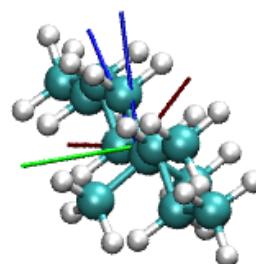
EingenValues - Molecule A

118.683	204.724	205.419
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EingenValues - Molecule B

34.6868	449.234	465.177
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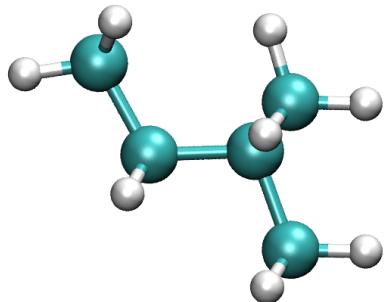
Different



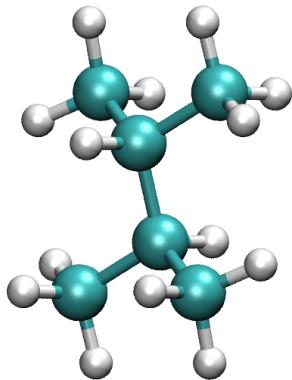
IsomerC6H14 Número 301

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

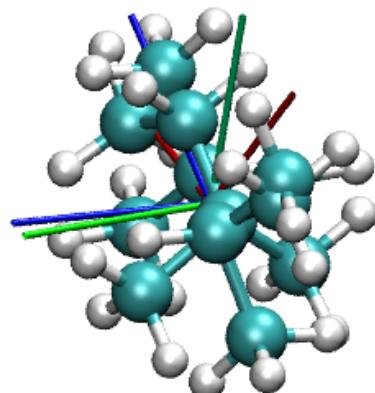
EingenValues - Molecule A

118.684	204.724	205.419
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EingenValues - Molecule B

120.611	177.08	272.075
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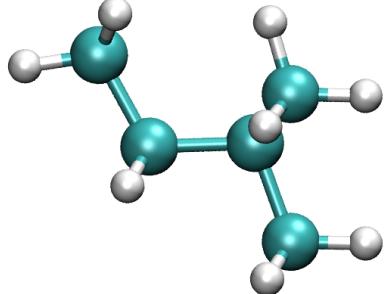
Different



IsomerC6H14 Número 302

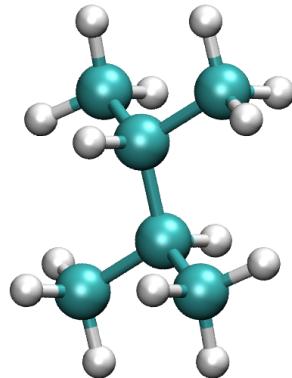
Molecule A

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

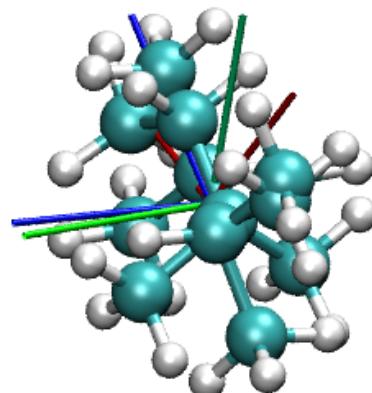
EingenValues - Molecule A

118.684	204.724	205.419
---------	---------	---------

EingenValues - Molecule B

120.611	177.08	272.076
---------	--------	---------

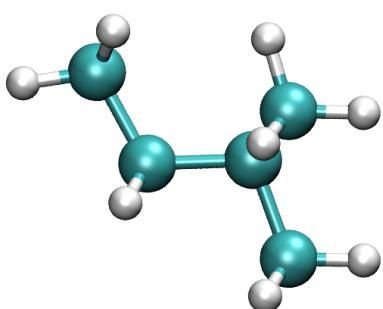
Different



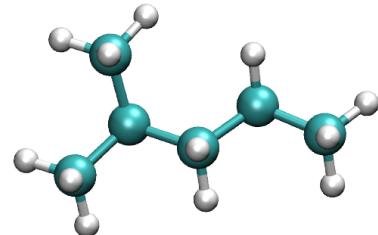
IsomerC6H14 Número 303

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

$$\begin{vmatrix} -0.999999 & -0.00105548 & -0.000587604 \\ -0.00105671 & 0.999997 & 0.00210321 \\ -0.000585382 & -0.00210383 & 0.999998 \end{vmatrix}$$

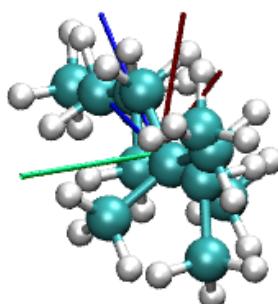
EingenValues - Molecule A

$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 76.7698 & 299.061 & 347.558 \end{vmatrix}$$

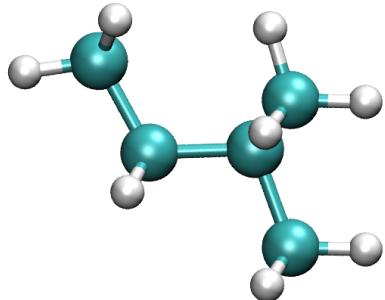
Different



IsomerC6H14 Número 304

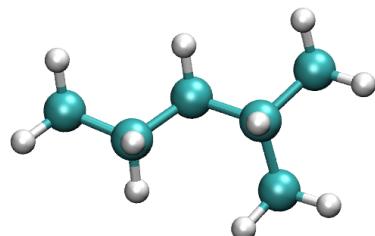
Molecule A

2,2-dimethyl-butane_out_G09_inversion



Molecule B

2-methyl-pentane_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

76.7702	-0.234595	-0.158982
-0.234595	299.061	-0.102162
-0.158982	-0.102162	347.558

EingenVectors - Molecule A

-0.869273	0.494332	0
0.494332	0.869273	0
0	0	1

EingenVectors - Molecule B

-0.999999	-0.00105562	-0.000587505
-0.00105685	0.999997	0.00210312
-0.000585284	-0.00210374	0.999998

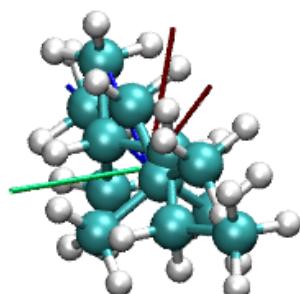
EingenValues - Molecule A

118.684	204.724	205.419
---------	---------	---------

EingenValues - Molecule B

76.7699	299.061	347.558
---------	---------	---------

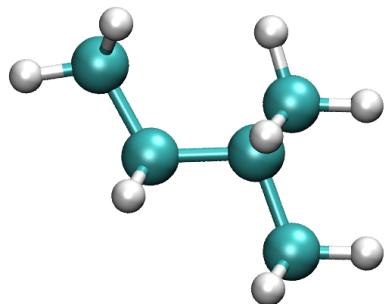
Different



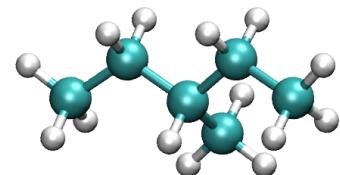
IsomerC6H14 Número 305

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

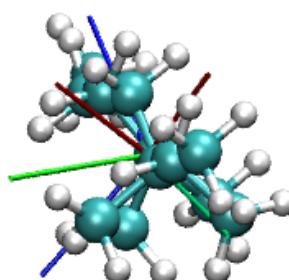
EingenValues - Molecule A

118.684	204.724	205.419
---------	---------	---------

EingenValues - Molecule B

77.8079	276.009	320.597
---------	---------	---------

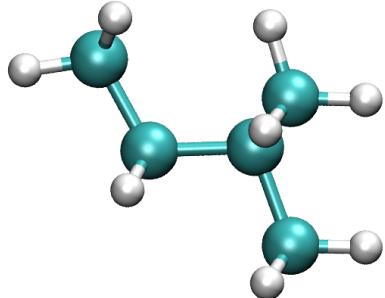
Different



IsomerC6H14 Número 306

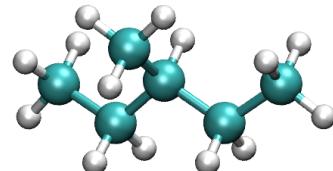
Molecule A

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

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

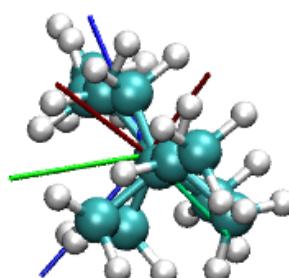
EingenValues - Molecule A

$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

EingenValues - Molecule B

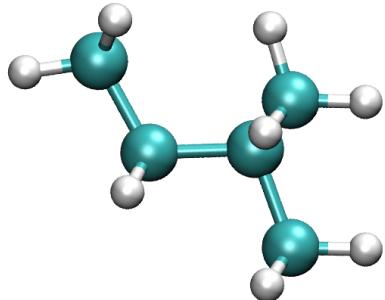
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Different

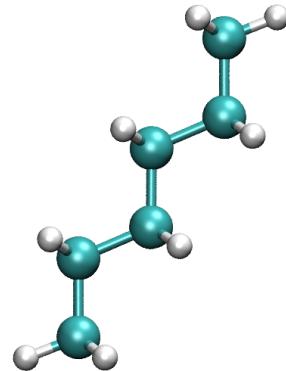


IsomerC6H14 Número 307

Molecule A
2,2-dimethyl-butane_out_G09_inversion



Molecule B hexane_out_G09



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869273 & 0.494332 & 0 \\ 0.494332 & 0.869273 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 346.244 & -179.129 & 0 \\ -179.129 & 137.676 & 0 \\ 0 & 0 & 465.177 \end{vmatrix}$$

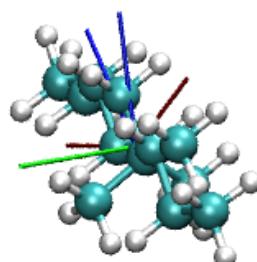
EingenVectors - Molecule B

$$\begin{vmatrix} -0.498436 & -0.866927 & 0 \\ 0.866927 & -0.498436 & -0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenValues - Molecule B

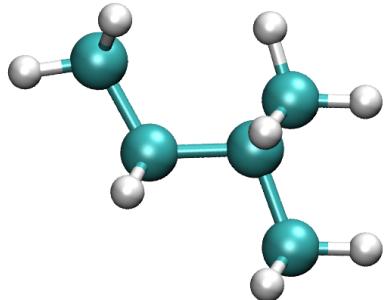
$$\begin{vmatrix} 34.6869 & 449.234 & 465.177 \end{vmatrix}$$

Different

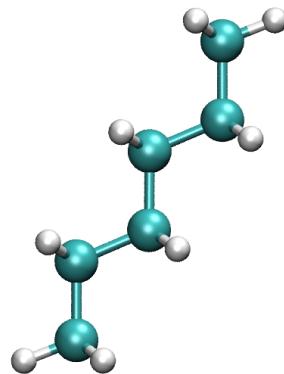


IsomerC6H14 Número 308

Molecule A
2,2-dimethyl-butane_out_G09_inversion



Molecule B hexane_out_G09_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 139.709 & 36.9725 & 0 \\ 36.9725 & 183.699 & 0 \\ 0 & 0 & 205.419 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.869273 & 0.494332 & 0 \\ 0.494332 & 0.869273 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 118.684 & 204.724 & 205.419 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 346.245 & -179.129 & 0 \\ -179.129 & 137.676 & 0 \\ 0 & 0 & 465.177 \end{vmatrix}$$

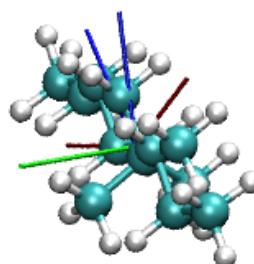
EingenVectors - Molecule B

$$\begin{vmatrix} -0.498435 & -0.866927 & 0 \\ 0.866927 & -0.498435 & -0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenValues - Molecule B

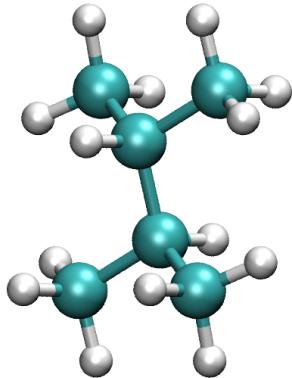
$$\begin{vmatrix} 34.6868 & 449.234 & 465.177 \end{vmatrix}$$

Different



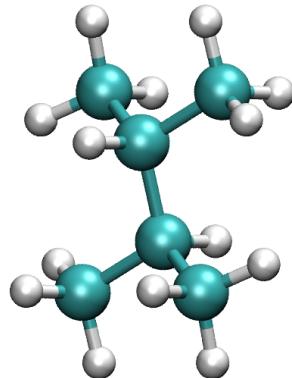
IsomerC6H14 Número 309

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

$$\begin{vmatrix} -0.112875 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112875 & -0 \end{vmatrix}$$

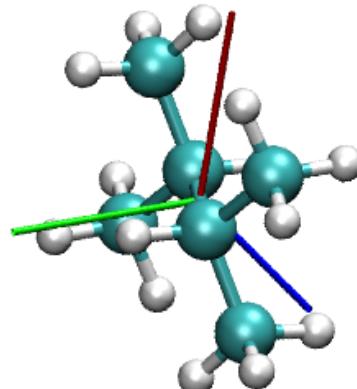
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.075 \end{vmatrix}$$

EingenValues - Molecule B

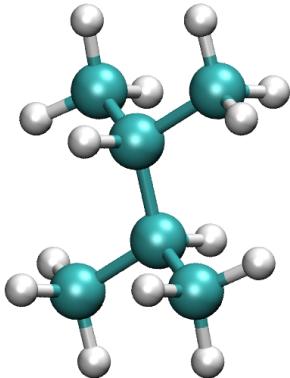
$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

Equal

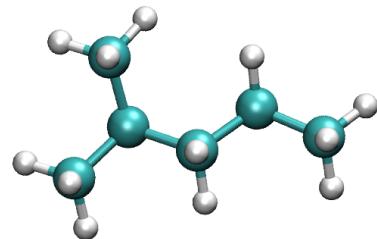


IsomerC6H14 Número 310

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

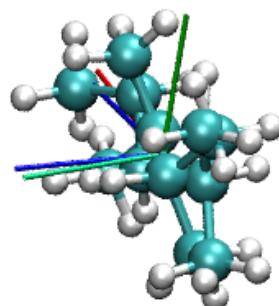
EingenValues - Molecule A

120.611	177.08	272.075
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EingenValues - Molecule B

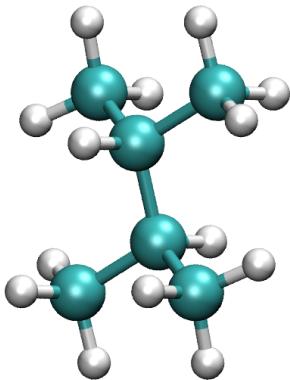
76.7698	299.061	347.558
---------	---------	---------

Different



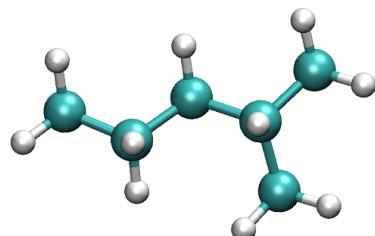
IsomerC6H14 Número 311

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

$$\begin{vmatrix} -0.999999 & -0.00105562 & -0.000587505 \\ -0.00105685 & 0.999997 & 0.00210312 \\ -0.000585284 & -0.00210374 & 0.999998 \end{vmatrix}$$

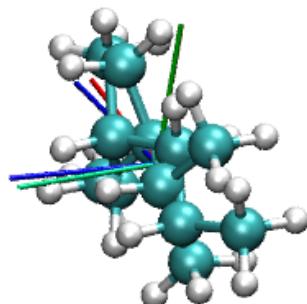
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.075 \end{vmatrix}$$

EingenValues - Molecule B

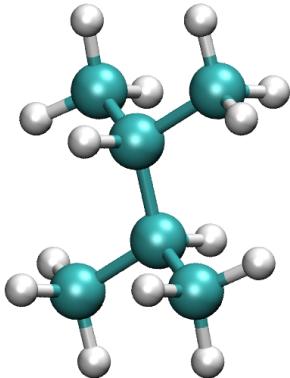
$$\begin{vmatrix} 76.7699 & 299.061 & 347.558 \end{vmatrix}$$

Different

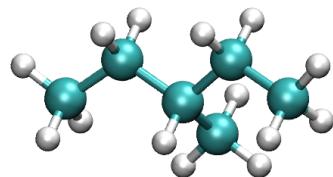


IsomerC6H14 Número 312

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

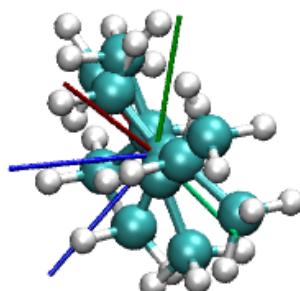
EingenValues - Molecule A

120.611	177.08	272.075
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EingenValues - Molecule B

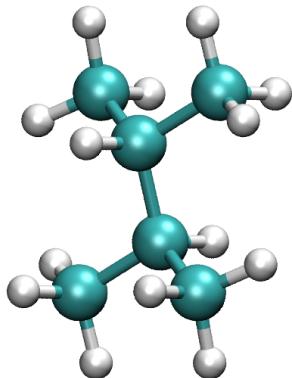
77.8079	276.009	320.597
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Different



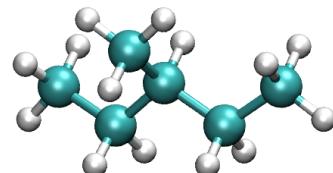
IsomerC6H14 Número 313

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

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

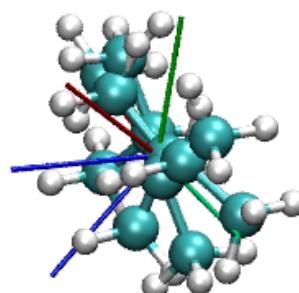
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.075 \end{vmatrix}$$

EingenValues - Molecule B

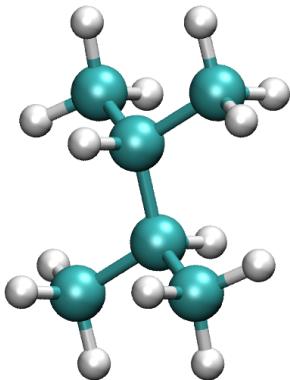
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Different

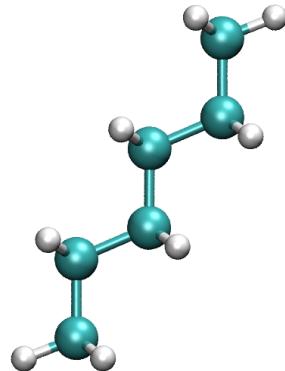


IsomerC6H14 Número 314

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

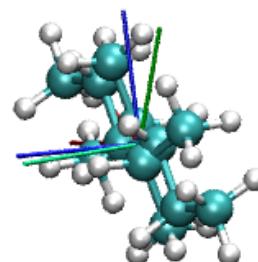
EingenValues - Molecule A

120.611	177.08	272.075
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EingenValues - Molecule B

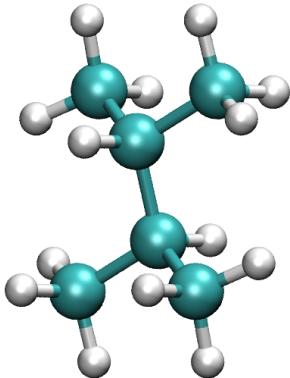
34.6869	449.234	465.177
---------	---------	---------

Different

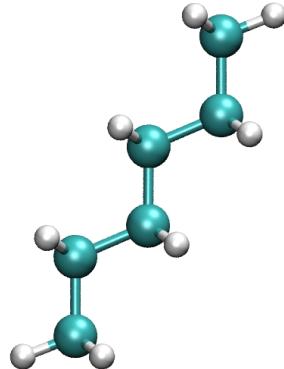


IsomerC6H14 Número 315

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

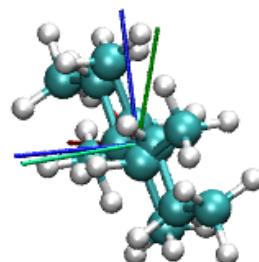
EingenValues - Molecule A

120.611	177.08	272.075
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EingenValues - Molecule B

34.6868	449.234	465.177
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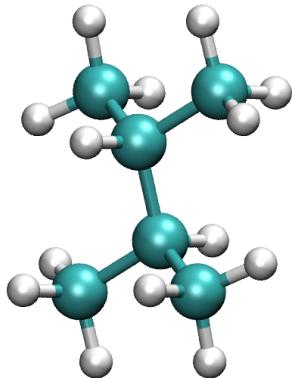
Different



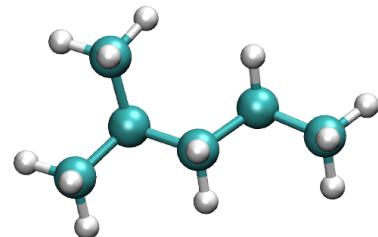
IsomerC6H14 Número 316

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

$$\begin{vmatrix} -0.999999 & -0.00105548 & -0.000587604 \\ -0.00105671 & 0.999997 & 0.00210321 \\ -0.000585382 & -0.00210383 & 0.999998 \end{vmatrix}$$

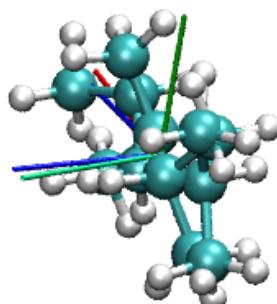
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 76.7698 & 299.061 & 347.558 \end{vmatrix}$$

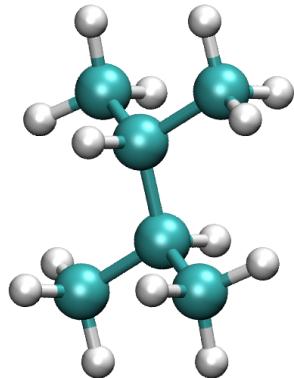
Different



IsomerC6H14 Número 317

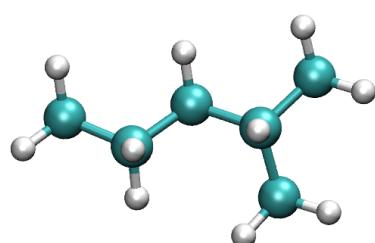
Molecule A

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

$$\begin{vmatrix} -0.999999 & -0.00105562 & -0.000587505 \\ -0.00105685 & 0.999997 & 0.00210312 \\ -0.000585284 & -0.00210374 & 0.999998 \end{vmatrix}$$

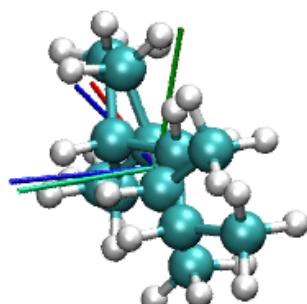
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 76.7699 & 299.061 & 347.558 \end{vmatrix}$$

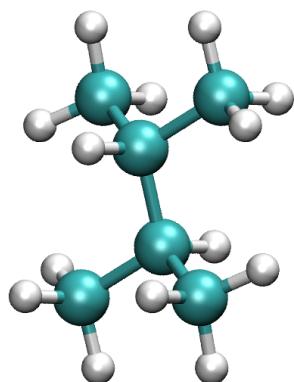
Different



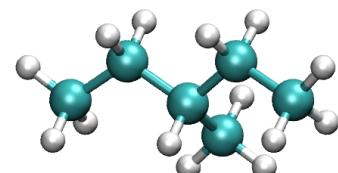
IsomerC6H14 Número 318

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

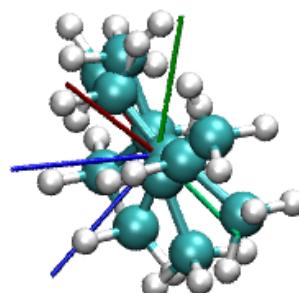
EingenValues - Molecule A

120.611	177.08	272.076
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EingenValues - Molecule B

77.8079	276.009	320.597
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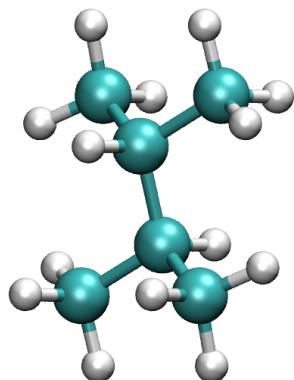
Different



IsomerC6H14 Número 319

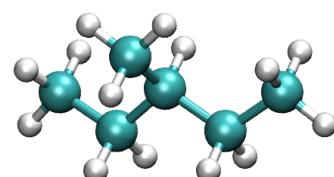
Molecule A

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

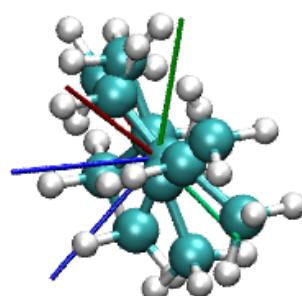
EingenValues - Molecule A

120.611	177.08	272.076
---------	--------	---------

EingenValues - Molecule B

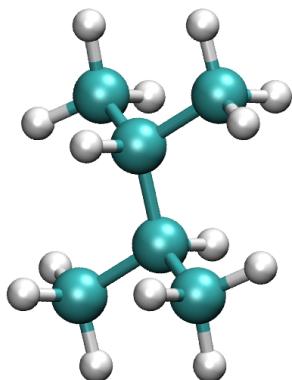
77.8081	276.009	320.598
---------	---------	---------

Different



IsomerC6H14 Número 320

Molecule A
2,3-dimethyl-butane_out_G09_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 270.146 & -16.9873 & 0 \\ -16.9873 & 122.541 & 0 \\ 0 & 0 & 177.08 \end{vmatrix}$$

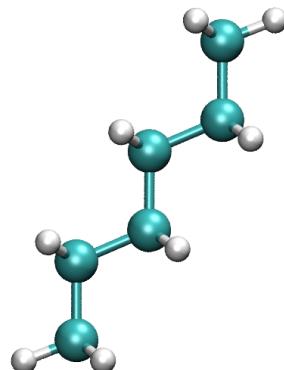
EingenVectors - Molecule A

$$\begin{vmatrix} -0.112875 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112875 & -0 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

Molecule B hexane_out_G09



Inertia Tensor - Molecule B

$$\begin{vmatrix} 346.244 & -179.129 & 0 \\ -179.129 & 137.676 & 0 \\ 0 & 0 & 465.177 \end{vmatrix}$$

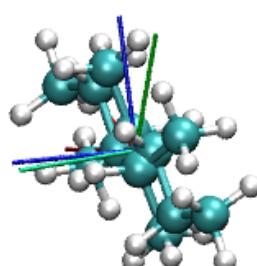
EingenVectors - Molecule B

$$\begin{vmatrix} -0.498436 & -0.866927 & 0 \\ 0.866927 & -0.498436 & -0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenValues - Molecule B

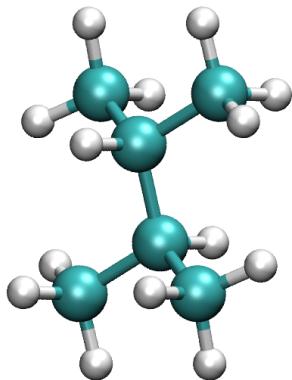
$$\begin{vmatrix} 34.6869 & 449.234 & 465.177 \end{vmatrix}$$

Different

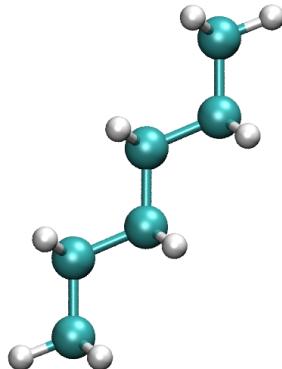


IsomerC6H14 Número 321

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

$$\begin{vmatrix} -0.498435 & -0.866927 & 0 \\ 0.866927 & -0.498435 & -0 \\ 0 & 0 & 1 \end{vmatrix}$$

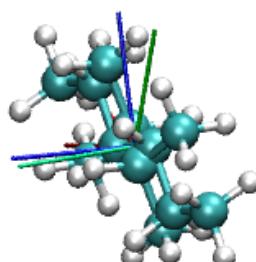
EingenValues - Molecule A

$$\begin{vmatrix} 120.611 & 177.08 & 272.076 \end{vmatrix}$$

EingenValues - Molecule B

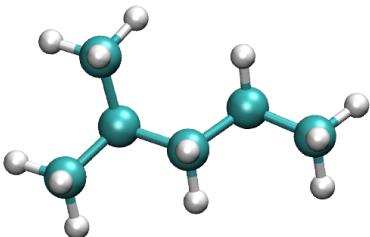
$$\begin{vmatrix} 34.6868 & 449.234 & 465.177 \end{vmatrix}$$

Different



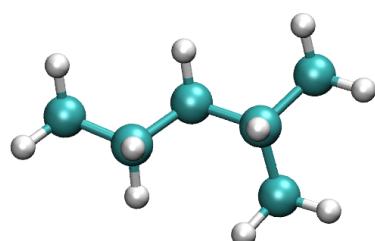
IsomerC6H14 Número 322

Molecule A 2-methyl-pentane_out_G09



Molecule B

2-methyl-pentane_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

76.7702	-0.234595	-0.158982
-0.234595	299.061	-0.102162
-0.158982	-0.102162	347.558

EingenVectors - Molecule A

-0.999999	-0.00105548	-0.000587604
-0.00105671	0.999997	0.00210321
-0.000585382	-0.00210383	0.999998

EingenVectors - Molecule B

-0.999999	-0.00105562	-0.000587505
-0.00105685	0.999997	0.00210312
-0.000585284	-0.00210374	0.999998

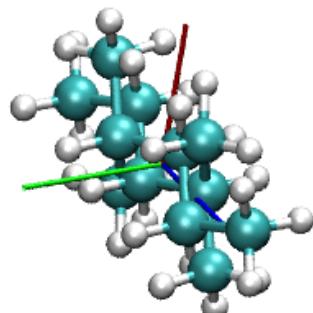
EingenValues - Molecule A

76.7698	299.061	347.558
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EingenValues - Molecule B

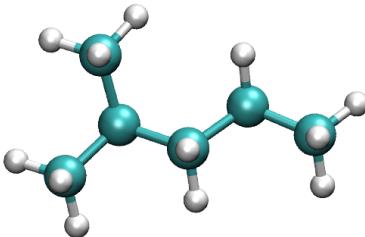
76.7699	299.061	347.558
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Enantiomers

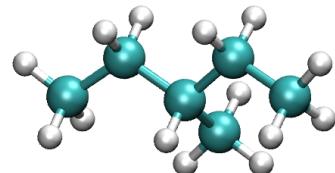


IsomerC6H14 Número 323

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

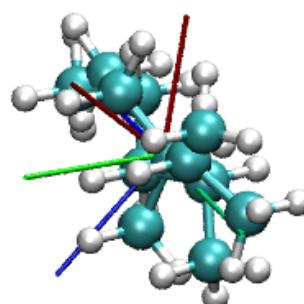
EingenValues - Molecule A

76.7698	299.061	347.558
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EingenValues - Molecule B

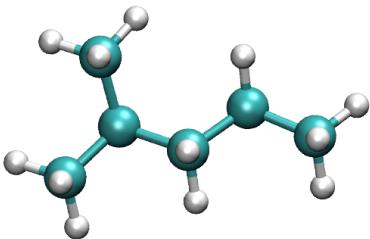
77.8079	276.009	320.597
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Different



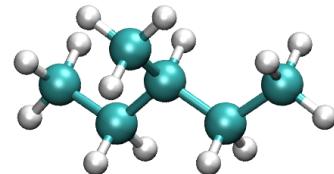
IsomerC6H14 Número 324

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

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

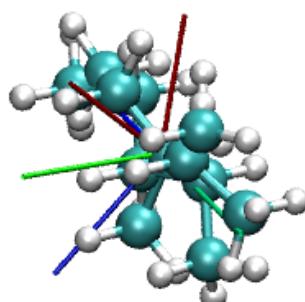
EingenValues - Molecule A

$$\begin{vmatrix} 76.7698 & 299.061 & 347.558 \end{vmatrix}$$

EingenValues - Molecule B

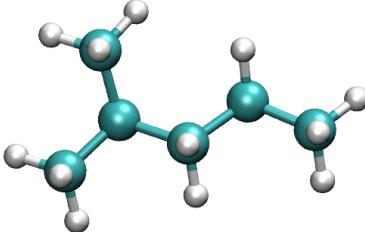
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Different

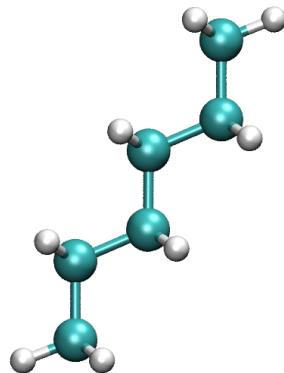


IsomerC6H14 Número 325

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

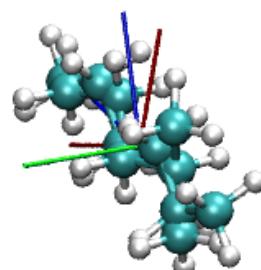
EingenValues - Molecule A

76.7698	299.061	347.558
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EingenValues - Molecule B

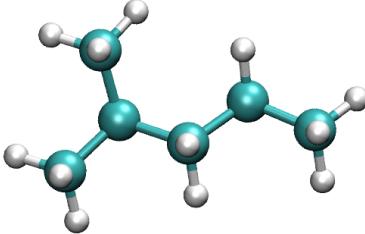
34.6869	449.234	465.177
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Different

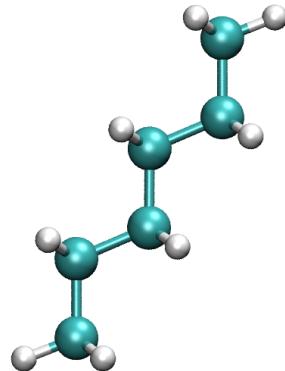


IsomerC6H14 Número 326

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

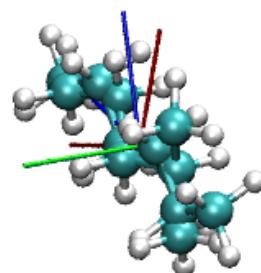
EingenValues - Molecule A

76.7698	299.061	347.558
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EingenValues - Molecule B

34.6868	449.234	465.177
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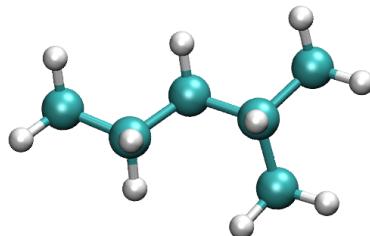
Different



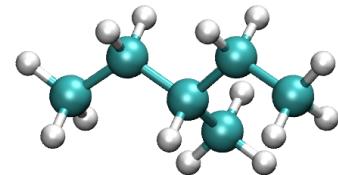
IsomerC6H14 Número 327

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

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
-0.767709	0.640799	0
0.640799	0.767709	0

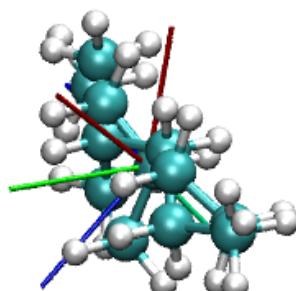
EingenValues - Molecule A

76.7699	299.061	347.558
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EingenValues - Molecule B

77.8079	276.009	320.597
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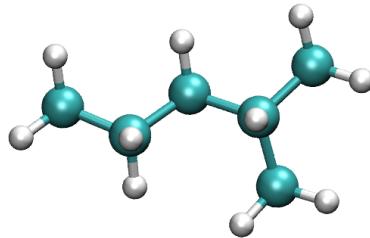
Different



IsomerC6H14 Número 328

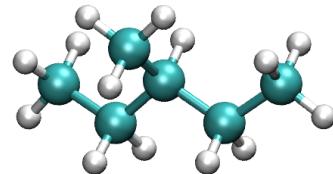
Molecule A

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

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
-0.76771	0.640798	0
0.640798	0.76771	0

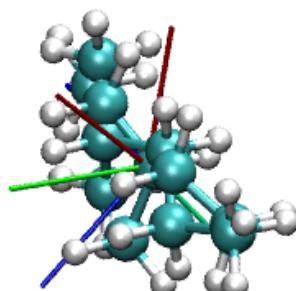
EigenValues - Molecule A

76.7699	299.061	347.558
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EigenValues - Molecule B

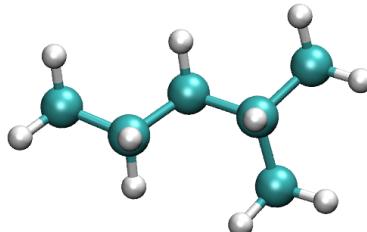
77.8081	276.009	320.598
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Different

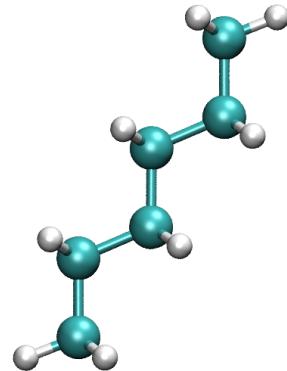


IsomerC6H14 Número 329

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

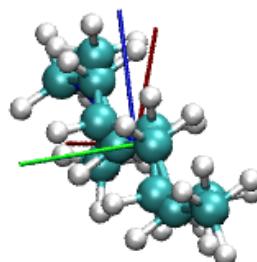
EingenVectors - Molecule A		
-0.999999	-0.00105562	-0.000587505
-0.00105685	0.999997	0.00210312
-0.000585284	-0.00210374	0.999998

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

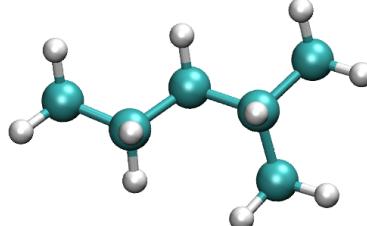
EingenValues - Molecule B		
34.6869	449.234	465.177

Different

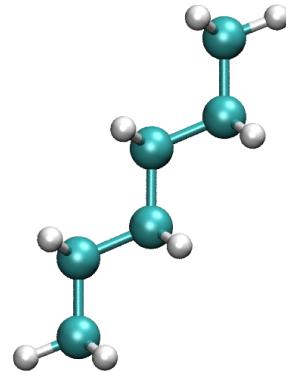


IsomerC6H14 Número 330

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

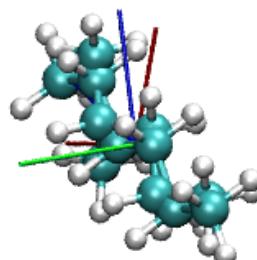
EingenVectors - Molecule A		
-0.999999	-0.00105562	-0.000587505
-0.00105685	0.999997	0.00210312
-0.000585284	-0.00210374	0.999998

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

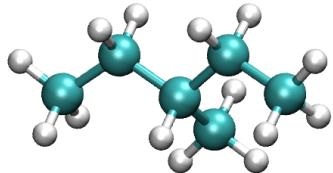
EingenValues - Molecule B		
34.6868	449.234	465.177

Different



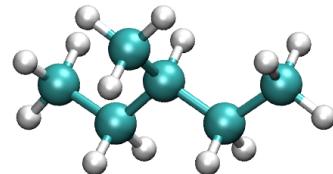
IsomerC6H14 Número 331

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

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

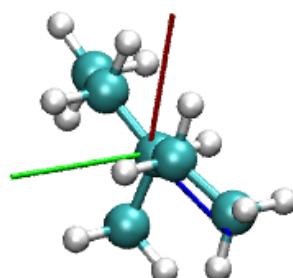
EingenValues - Molecule A

$$\begin{vmatrix} 77.8079 & 276.009 & 320.597 \end{vmatrix}$$

EingenValues - Molecule B

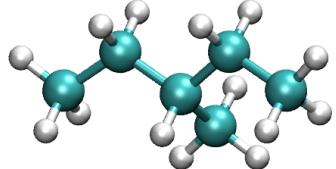
$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Equal

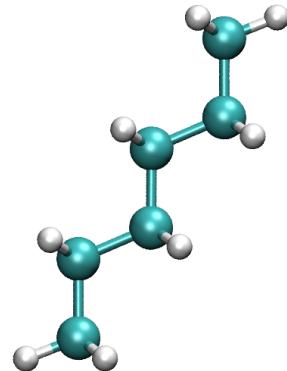


IsomerC6H14 Número 332

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

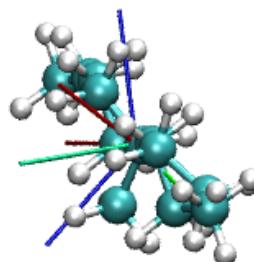
EingenValues - Molecule A

77.8079	276.009	320.597
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EingenValues - Molecule B

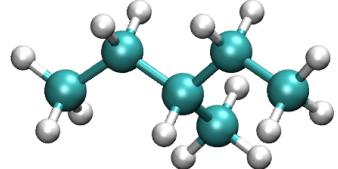
34.6869	449.234	465.177
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Different

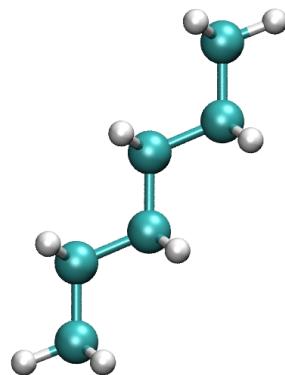


IsomerC6H14 Número 333

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

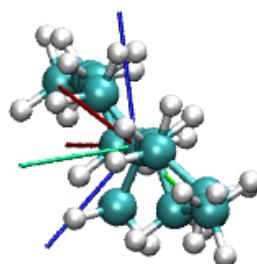
EingenValues - Molecule A

77.8079	276.009	320.597
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EingenValues - Molecule B

34.6868	449.234	465.177
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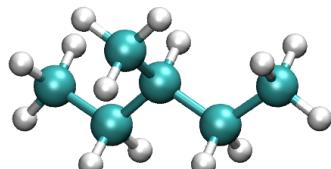
Different



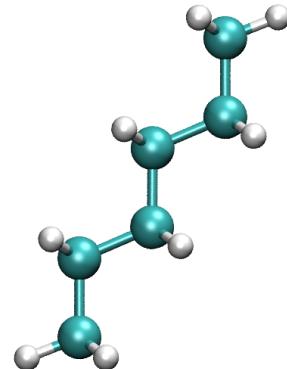
IsomerC6H14 Número 334

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

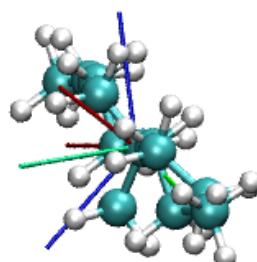
EingenValues - Molecule A

77.8081	276.009	320.598
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EingenValues - Molecule B

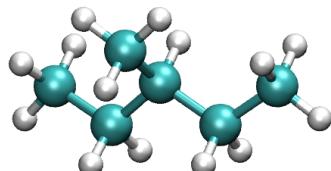
34.6869	449.234	465.177
---------	---------	---------

Different

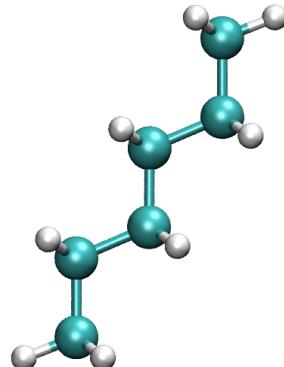


IsomerC6H14 Número 335

Molecule A
3-methyl-pentane_out_G09_inversion



Molecule B hexane_out_G09_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 294.318 & 21.9353 & 0 \\ 21.9353 & 302.289 & 0 \\ 0 & 0 & 77.8081 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.76771 & 0.640798 & 0 \\ 0.640798 & 0.76771 & 0 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 77.8081 & 276.009 & 320.598 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 346.245 & -179.129 & 0 \\ -179.129 & 137.676 & 0 \\ 0 & 0 & 465.177 \end{vmatrix}$$

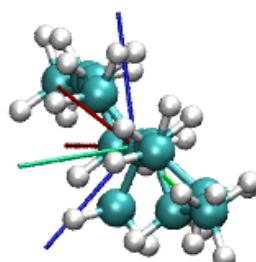
EingenVectors - Molecule B

$$\begin{vmatrix} -0.498435 & -0.866927 & 0 \\ 0.866927 & -0.498435 & -0 \\ 0 & 0 & 1 \end{vmatrix}$$

EingenValues - Molecule B

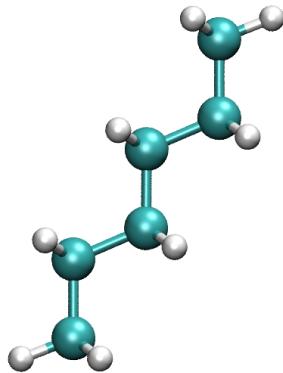
$$\begin{vmatrix} 34.6868 & 449.234 & 465.177 \end{vmatrix}$$

Different

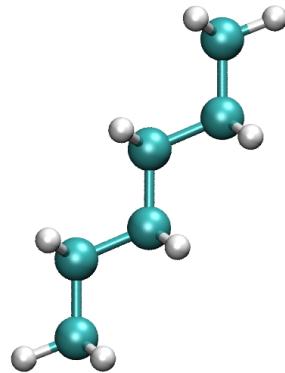


IsomerC6H14 Número 336

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

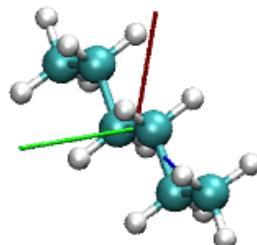
EingenValues - Molecule A

34.6869	449.234	465.177
---------	---------	---------

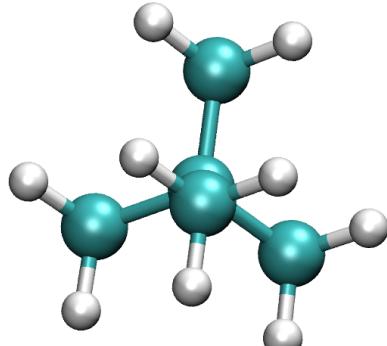
EingenValues - Molecule B

34.6868	449.234	465.177
---------	---------	---------

Equal

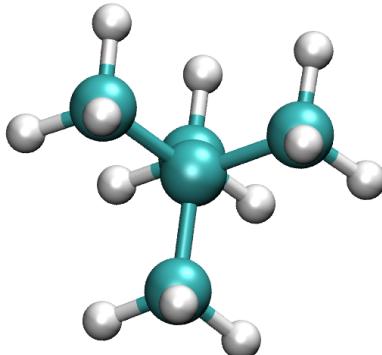


Molecule A neopentane_Symmetry_out_G09



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

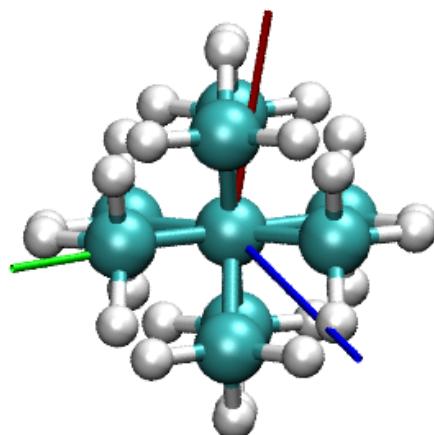
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

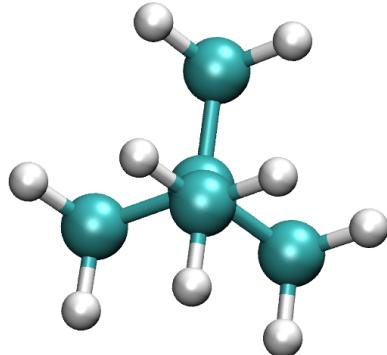
114.662	114.667	114.672
---------	---------	---------

Equal

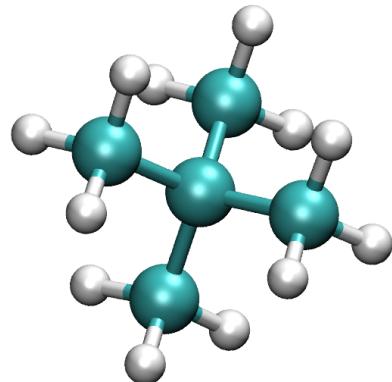


NeoConformation Número 338

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

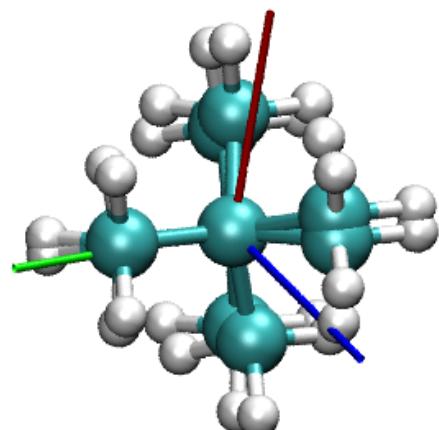
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

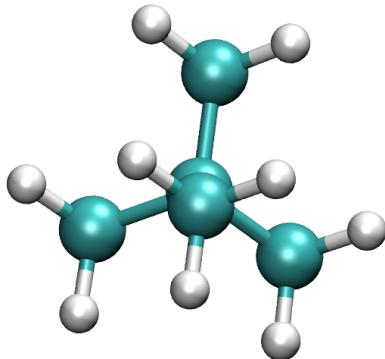
114.662	114.667	114.672
---------	---------	---------

Equal

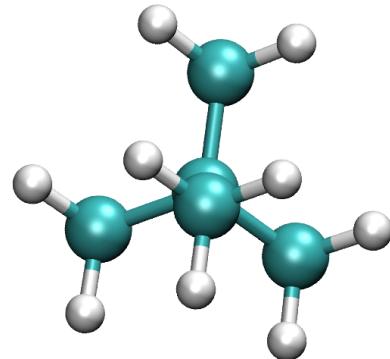


NeoConformation Número 339

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

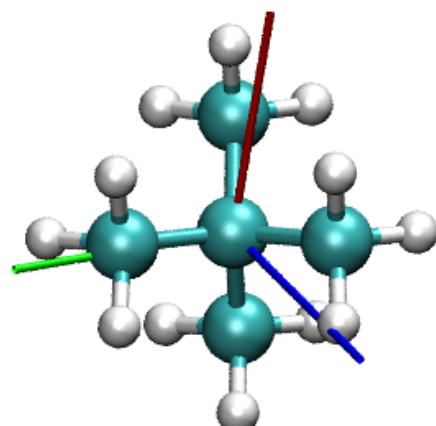
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

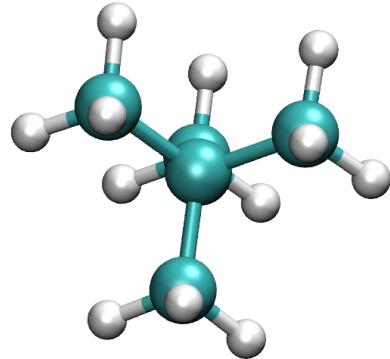
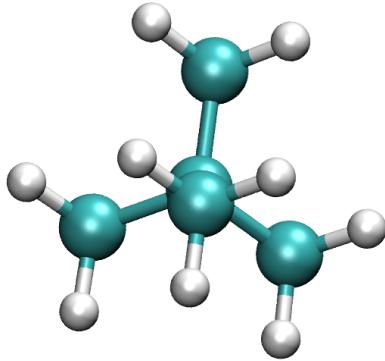
114.662	114.667	114.672
---------	---------	---------

Equal



NeoConformation Número 340

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

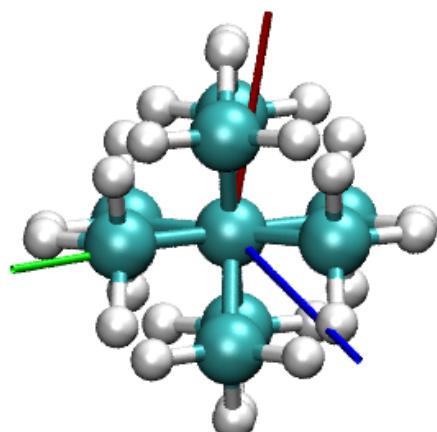
EingenValues - Molecule A

114.662	114.667	114.672
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EingenValues - Molecule B

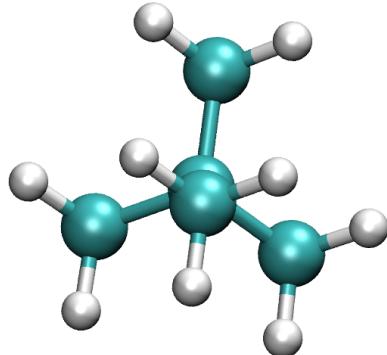
114.662	114.667	114.672
---------	---------	---------

Equal



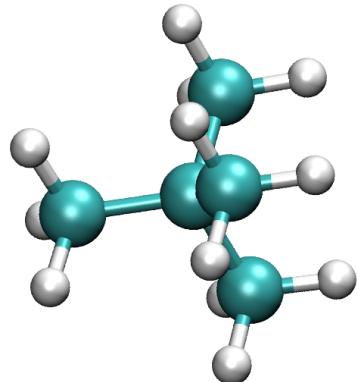
NeoConformation Número 341

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

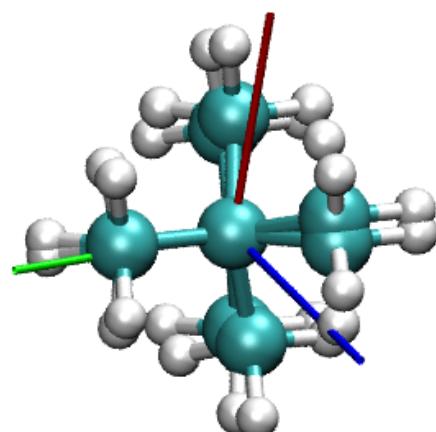
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

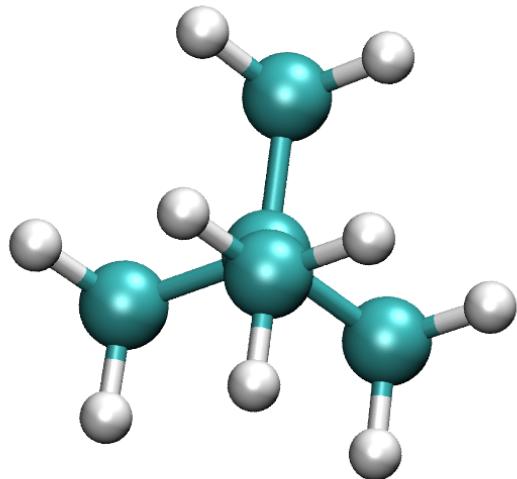
Equal



NeoConformation Número 342

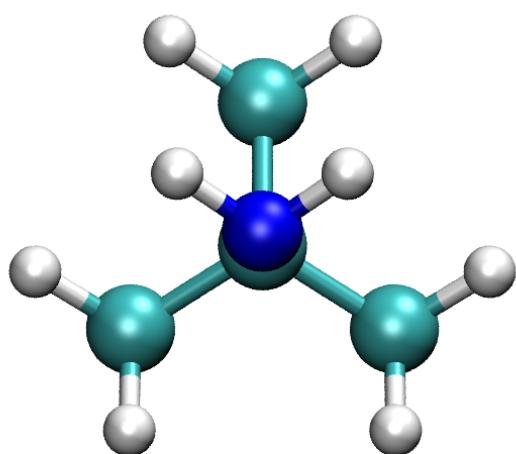
Molecule A

neopentane_Symmetry_out_G09



Molecule B

tert-butylamine_out_G09

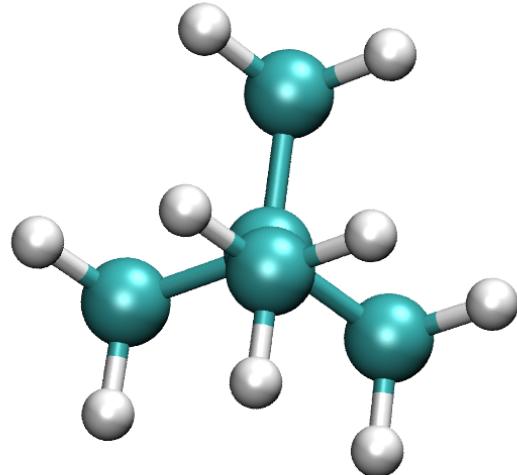


Different

NeoConformation Número 343

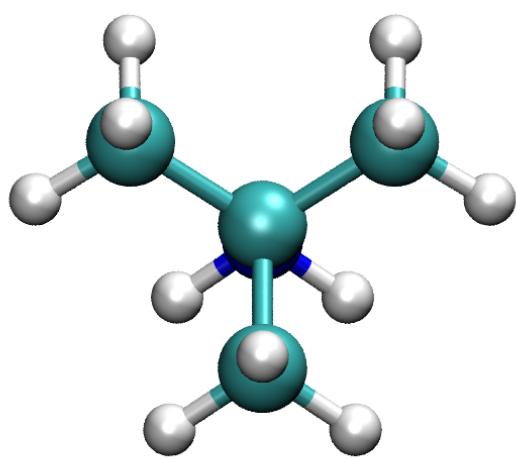
Molecule A

neopentane_Symmetry_out_G09



Molecule B

tert-butylamine_out_G09_inversion



Different

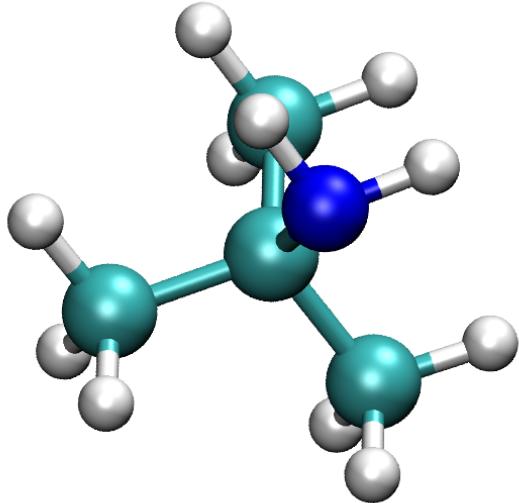
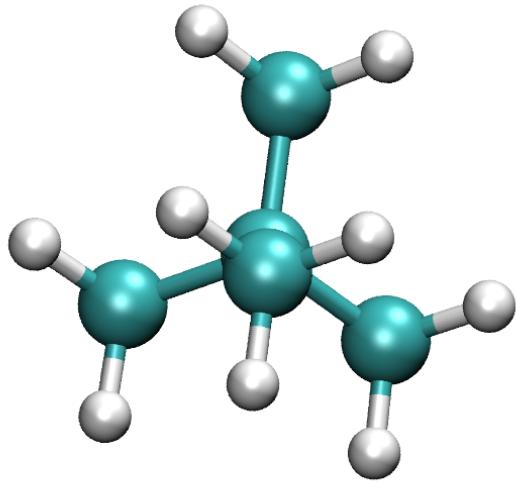
NeoConformation Número 344

Molecule A

neopentane_Symmetry_out_G09

Molecule B

tert-butylamine_out_G09_rot_x15_y15_z15

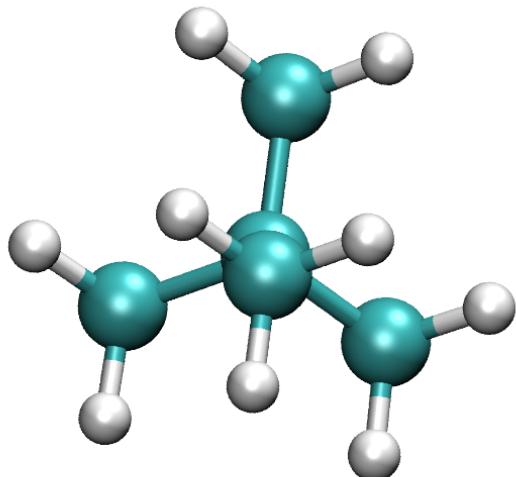


Different

NeoConformation Número 345

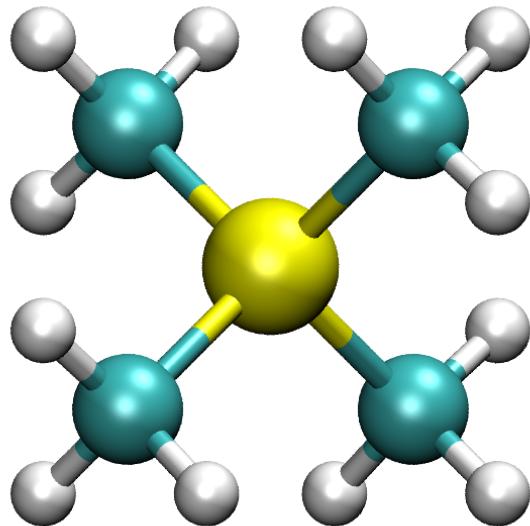
Molecule A

neopentane_Symmetry_out_G09



Molecule B

tetramethylsilane_out_G09

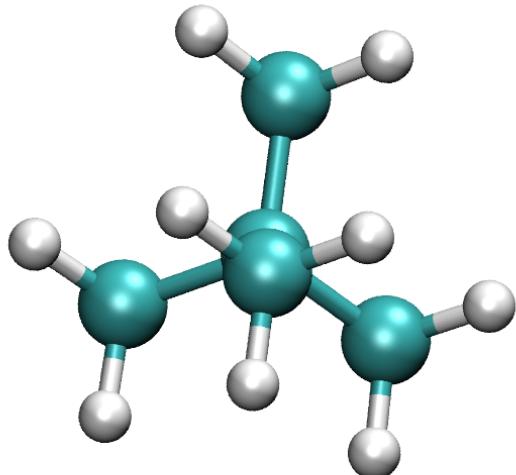


Different

NeoConformation Número 346

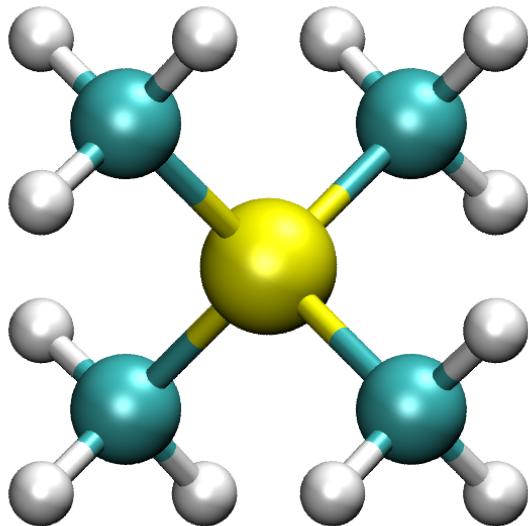
Molecule A

neopentane_Symmetry_out_G09



Molecule B

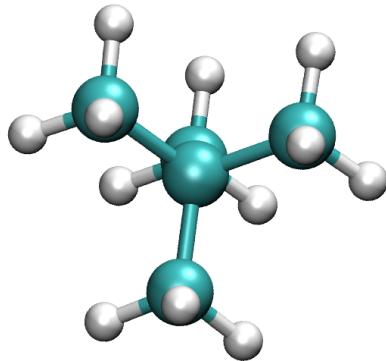
tetramethylsilane_out_G09_inversion



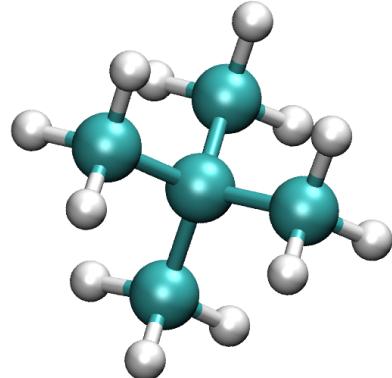
Different

NeoConformation Número 347

Molecule A
neopentane_Symmetry_out_G09_inversion



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

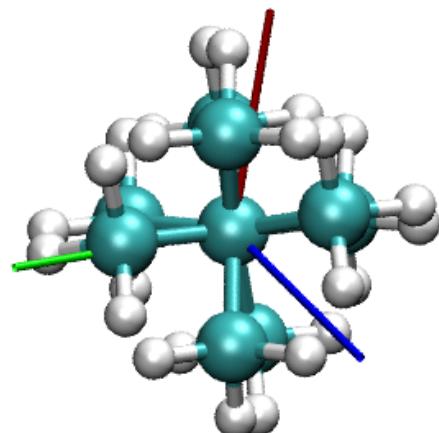
EingenVectors - Molecule A		
-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

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

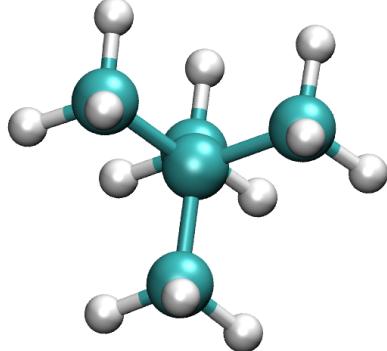
Equal



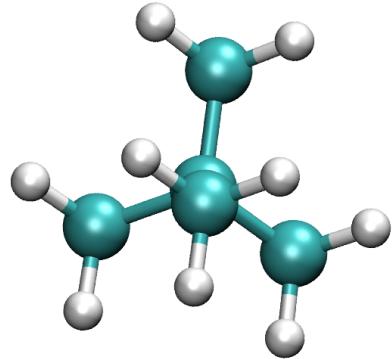
NeoConformation Número 348

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

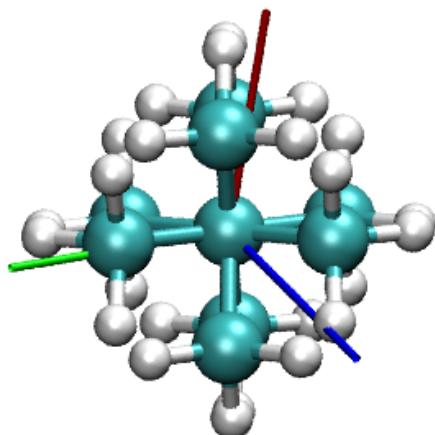
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

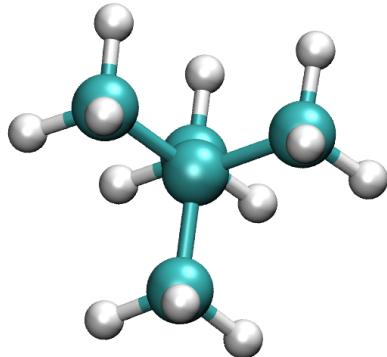
114.662	114.667	114.672
---------	---------	---------

Equal

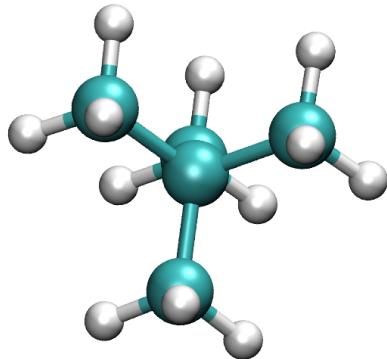


NeoConformation Número 349

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

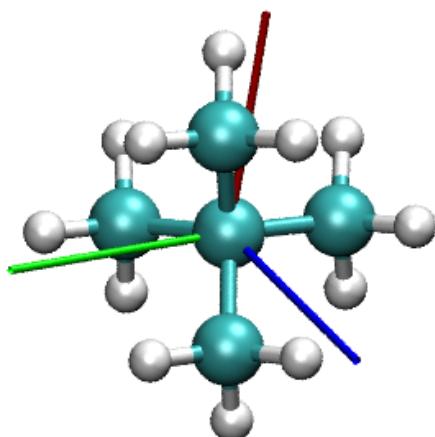
EingenVectors - Molecule A		
-0.999243	0.0340426	0.0188303
-0.0350564	-0.997791	-0.0564246
0.0168679	-0.057042	0.998229

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

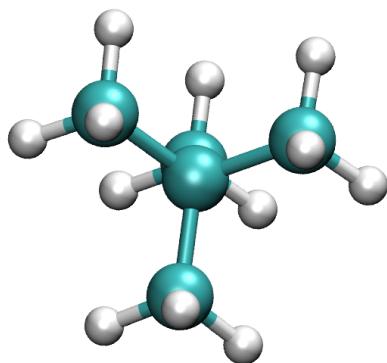
Equal



NeoConformation Número 350

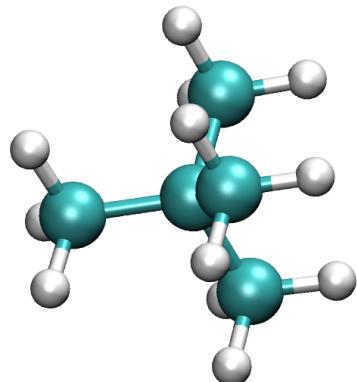
Molecule A

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

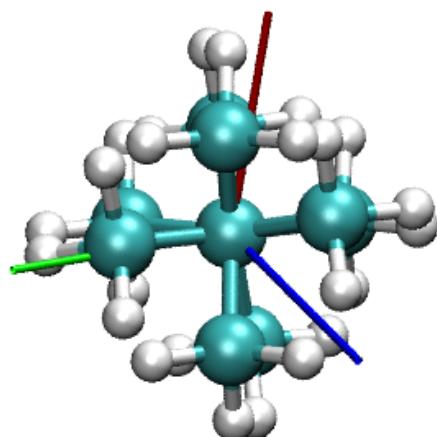
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

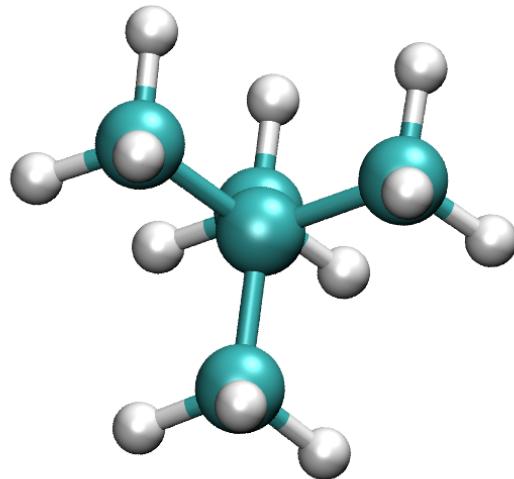
Equal



NeoConformation Número 351

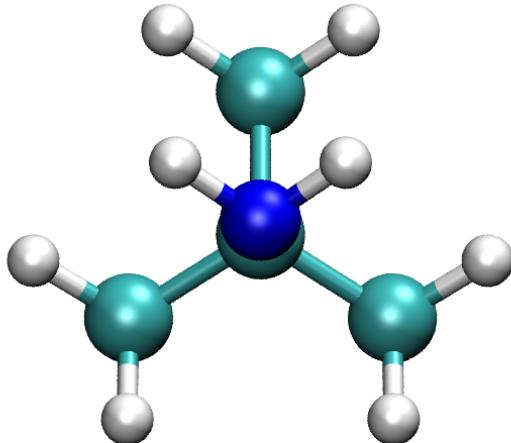
Molecule A

neopentane_Symmetry_out_G09_inversion



Molecule B

tert-butylamine_out_G09

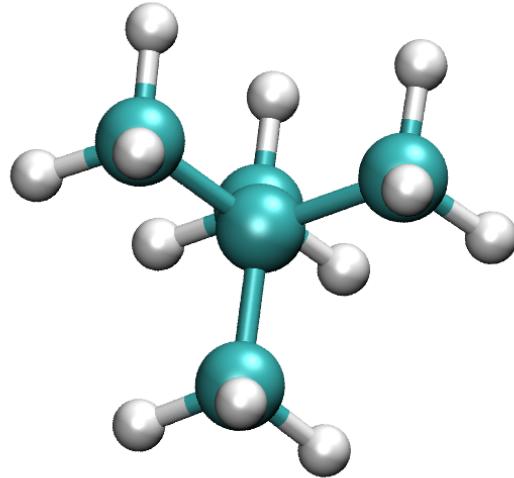


Different

NeoConformation Número 352

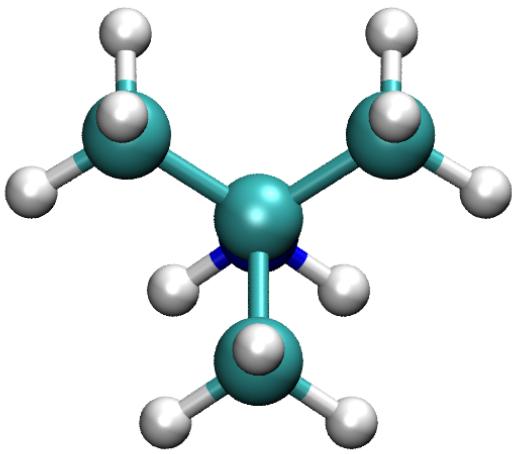
Molecule A

neopentane_Symmetry_out_G09_inversion



Molecule B

tert-butylamine_out_G09_inversion

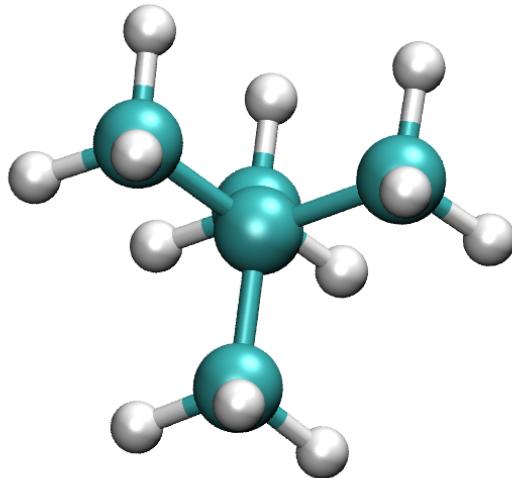


Different

NeoConformation Número 353

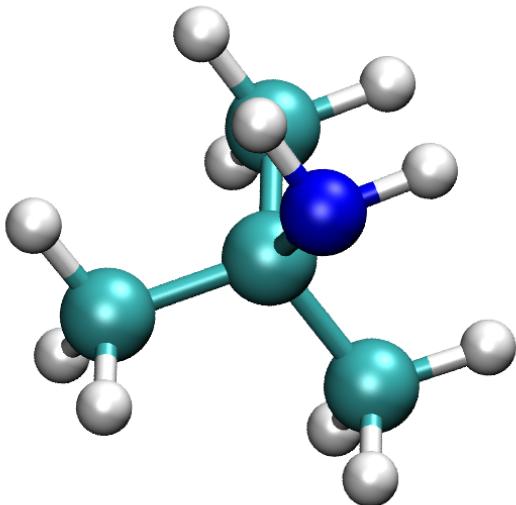
Molecule A

neopentane_Symmetry_out_G09_inversion



Molecule B

tert-butylamine_out_G09_rot_x15_y15_z15

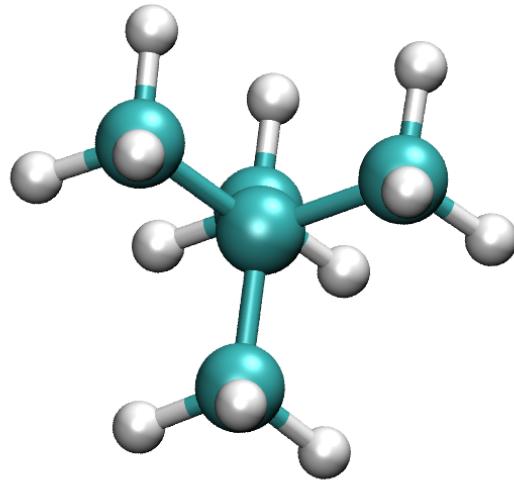


Different

NeoConformation Número 354

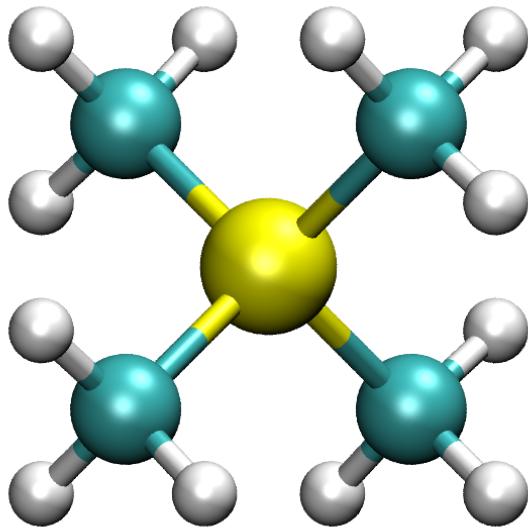
Molecule A

neopentane_Symmetry_out_G09_inversion



Molecule B

tetramethylsilane_out_G09

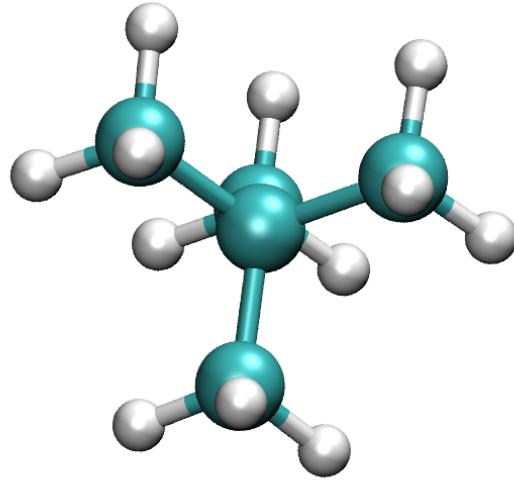


Different

NeoConformation Número 355

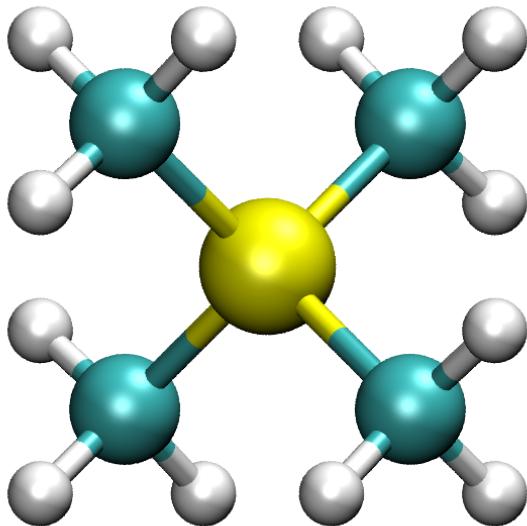
Molecule A

neopentane_Symmetry_out_G09_inversion



Molecule B

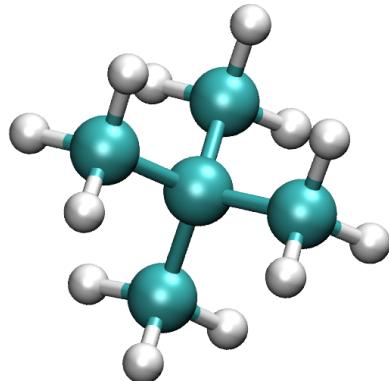
tetramethylsilane_out_G09_inversion



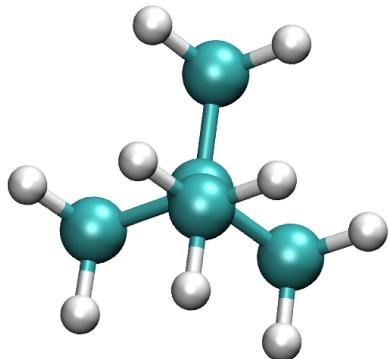
Different

NeoConformation Número 356

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

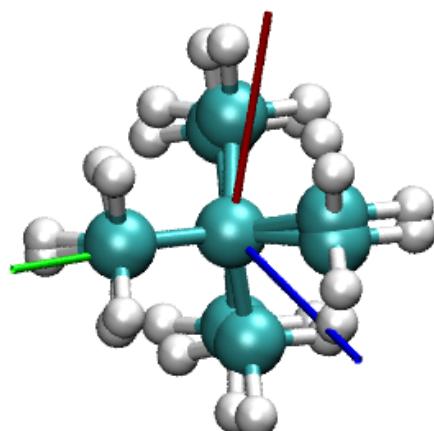
EingenValues - Molecule A

114.662	114.667	114.672
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EingenValues - Molecule B

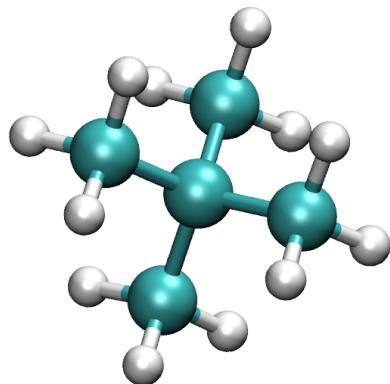
114.662	114.667	114.672
---------	---------	---------

Equal

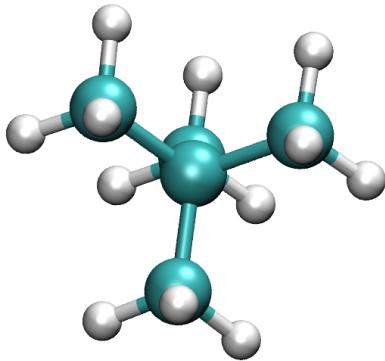


NeoConformation Número 357

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

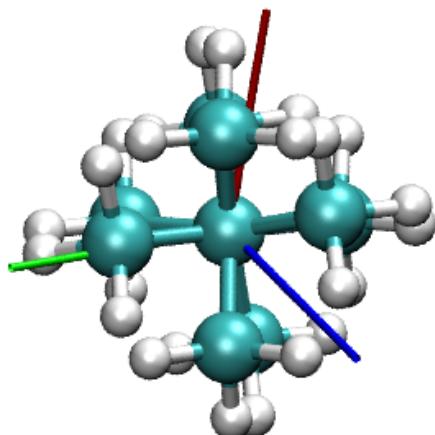
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

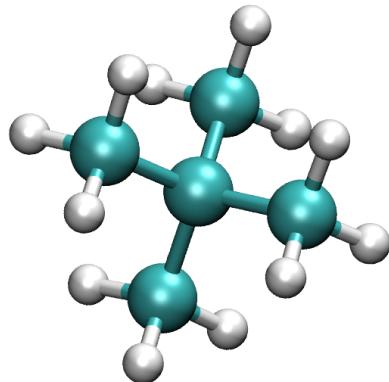
EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

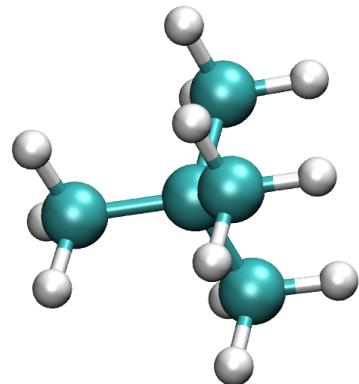
Equal



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

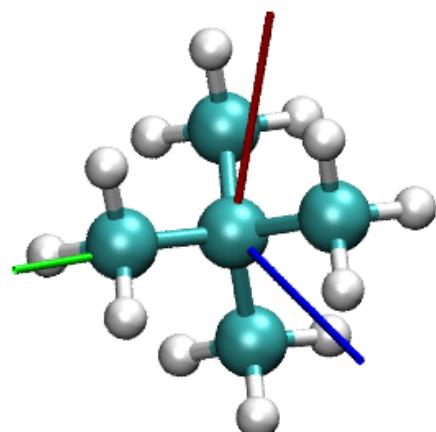
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

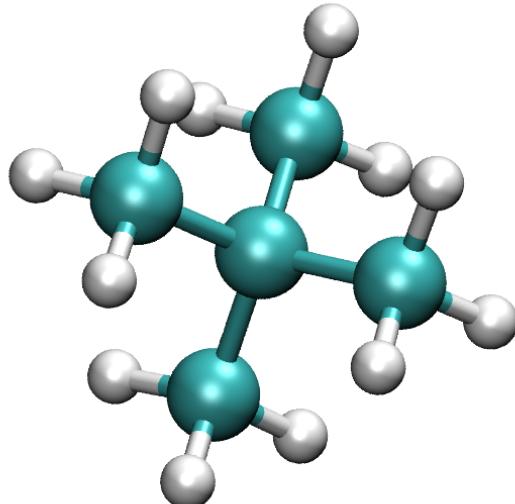
Equal



NeoConformation Número 359

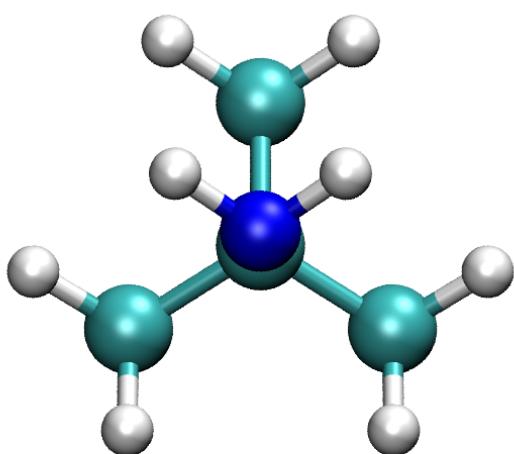
Molecule A

neopentane_Symmetry_out_G09_rot_x45_y45_z60



Molecule B

tert-butylamine_out_G09

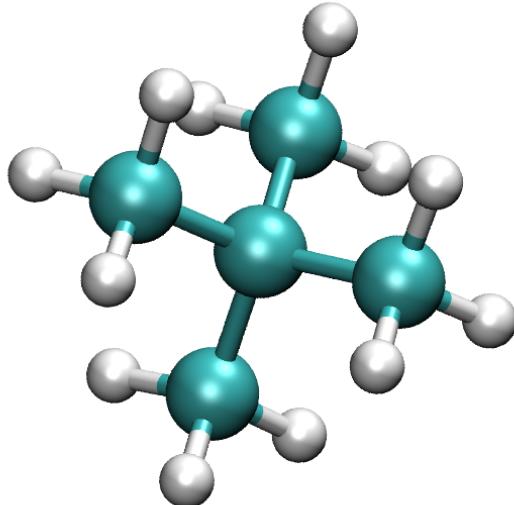


Different

NeoConformation Número 360

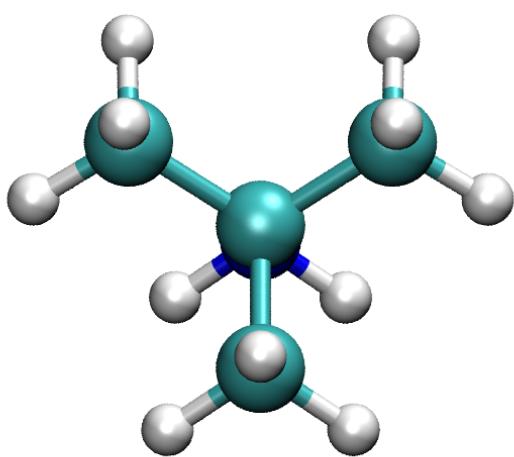
Molecule A

neopentane_Symmetry_out_G09_rot_x45_y45_z60



Molecule B

tert-butylamine_out_G09_inversion

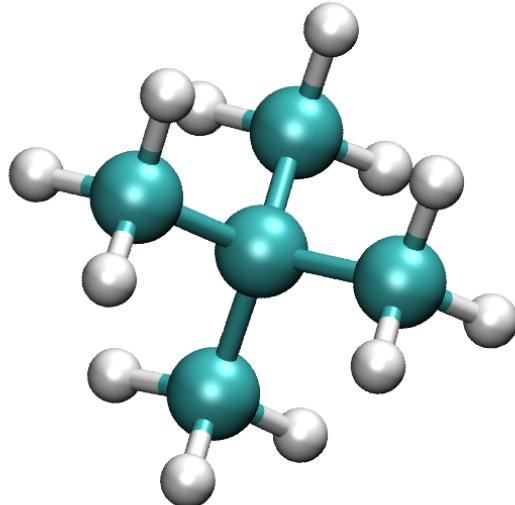


Different

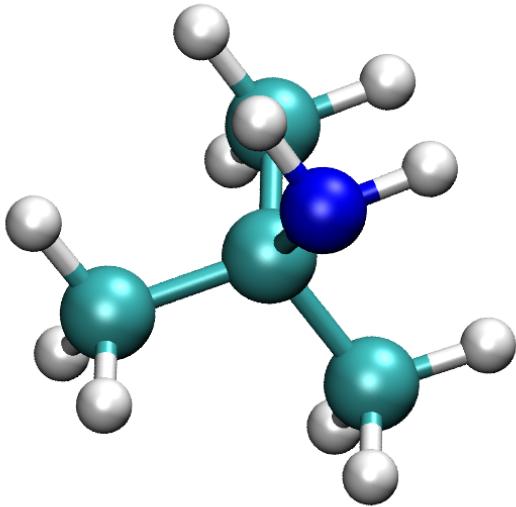
NeoConformation Número 361

Molecule A

neopentane_Symmetry_out_G09_rot_x45_y45_z60



Molecule B

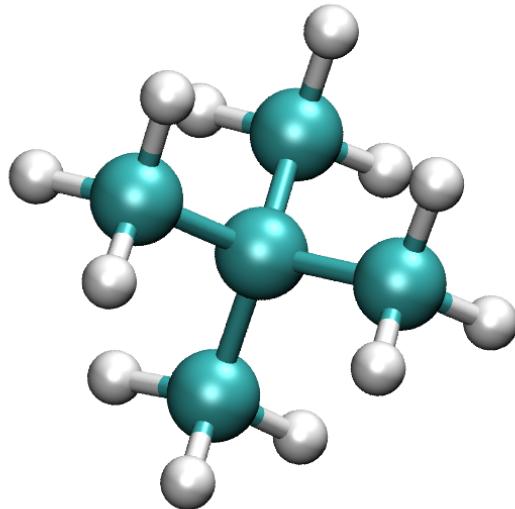


Different

NeoConformation Número 362

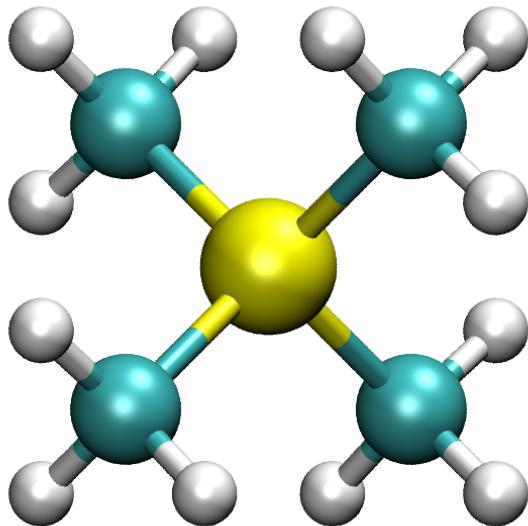
Molecule A

neopentane_Symmetry_out_G09_rot_x45_y45_z60



Molecule B

tetramethylsilane_out_G09

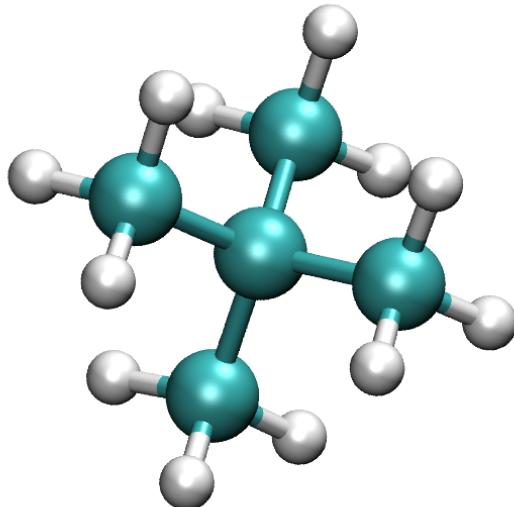


Different

NeoConformation Número 363

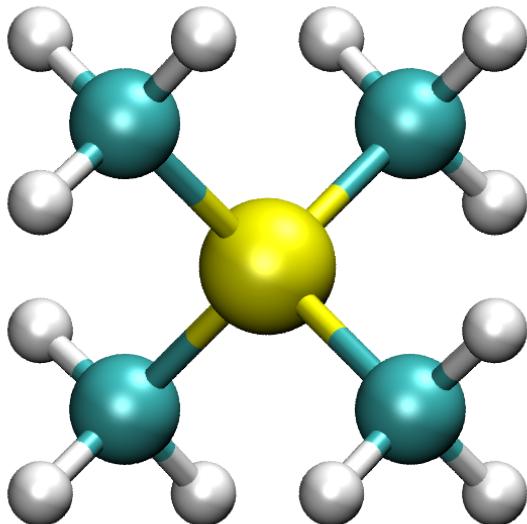
Molecule A

neopentane_Symmetry_out_G09_rot_x45_y45_z60



Molecule B

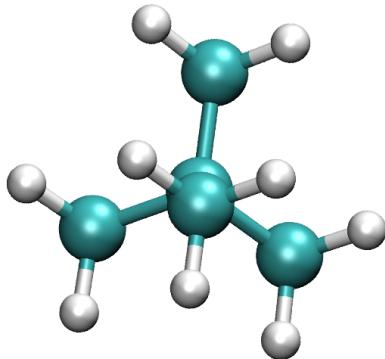
tetramethylsilane_out_G09_inversion



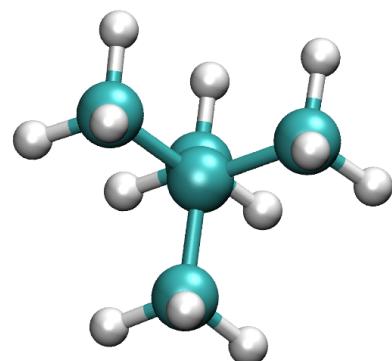
Different

NeoConformation Número 364

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

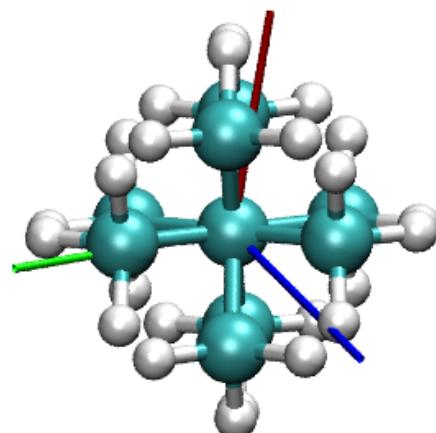
EingenValues - Molecule A

114.662	114.667	114.672
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EingenValues - Molecule B

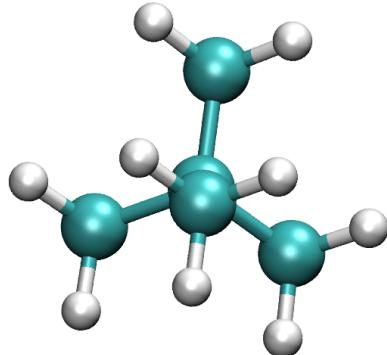
114.662	114.667	114.672
---------	---------	---------

Equal



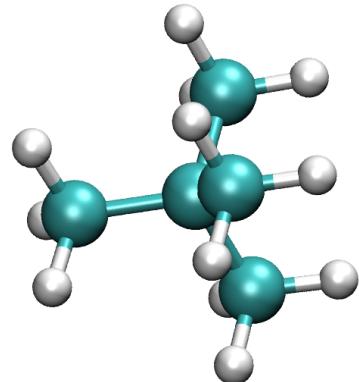
NeoConformation Número 365

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

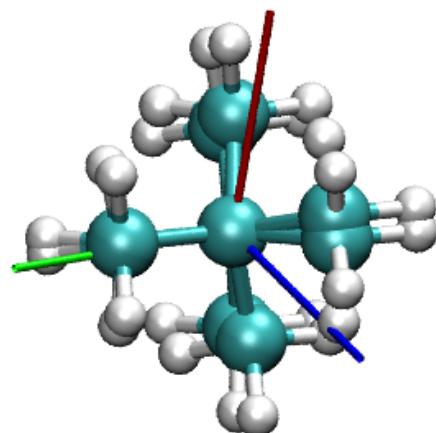
EingenValues - Molecule A

114.662	114.667	114.672
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EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

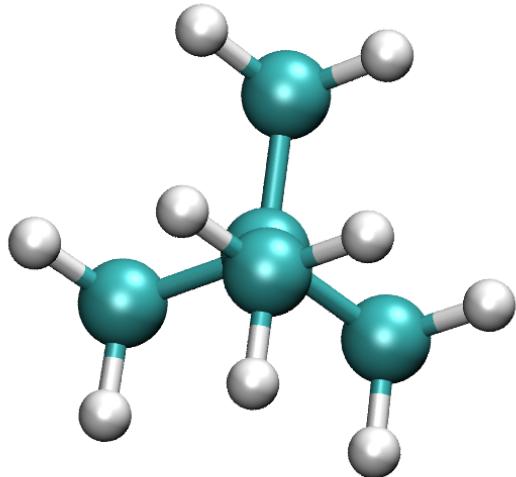
Equal



NeoConformation Número 366

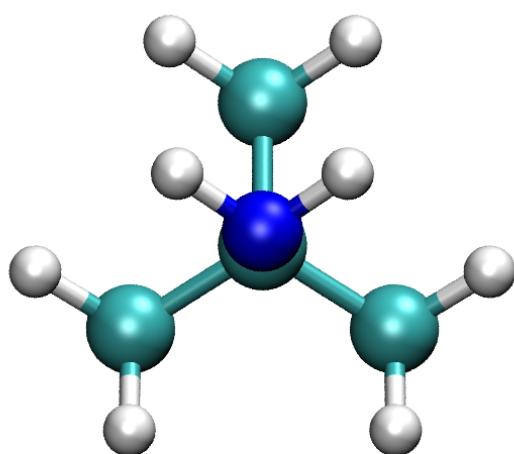
Molecule A

neopentane_out_G09



Molecule B

tert-butylamine_out_G09

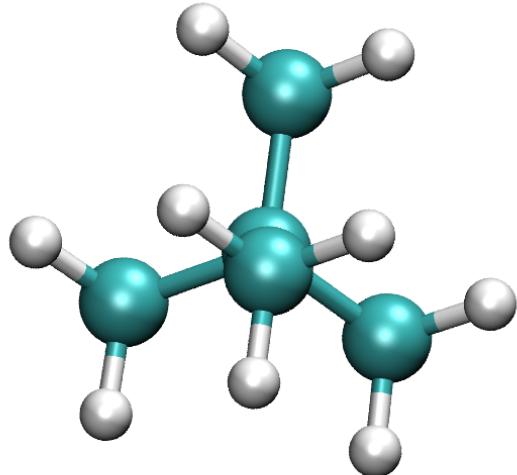


Different

NeoConformation Número 367

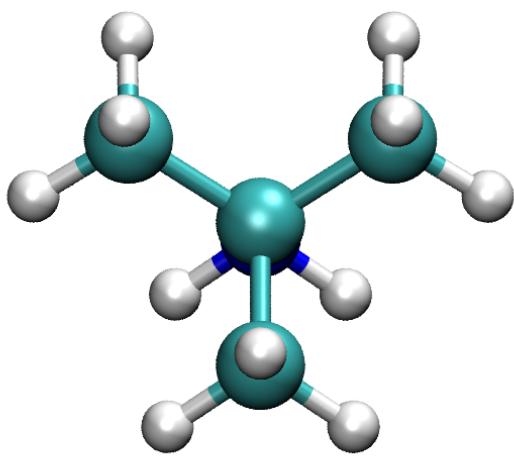
Molecule A

neopentane_out_G09



Molecule B

tert-butylamine_out_G09_inversion

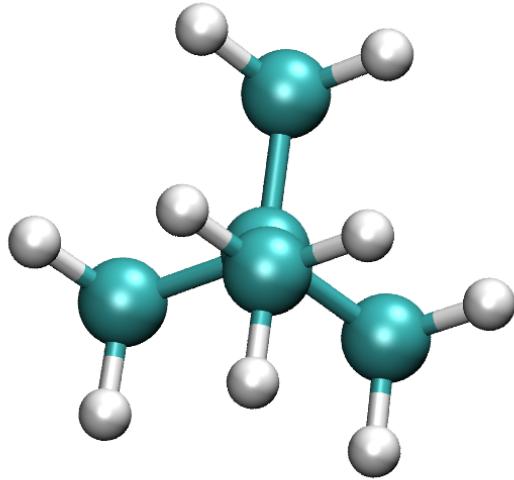


Different

NeoConformation Número 368

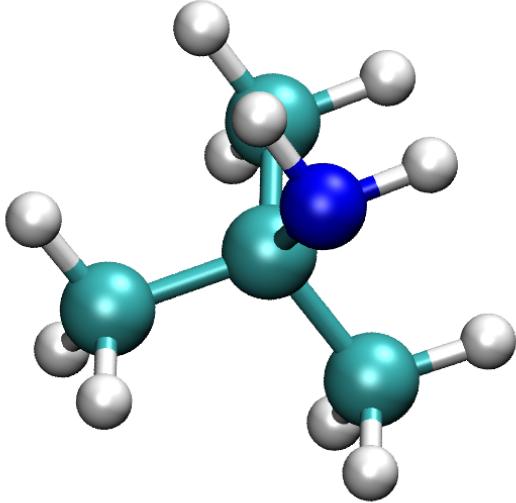
Molecule A

neopentane_out_G09



Molecule B

tert-butylamine_out_G09_rot_x15_y15_z15

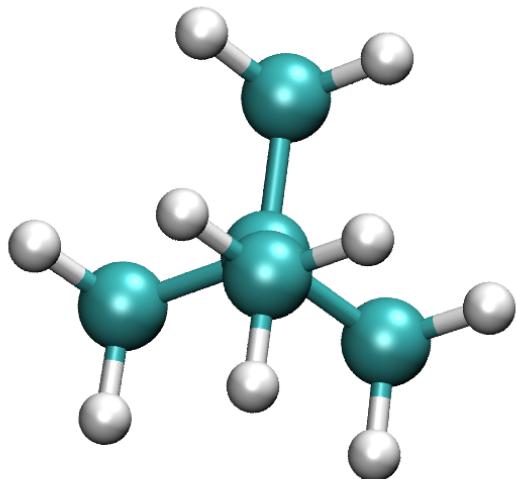


Different

NeoConformation Número 369

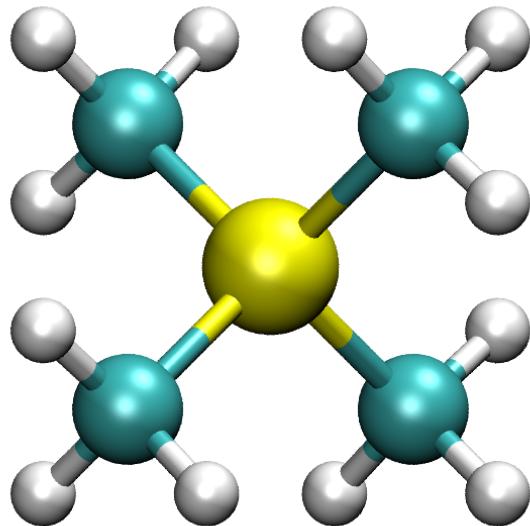
Molecule A

neopentane_out_G09



Molecule B

tetramethylsilane_out_G09

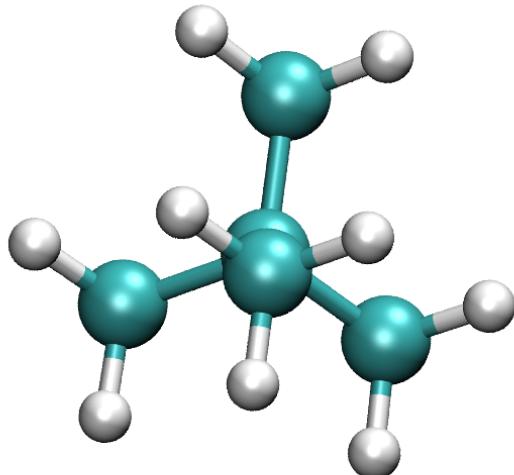


Different

NeoConformation Número 370

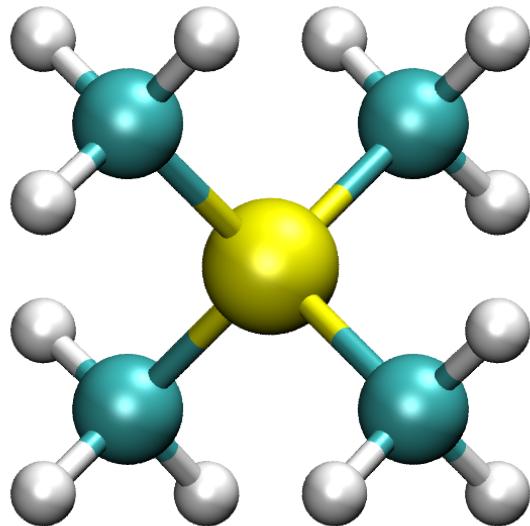
Molecule A

neopentane_out_G09



Molecule B

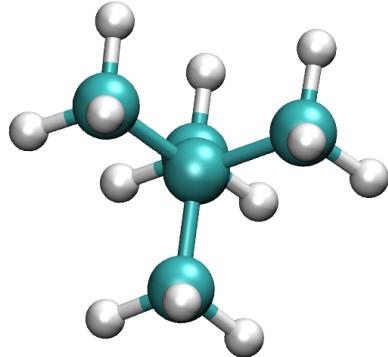
tetramethylsilane_out_G09_inversion



Different

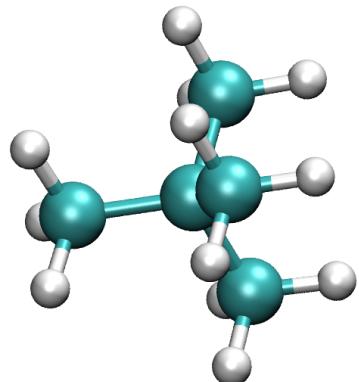
NeoConformation Número 371

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

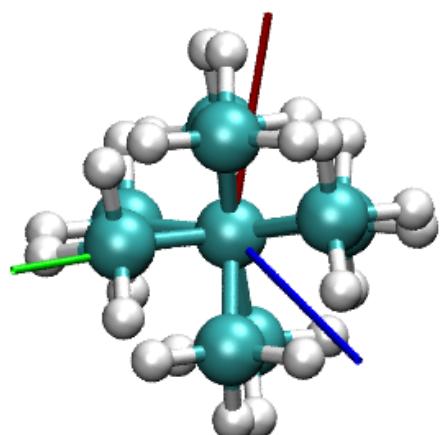
EingenValues - Molecule A

114.662	114.667	114.672
---------	---------	---------

EingenValues - Molecule B

114.662	114.667	114.672
---------	---------	---------

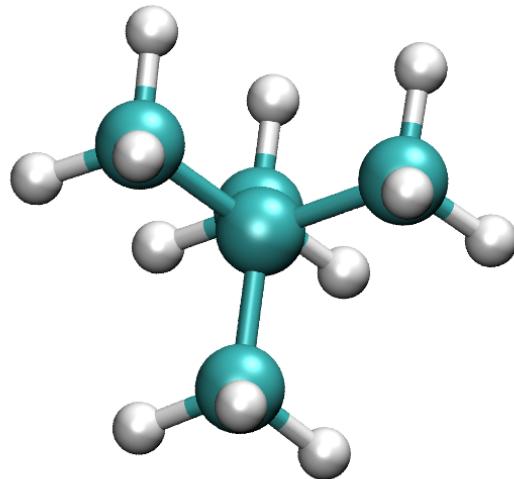
Equal



NeoConformation Número 372

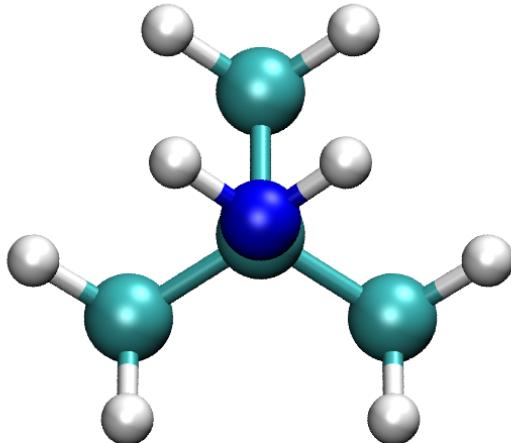
Molecule A

neopentane.out_G09_inversion



Molecule B

tert-butylamine.out_G09

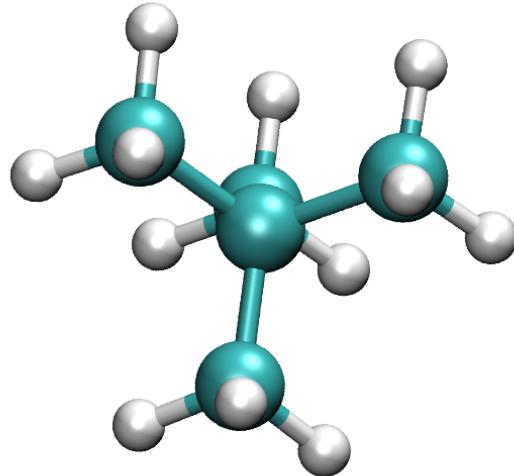


Different

NeoConformation Número 373

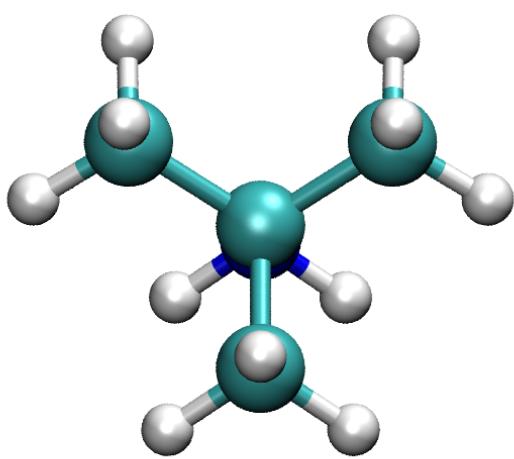
Molecule A

neopentane_out_G09_inversion



Molecule B

tert-butylamine_out_G09_inversion

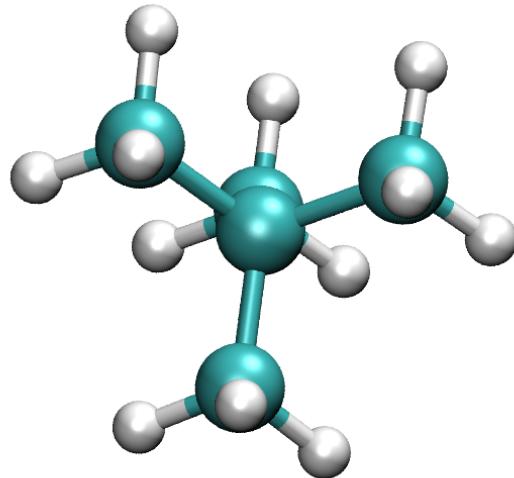


Different

NeoConformation Número 374

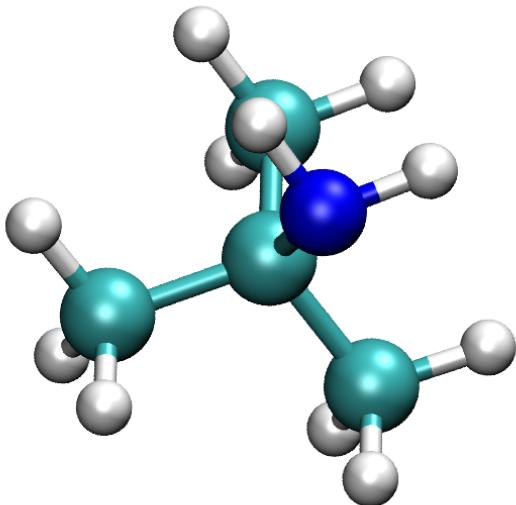
Molecule A

neopentane_out_G09_inversion



Molecule B

tert-butylamine_out_G09_rot_x15_y15_z15

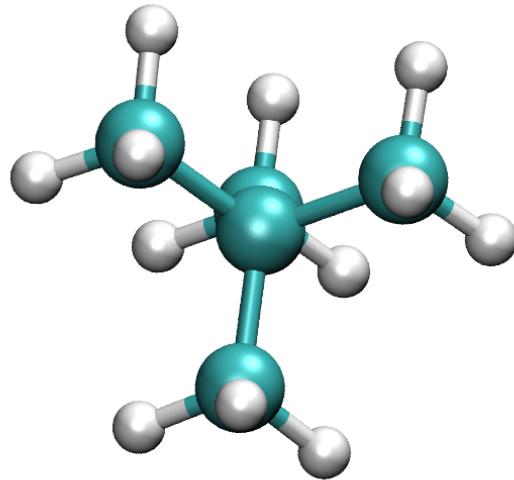


Different

NeoConformation Número 375

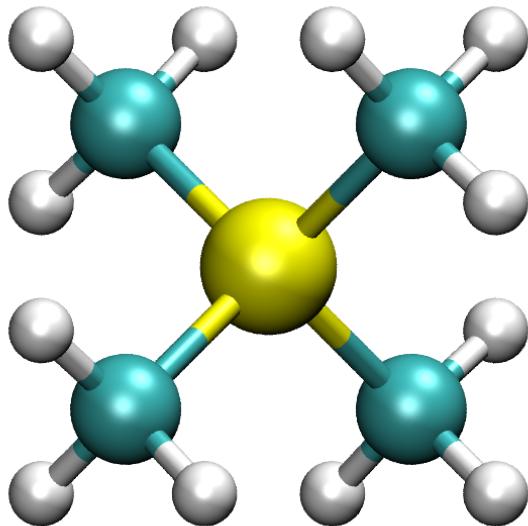
Molecule A

neopentane_out_G09_inversion



Molecule B

tetramethylsilane_out_G09

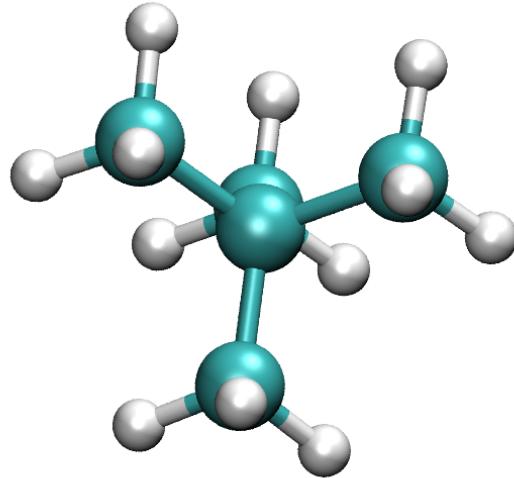


Different

NeoConformation Número 376

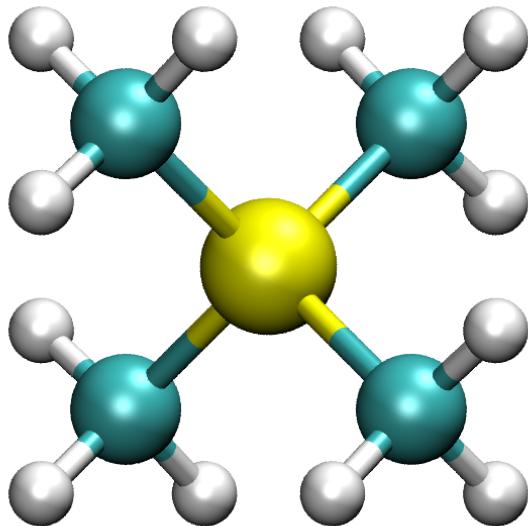
Molecule A

neopentane_out_G09_inversion



Molecule B

tetramethylsilane_out_G09_inversion

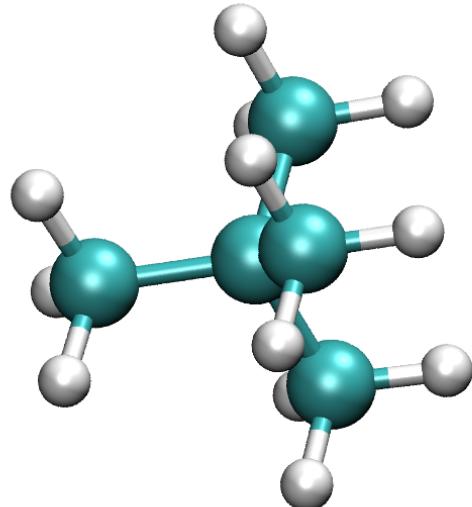


Different

NeoConformation Número 377

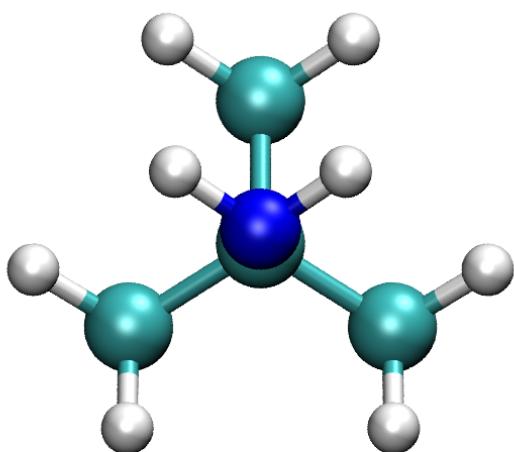
Molecule A

neopentane_out_G09_rot_x15-y15-z15



Molecule B

tert-butylamine_out_G09

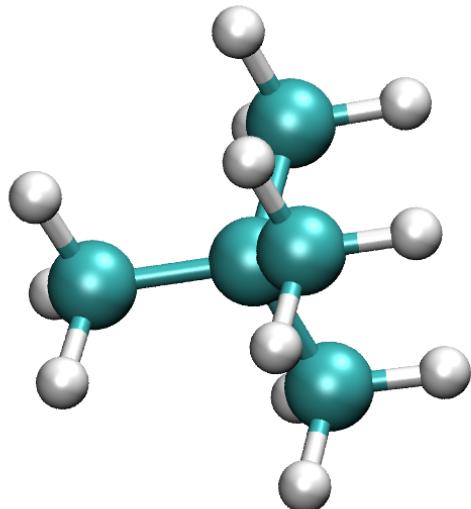


Different

NeoConformation Número 378

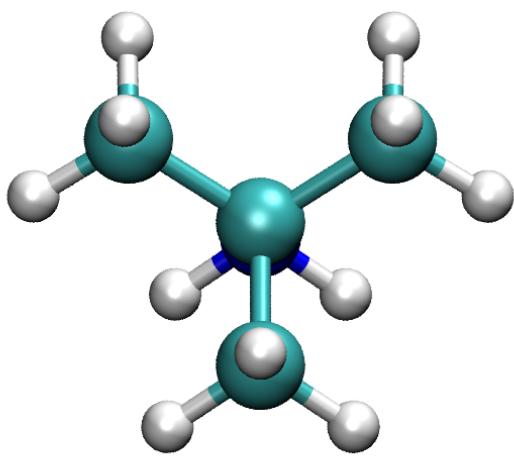
Molecule A

neopentane_out_G09_rot_x15-y15-z15



Molecule B

tert-butylamine_out_G09_inversion

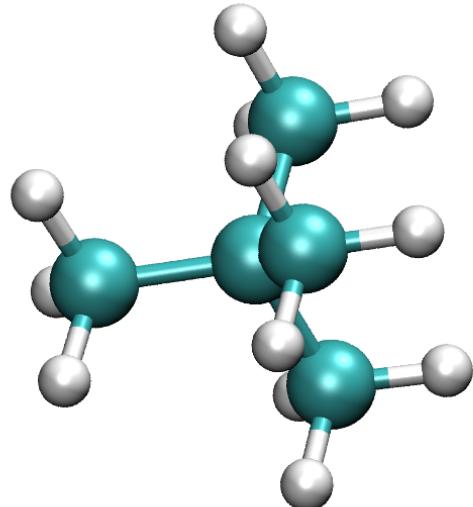


Different

NeoConformation Número 379

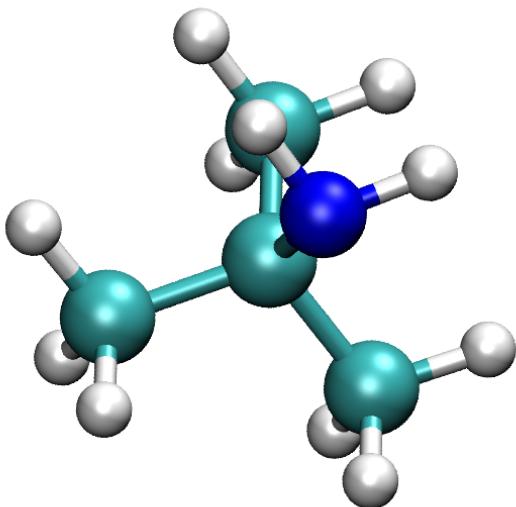
Molecule A

neopentane_out_G09_rot_x15-y15-z15



Molecule B

tert-butylamine_out_G09_rot_x15_y15_z15

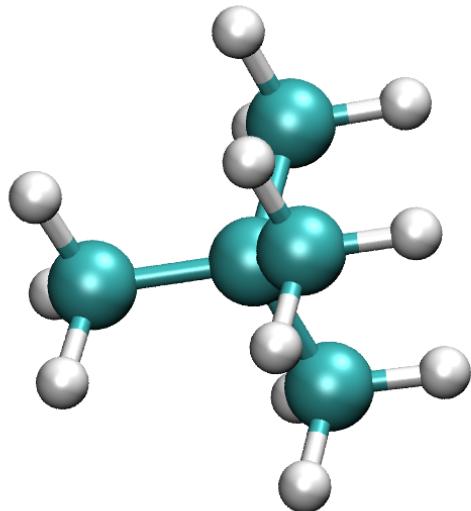


Different

NeoConformation Número 380

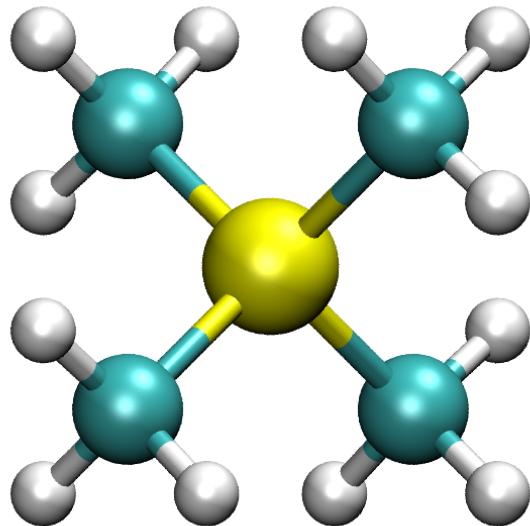
Molecule A

neopentane_out_G09_rot_x15-y15-z15



Molecule B

tetramethylsilane_out_G09

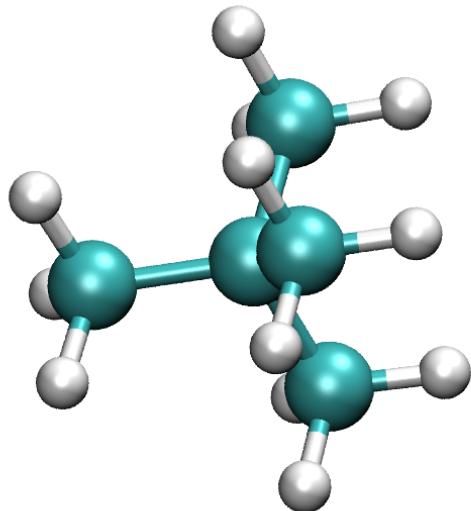


Different

NeoConformation Número 381

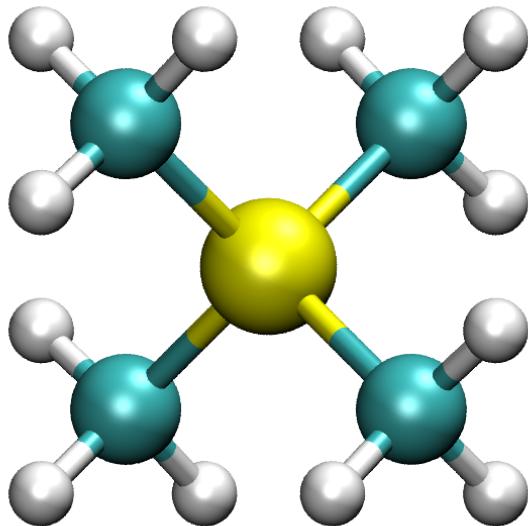
Molecule A

neopentane_out_G09_rot_x15-y15-z15



Molecule B

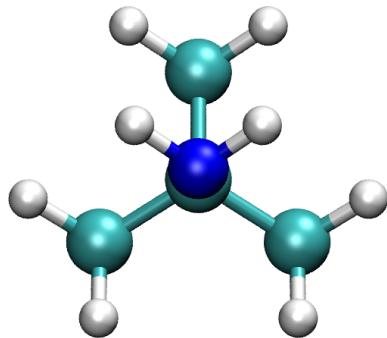
tetramethylsilane_out_G09_inversion



Different

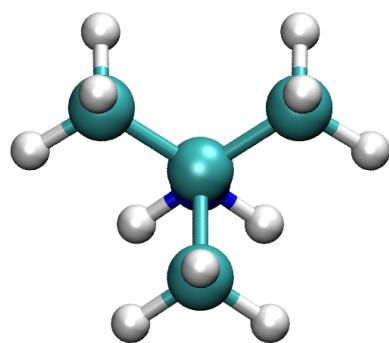
NeoConformation Número 382

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

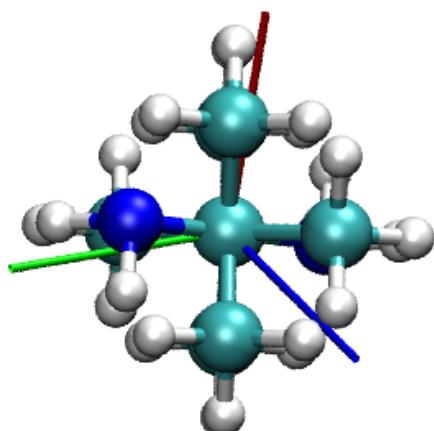
EingenValues - Molecule A

110.655	111.213	113.693
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EingenValues - Molecule B

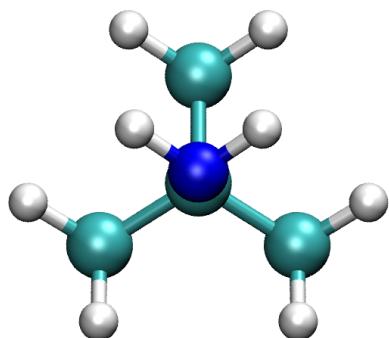
110.655	111.213	113.693
---------	---------	---------

Enantiomers



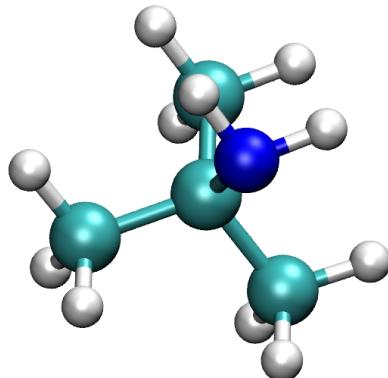
NeoConformation Número 383

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

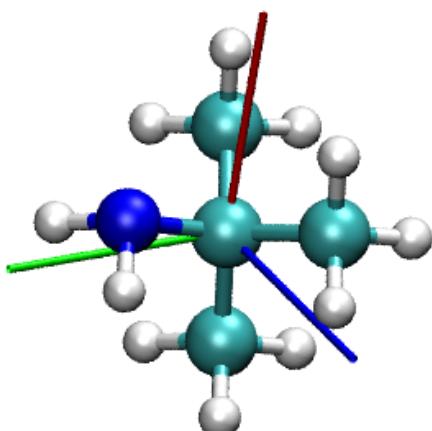
EingenValues - Molecule A

110.655	111.213	113.693
---------	---------	---------

EingenValues - Molecule B

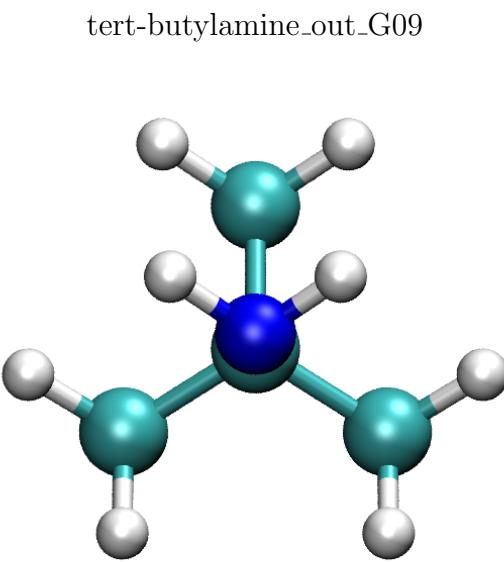
110.655	111.213	113.693
---------	---------	---------

Equal



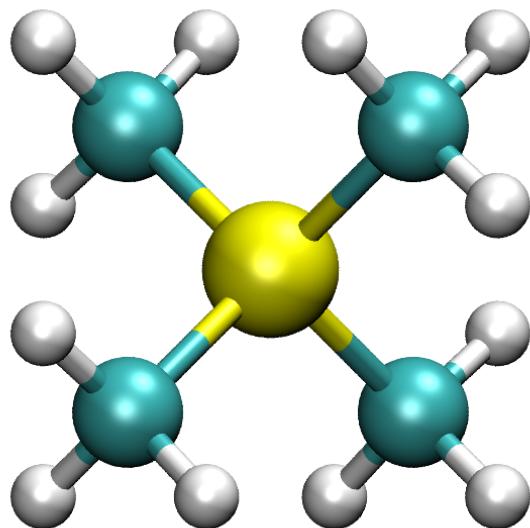
NeoConformation Número 384

Molecule A



Molecule B

tetramethylsilane_out_G09

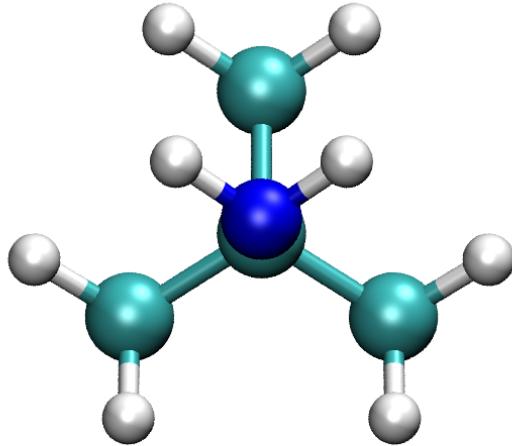


Different

NeoConformation Número 385

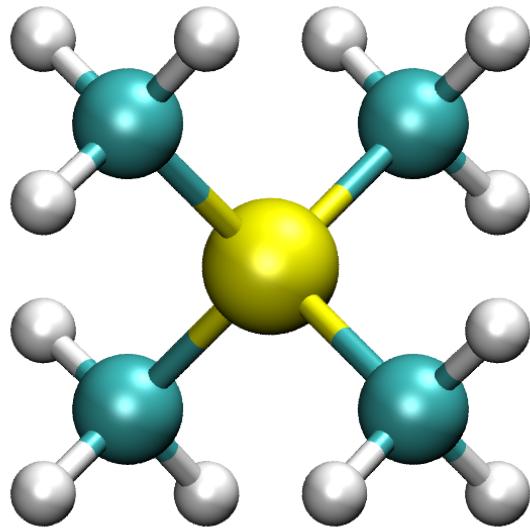
Molecule A

tert-butylamine_out_G09



Molecule B

tetramethylsilane_out_G09_inversion

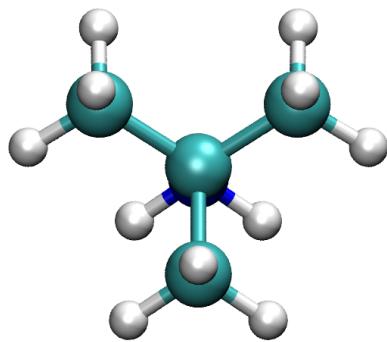


Different

NeoConformation Número 386

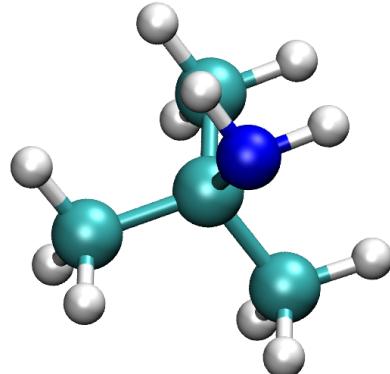
Molecule A

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

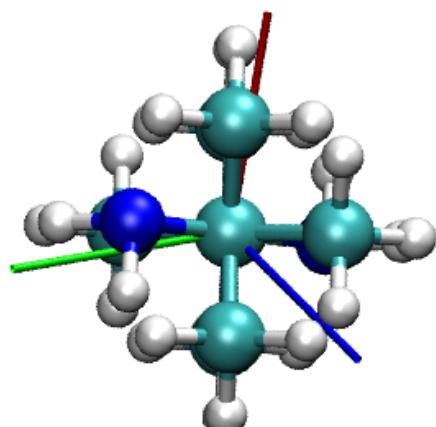
EingenValues - Molecule A

110.655	111.213	113.693
---------	---------	---------

EingenValues - Molecule B

110.655	111.213	113.693
---------	---------	---------

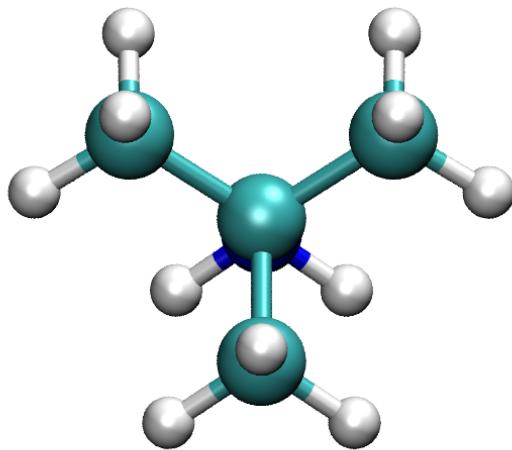
Enantiomers



NeoConformation Número 387

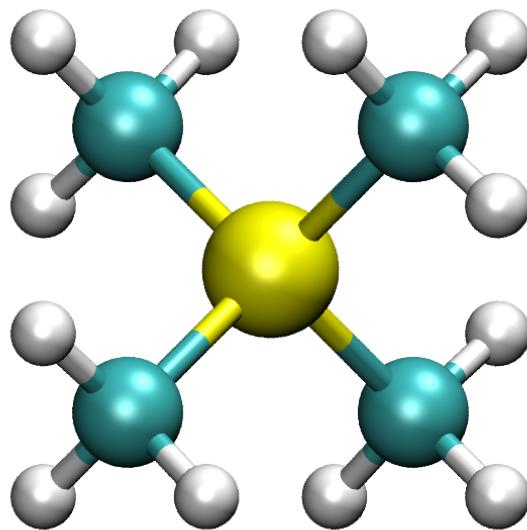
Molecule A

tert-butylamine_out_G09_inversion



Molecule B

tetramethylsilane_out_G09

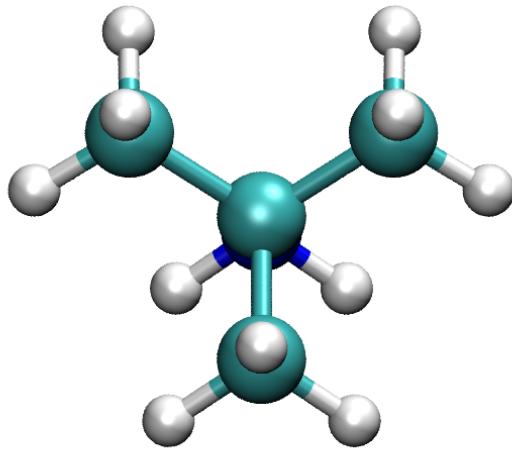


Different

NeoConformation Número 388

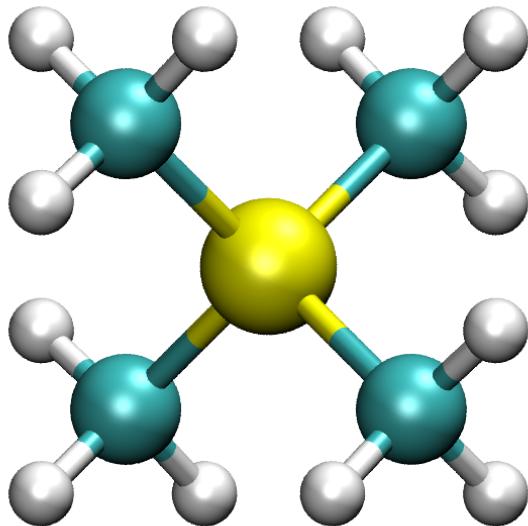
Molecule A

tert-butylamine_out_G09_inversion



Molecule B

tetramethylsilane_out_G09_inversion

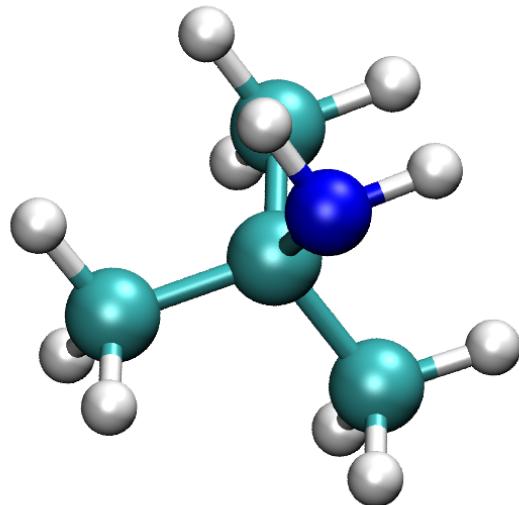


Different

NeoConformation Número 389

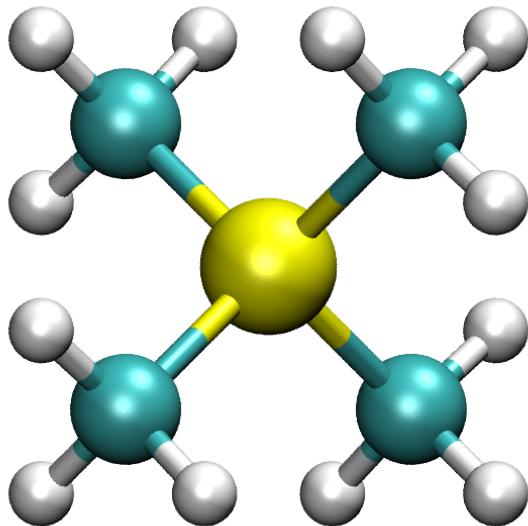
Molecule A

tert-butylamine_out_G09_rot_x15_y15_z15



Molecule B

tetramethylsilane_out_G09

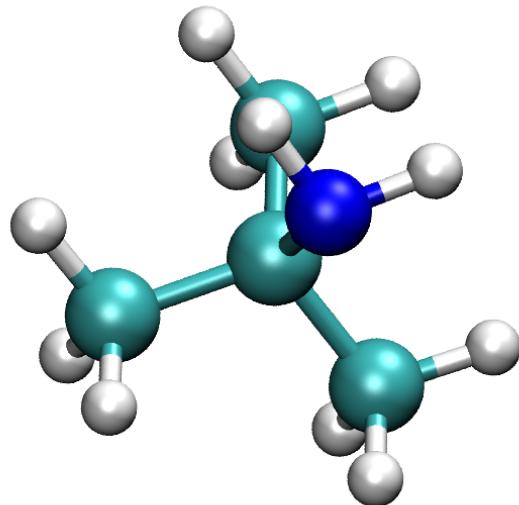


Different

NeoConformation Número 390

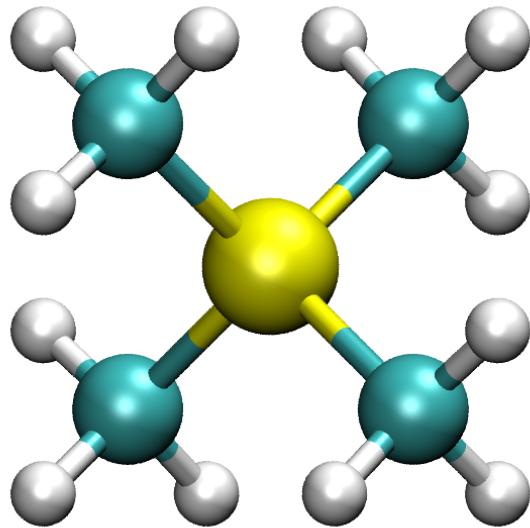
Molecule A

tert-butylamine_out_G09_rot_x15_y15_z15



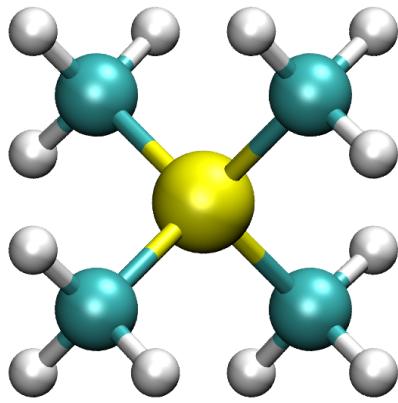
Molecule B

tetramethylsilane_out_G09_inversion



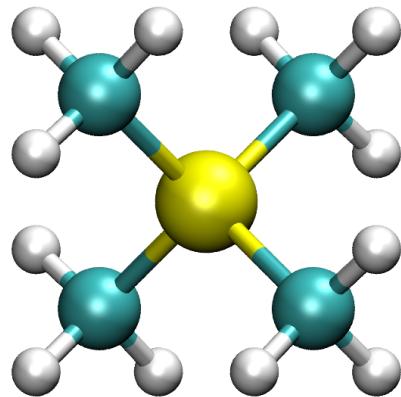
Different

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

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

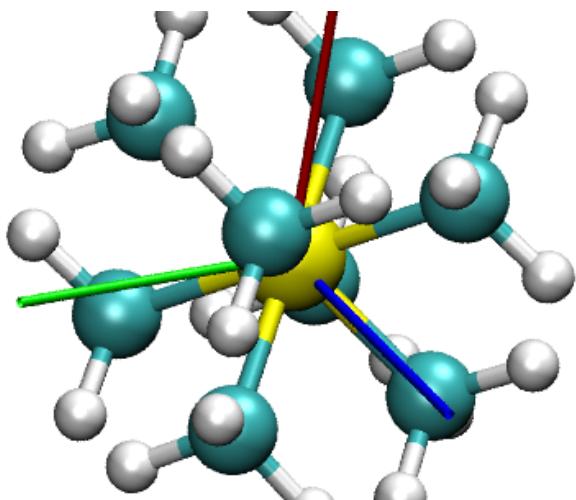
EingenValues - Molecule A

$$\begin{vmatrix} 166.054 & 166.054 & 166.054 \end{vmatrix}$$

EingenValues - Molecule B

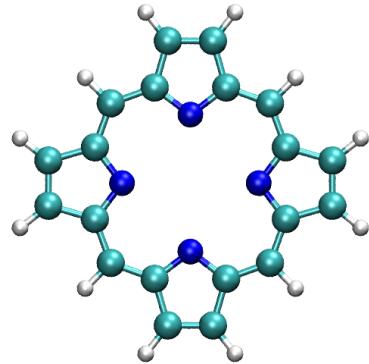
$$\begin{vmatrix} 166.053 & 166.053 & 166.053 \end{vmatrix}$$

Equal

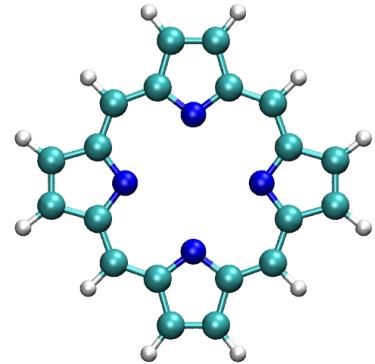


RotationSameMolecule Número 392

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

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

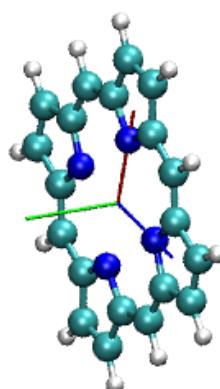
EingenValues - Molecule A

$$\begin{vmatrix} 1914.06 & 1914.06 & 3828.12 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 1914.06 & 1914.06 & 3828.12 \end{vmatrix}$$

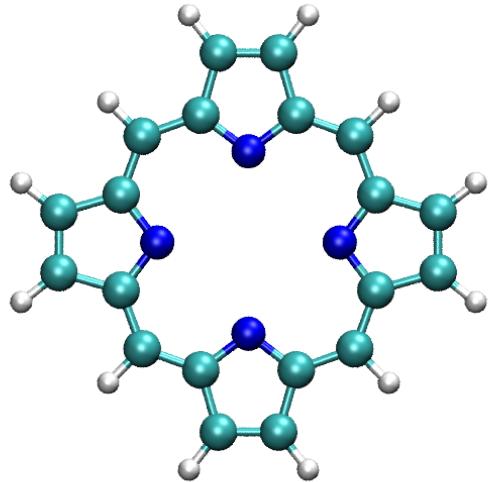
Equal



RotationSameMolecule Número 393

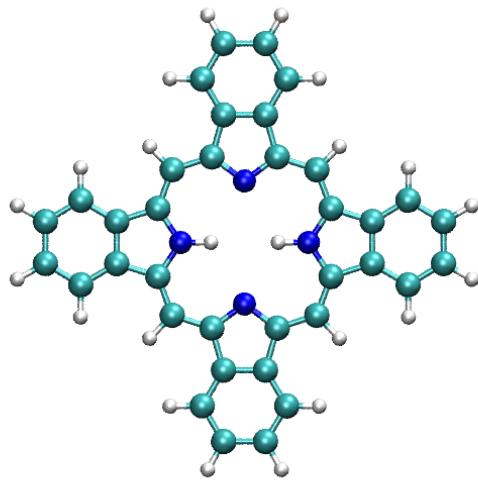
Molecule A

Porphin_out_G09



Molecule B

Tetrabenzoporphyrin_out_G09

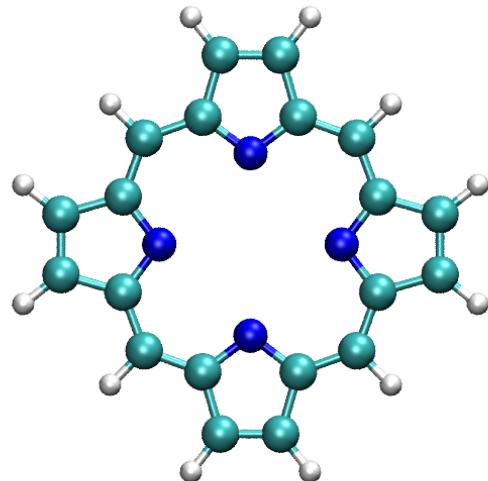


Different

RotationSameMolecule Número 394

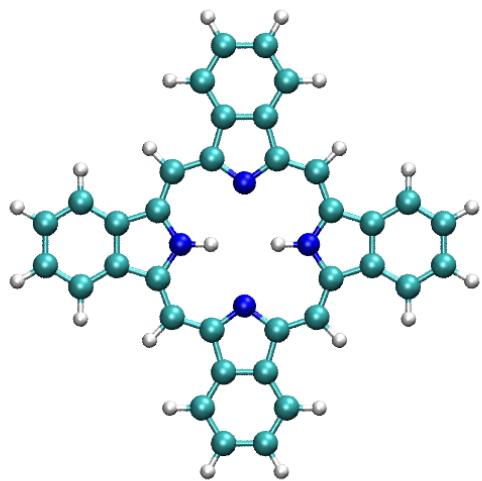
Molecule A

Porphin_out_G09



Molecule B

Tetrabenzoporphyrin_out_G09_inversion

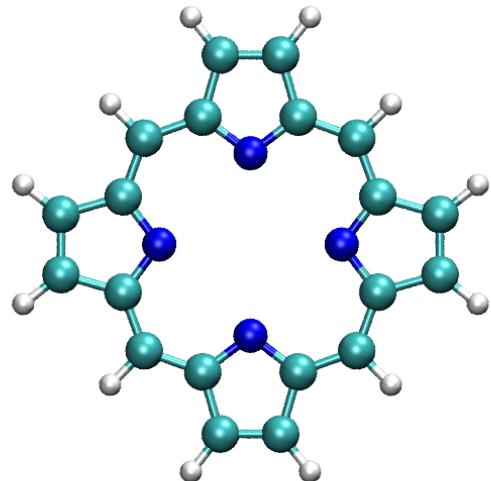


Different

RotationSameMolecule Número 395

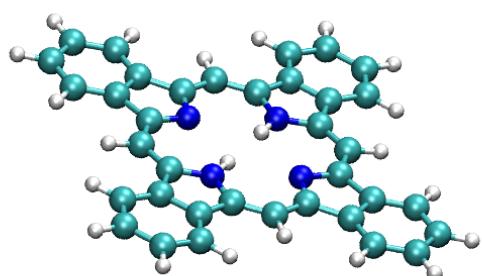
Molecule A

Porphin_out_G09



Molecule B

Tetrabenzoporphyrin_rotated02_out_G09

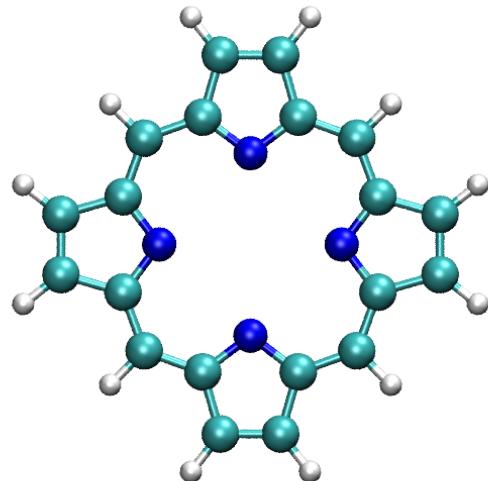


Different

RotationSameMolecule Número 396

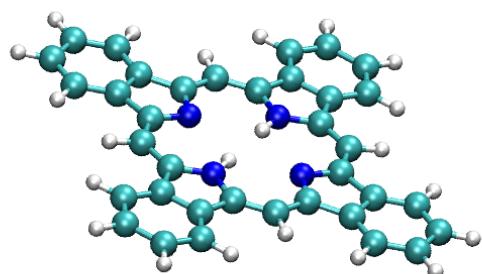
Molecule A

Porphin_out_G09



Molecule B

Tetrabenzoporphyrin_rotated02_out_G09_inversion

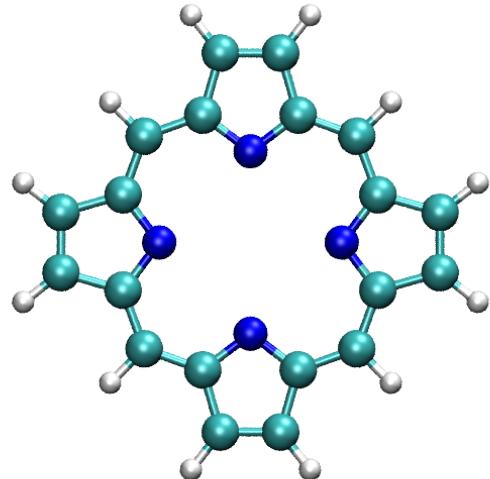


Different

RotationSameMolecule Número 397

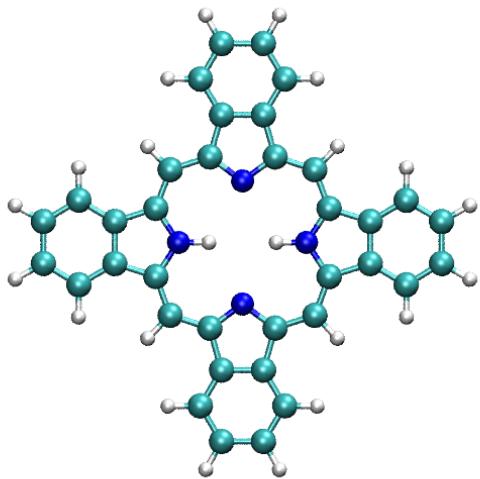
Molecule A

Porphin_out_G09



Molecule B

Tetrabenzoporphyrin_rotated_out_G09

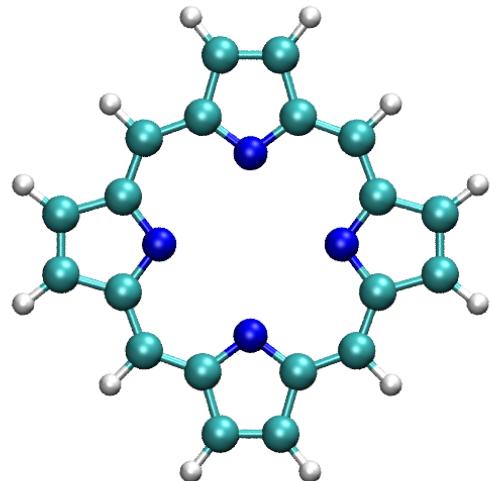


Different

RotationSameMolecule Número 398

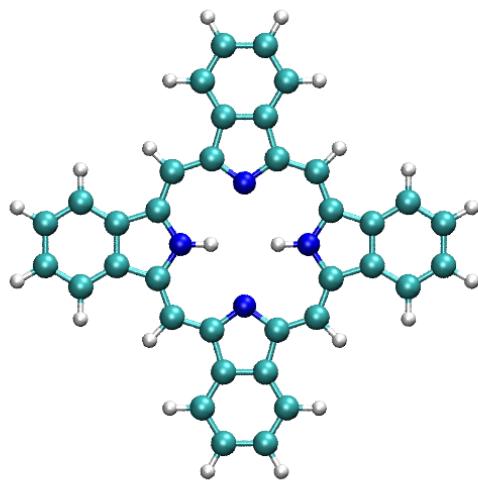
Molecule A

Porphin_out_G09



Molecule B

Tetrabenzoporphyrin_rotated_out_G09_inversion

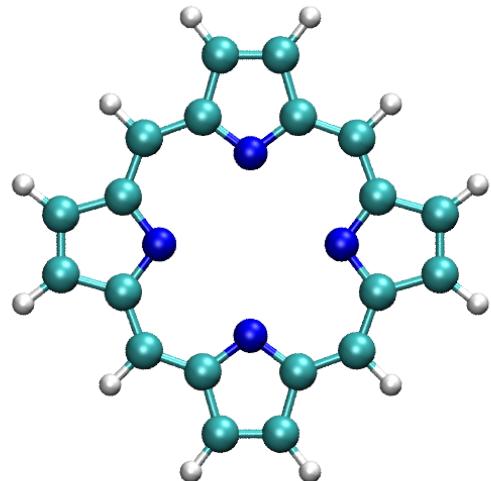


Different

RotationSameMolecule Número 399

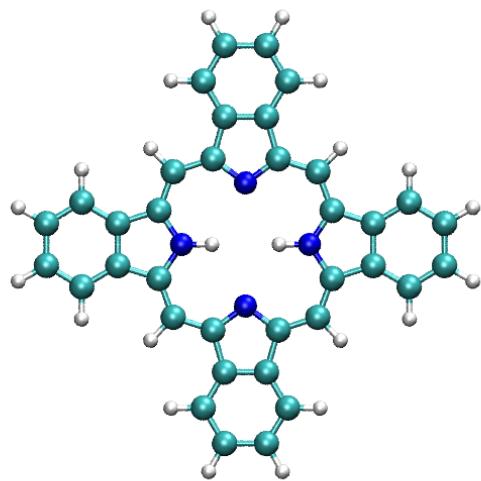
Molecule A

Porphin_out_G09_inversion



Molecule B

Tetrabenzoporphyrin_out_G09

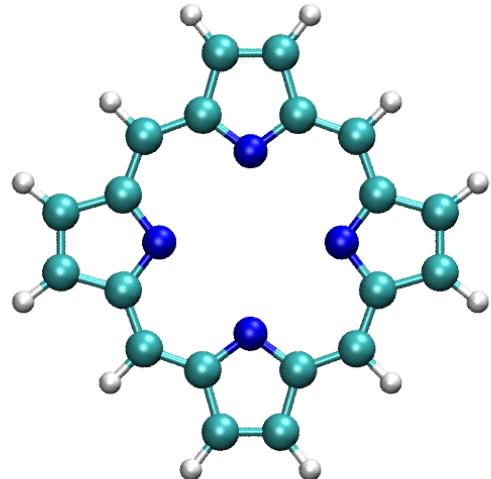


Different

RotationSameMolecule Número 400

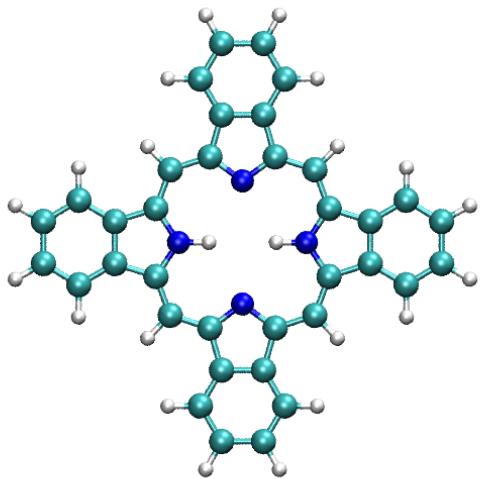
Molecule A

Porphin_out_G09_inversion



Molecule B

Tetrabenzoporphyrin_out_G09_inversion

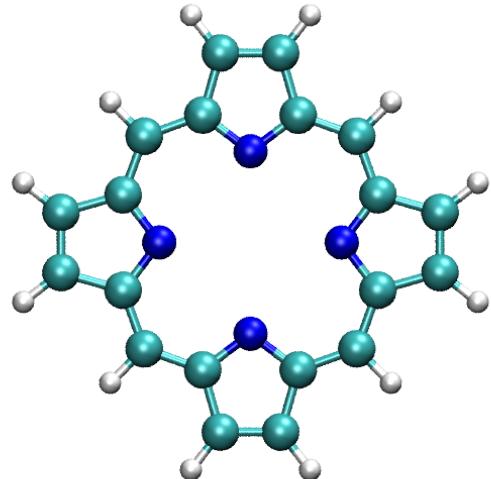


Different

RotationSameMolecule Número 401

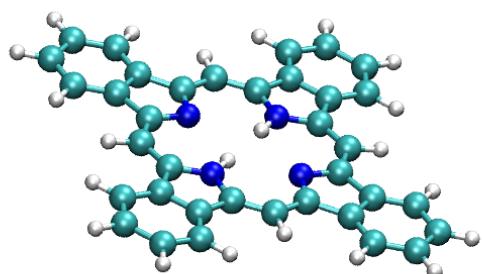
Molecule A

Porphin_out_G09_inversion



Molecule B

Tetrabenzoporphyrin_rotated02_out_G09

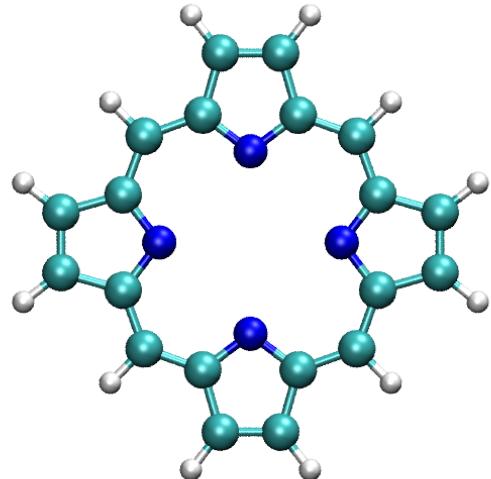


Different

RotationSameMolecule Número 402

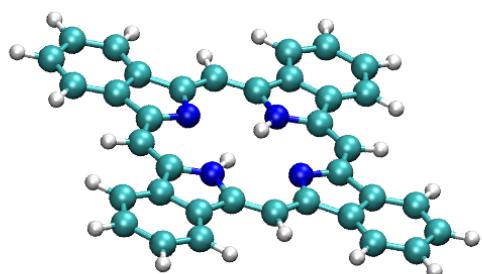
Molecule A

Porphin_out_G09_inversion



Molecule B

Tetrabenzoporphyrin_rotated02_out_G09_inversion

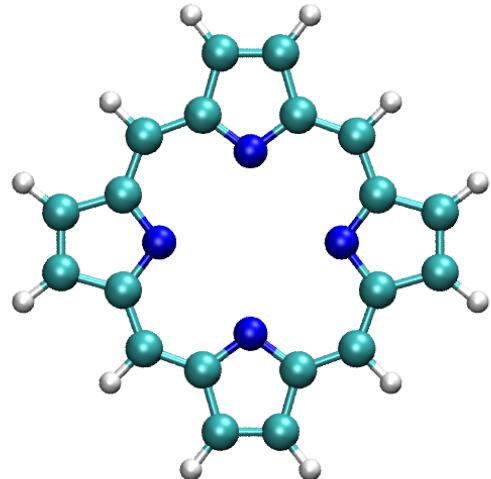


Different

RotationSameMolecule Número 403

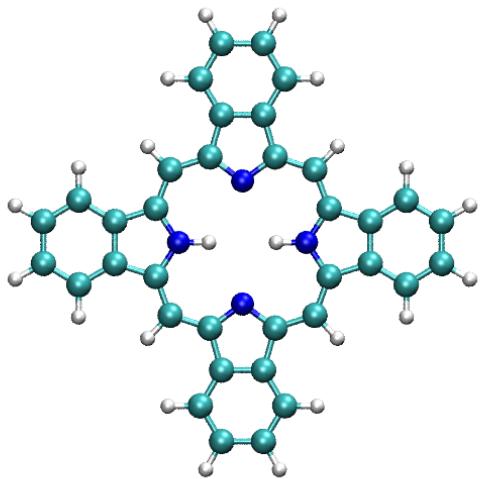
Molecule A

Porphin_out_G09_inversion



Molecule B

Tetrabenzoporphyrin_rotated_out_G09

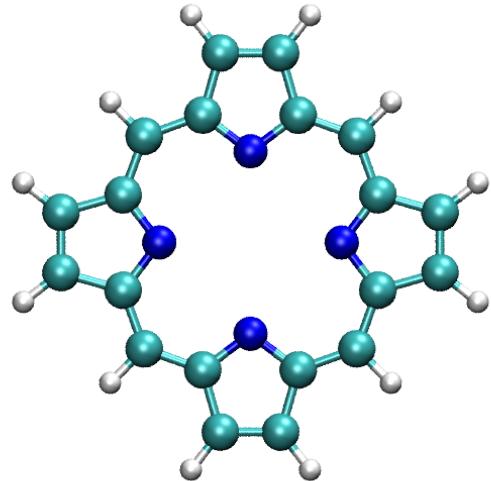


Different

RotationSameMolecule Número 404

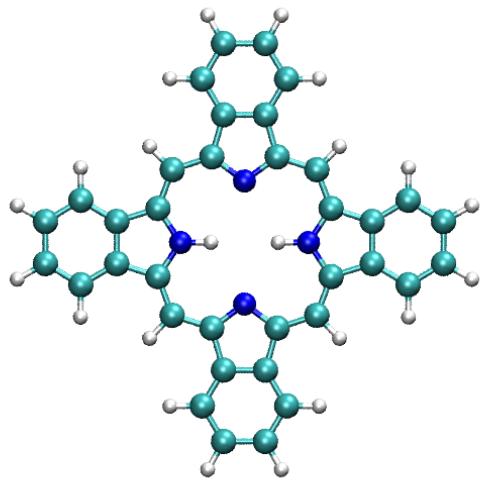
Molecule A

Porphin_out_G09_inversion



Molecule B

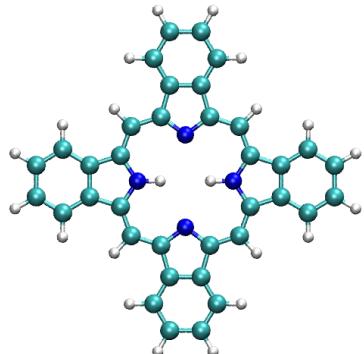
Tetrabenzoporphyrin_rotated_out_G09_inversion



Different

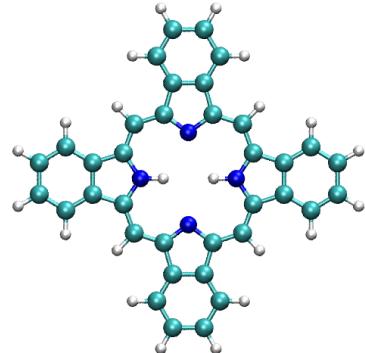
RotationSameMolecule Número 405

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

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

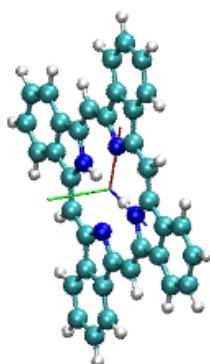
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

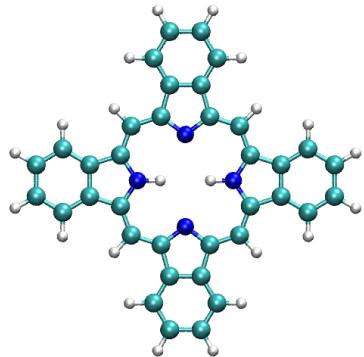
$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Equal



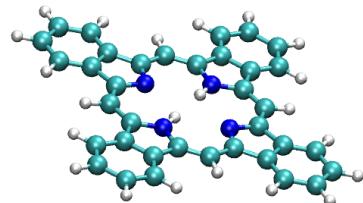
RotationSameMolecule Número 406

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

$$\begin{vmatrix} -0.771476 & 0.397136 & -0.497099 \\ 0.301236 & -0.460189 & -0.835154 \\ -0.56043 & -0.794046 & 0.235394 \end{vmatrix}$$

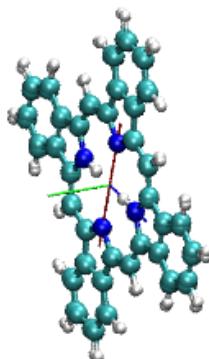
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

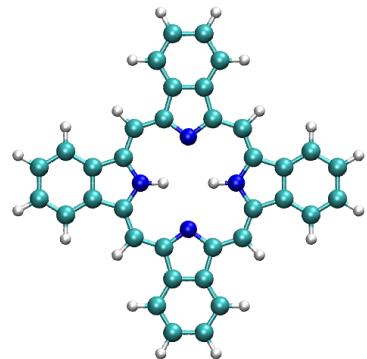
EingenValues - Molecule B

$$\begin{vmatrix} 5923.93 & 5941.33 & 11865.3 \end{vmatrix}$$

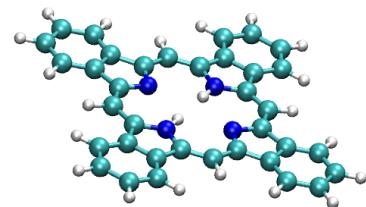
Enantiomers



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

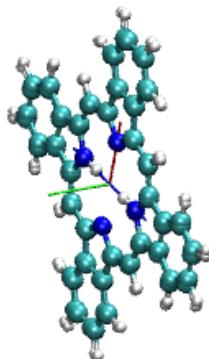
EingenValues - Molecule A

5922.88	5941.95	11864.8
---------	---------	---------

EingenValues - Molecule B

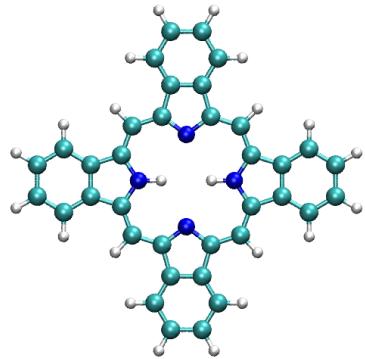
5923.93	5941.33	11865.3
---------	---------	---------

Enantiomers



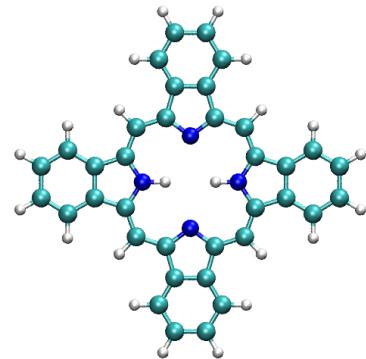
RotationSameMolecule Número 408

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

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

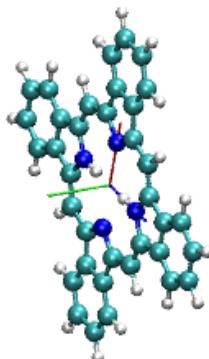
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

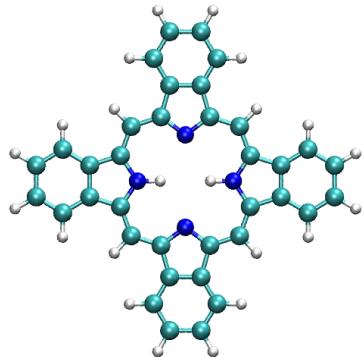
$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Equal

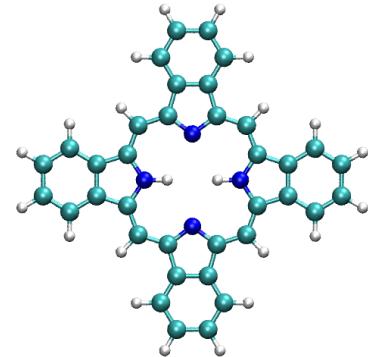


RotationSameMolecule Número 409

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

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

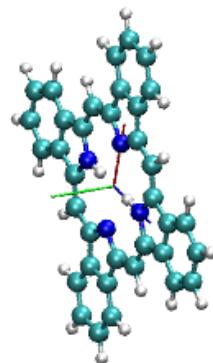
EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

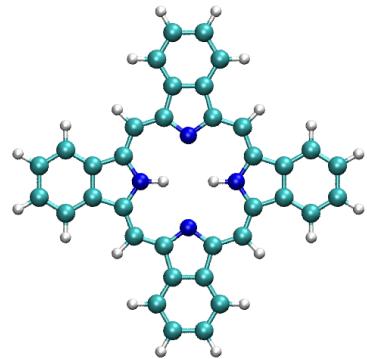
Equal



RotationSameMolecule Número 410

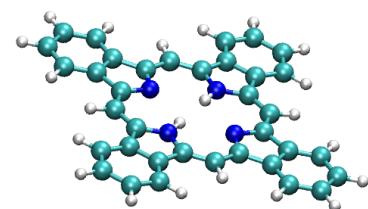
Molecule A

Tetrabenzoporphyrin.out.G09.inversion



Molecule B

Tetrabenzoporphyrin_rotated02.out.G09



Inertia Tensor - Molecule A

11864.8	0	0
0	5941.95	0
0	0	5922.88

Inertia Tensor - Molecule B

7791.57	2641.52	-788.168
2641.52	9673.67	-1103.82
-788.168	-1103.82	6265.27

EingenVectors - Molecule A

0	0	1
0	1	0
1	0	0

EingenVectors - Molecule B

-0.771476	0.397136	-0.497099
0.301236	-0.460189	-0.835154
-0.56043	-0.794046	0.235394

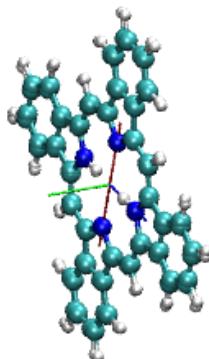
EingenValues - Molecule A

5922.88	5941.95	11864.8
---------	---------	---------

EingenValues - Molecule B

5923.93	5941.33	11865.3
---------	---------	---------

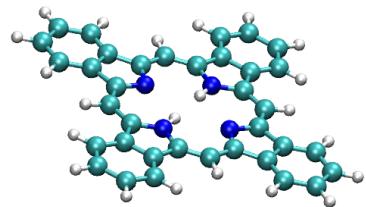
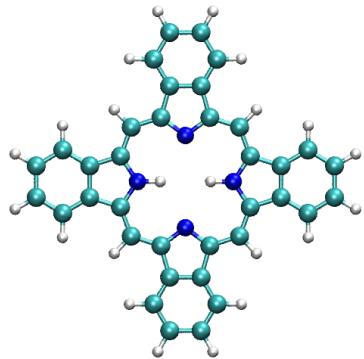
Enantiomers



RotationSameMolecule Número 411

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

$$\begin{vmatrix} -0.771478 & 0.39714 & -0.497093 \\ 0.30123 & -0.460186 & -0.835158 \\ -0.56043 & -0.794046 & 0.235393 \end{vmatrix}$$

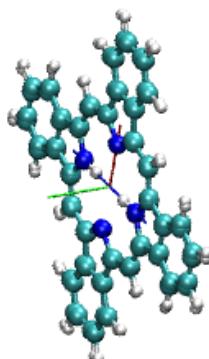
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

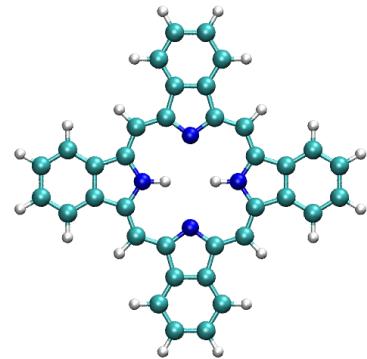
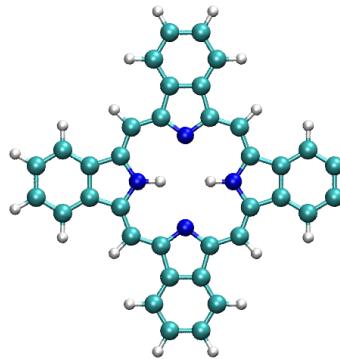
$$\begin{vmatrix} 5923.93 & 5941.33 & 11865.3 \end{vmatrix}$$

Enantiomers



RotationSameMolecule Número 412

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

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

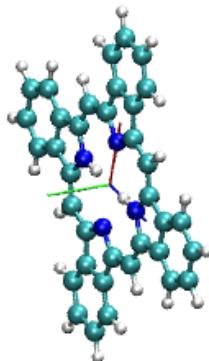
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

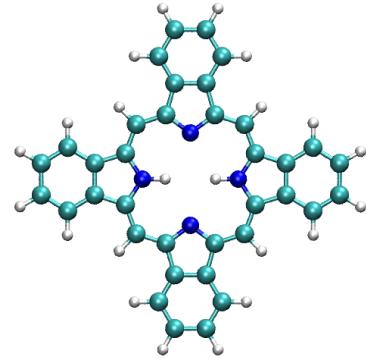
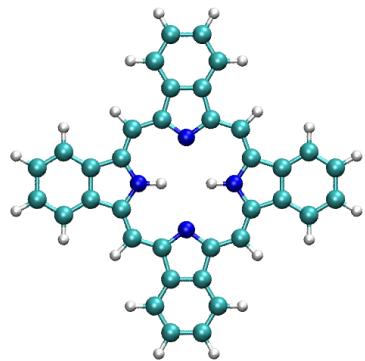
Equal



RotationSameMolecule Número 413

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

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

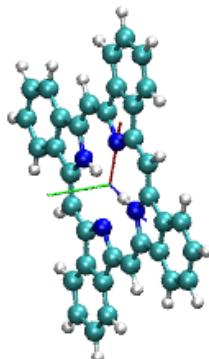
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

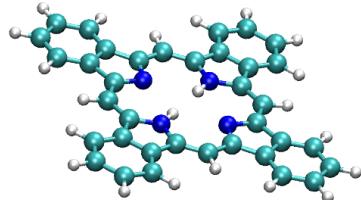
$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Equal

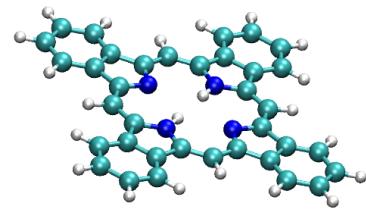


RotationSameMolecule Número 414

Molecule A
Tetrabenzoporphyrin_rotated02_out_G09



Molecule B Tetrabenzoporphyrin_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

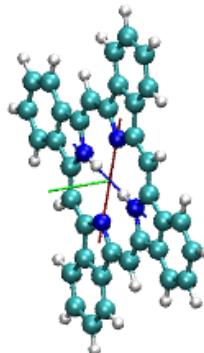
EingenValues - Molecule A

5923.93	5941.33	11865.3
---------	---------	---------

EingenValues - Molecule B

5923.93	5941.33	11865.3
---------	---------	---------

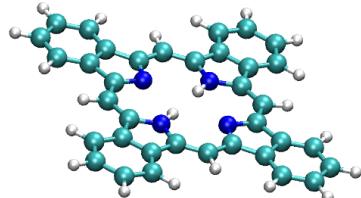
Equal



RotationSameMolecule Número 415

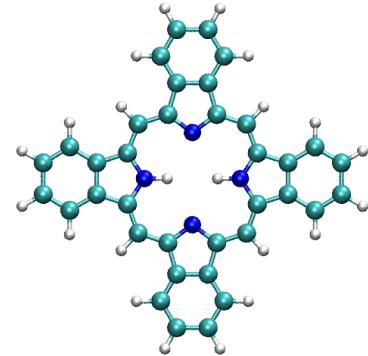
Molecule A

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

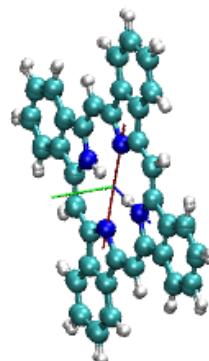
EigenValues - Molecule A

5923.93	5941.33	11865.3
---------	---------	---------

EigenValues - Molecule B

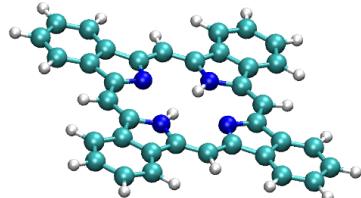
5922.88	5941.95	11864.8
---------	---------	---------

Enantiomers

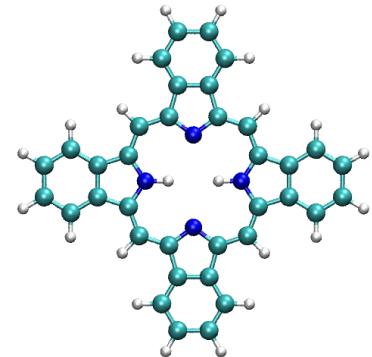


RotationSameMolecule Número 416

Molecule A
Tetrabenzoporphyrin_rotated02_out_G09



Molecule B Tetrabenzoporphyrin_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

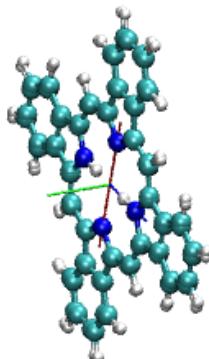
EingenVectors - Molecule A		
-0.771476	0.397136	-0.497099
0.301236	-0.460189	-0.835154
-0.56043	-0.794046	0.235394

EingenVectors - Molecule B		
0	0	1
0	1	0
1	0	0

EingenValues - Molecule A		
5923.93	5941.33	11865.3

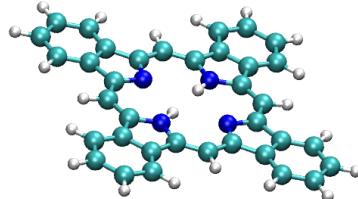
EingenValues - Molecule B		
5922.88	5941.95	11864.8

Enantiomers

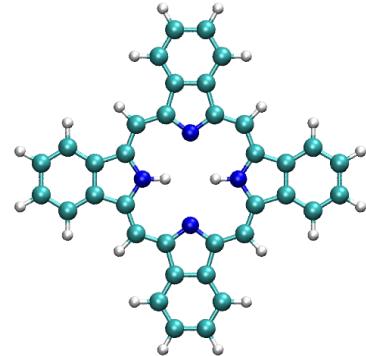


RotationSameMolecule Número 417

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

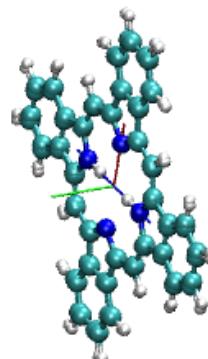
EigenValues - Molecule A

5923.93	5941.33	11865.3
---------	---------	---------

EigenValues - Molecule B

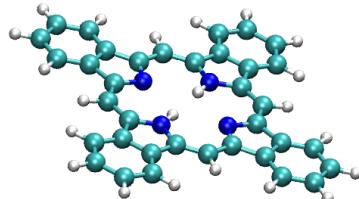
5922.88	5941.95	11864.8
---------	---------	---------

Enantiomers

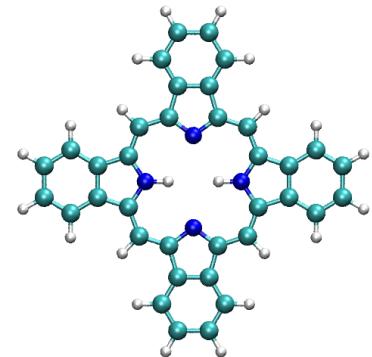


RotationSameMolecule Número 418

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

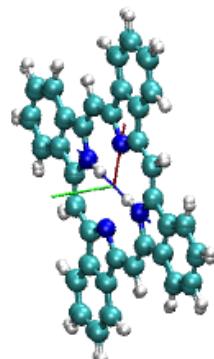
EingenValues - Molecule A

5923.93	5941.33	11865.3
---------	---------	---------

EingenValues - Molecule B

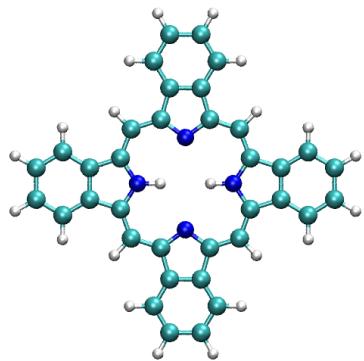
5922.88	5941.95	11864.8
---------	---------	---------

Enantiomers

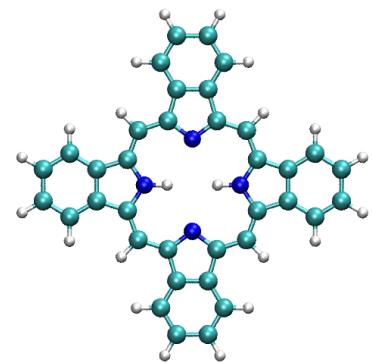


RotationSameMolecule Número 419

Molecule A
Tetrabenzoporphyrin_rotated_out_G09



Molecule B Tetrabenzoporphyrin_rotated_out_G09_inversion



Inertia Tensor - Molecule A

$$\begin{vmatrix} 11864.8 & 0 & 0 \\ 0 & 5941.95 & 0 \\ 0 & 0 & 5922.88 \end{vmatrix}$$

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

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

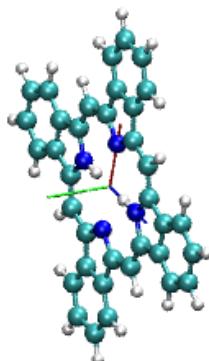
EingenValues - Molecule A

$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

EingenValues - Molecule B

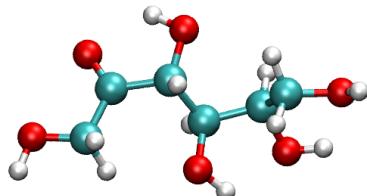
$$\begin{vmatrix} 5922.88 & 5941.95 & 11864.8 \end{vmatrix}$$

Equal

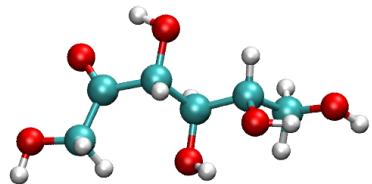


Sugars Número 420

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

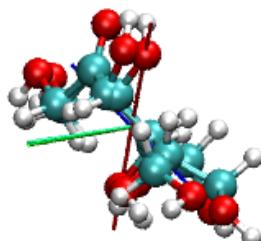
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

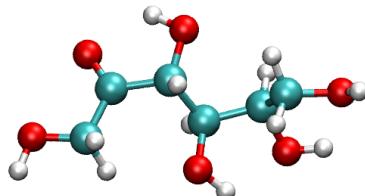
257.858	1154.77	1276.75
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Different

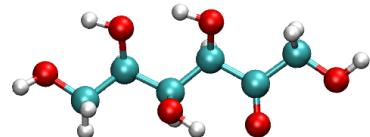


Sugars Número 421

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

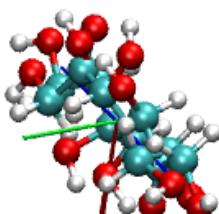
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

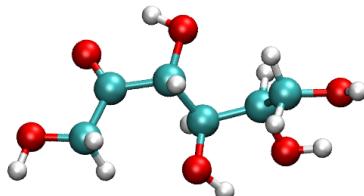
203.032	1215.85	1332.21
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Different

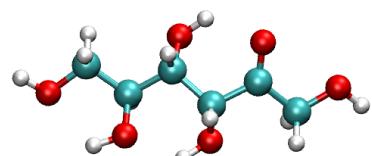


Sugars Número 422

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

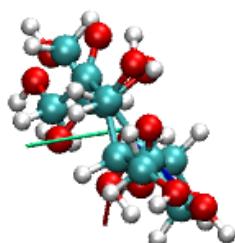
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

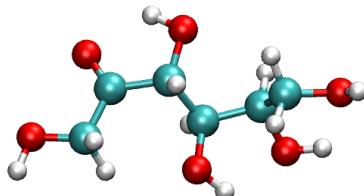
214.698	1187.04	1322.41
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Different

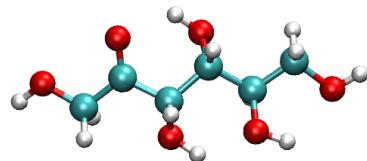


Sugars Número 423

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

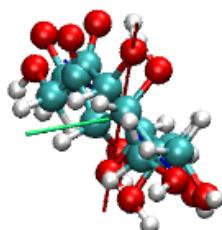
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

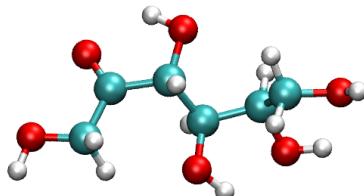
214.739	1186.84	1322.13
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Different

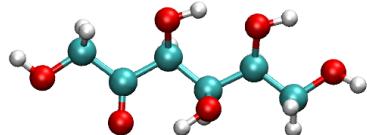


Sugars Número 424

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

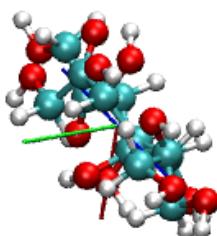
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

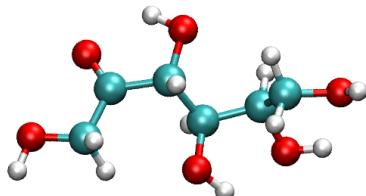
203.048	1215.85	1332.24
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Different

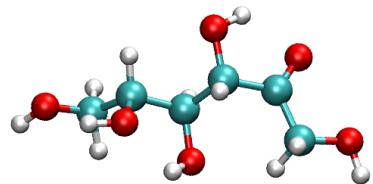


Sugars Número 425

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

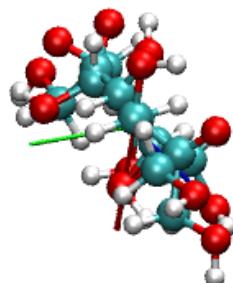
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

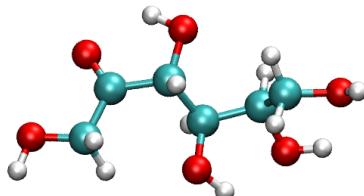
257.845	1154.78	1276.78
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Different

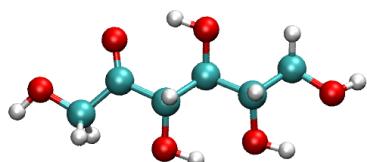


Sugars Número 426

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

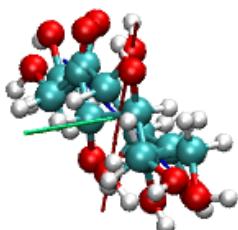
EingenValues - Molecule A

270.084	1104.35	1244.51
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EingenValues - Molecule B

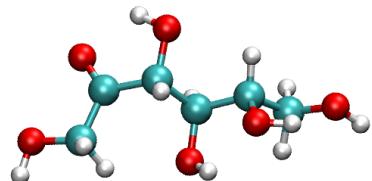
224.041	1180.31	1363.9
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Different

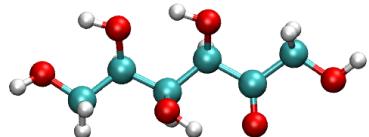


Sugars Número 427

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

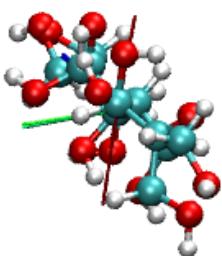
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

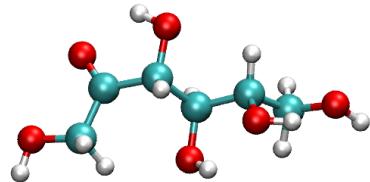
203.032	1215.85	1332.21
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Different

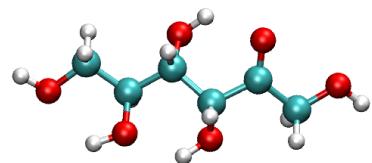


Sugars Número 428

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

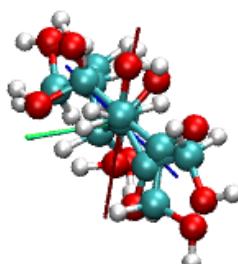
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

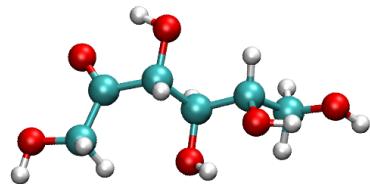
214.698	1187.04	1322.41
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Different

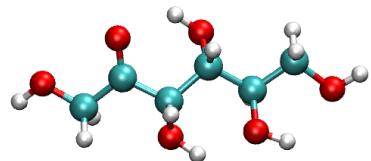


Sugars Número 429

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

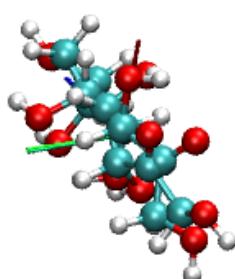
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

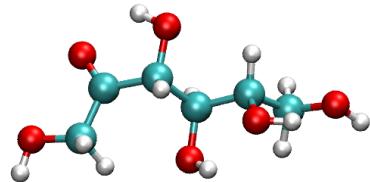
214.739	1186.84	1322.13
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Different

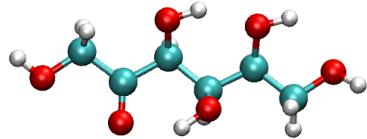


Sugars Número 430

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

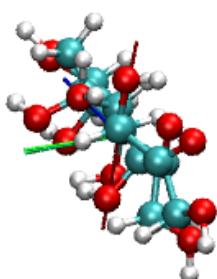
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

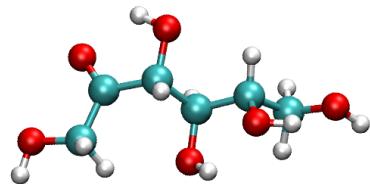
203.048	1215.85	1332.24
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Different

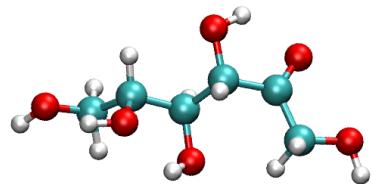


Sugars Número 431

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

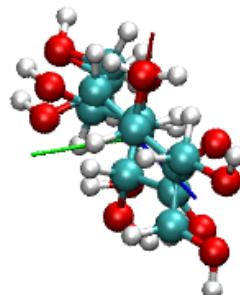
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

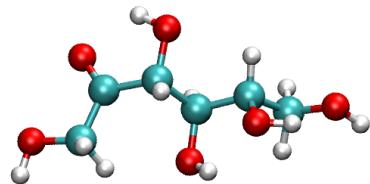
257.845	1154.78	1276.78
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Enantiomers

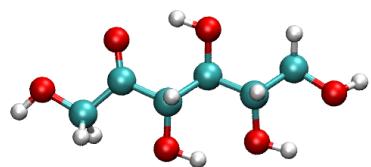


Sugars Número 432

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

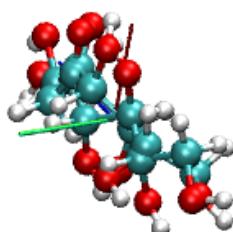
EingenValues - Molecule A

257.858	1154.77	1276.75
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EingenValues - Molecule B

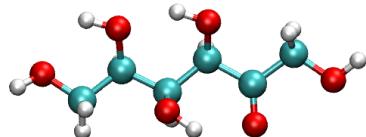
224.041	1180.31	1363.9
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Different

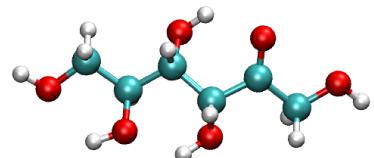


Sugars Número 433

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

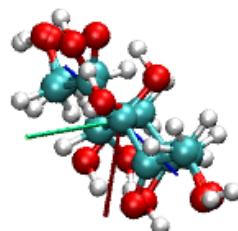
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

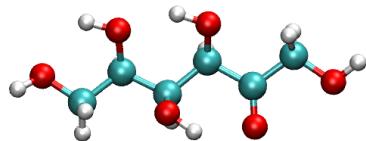
214.698	1187.04	1322.41
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Different

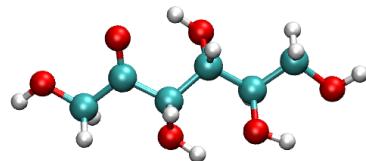


Sugars Número 434

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

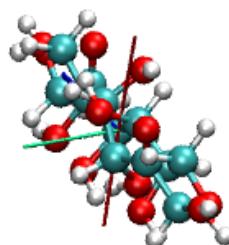
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

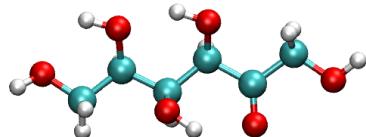
214.739	1186.84	1322.13
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Different

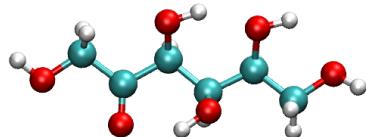


Sugars Número 435

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

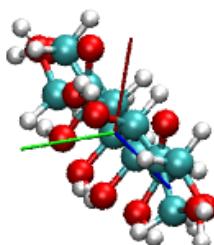
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

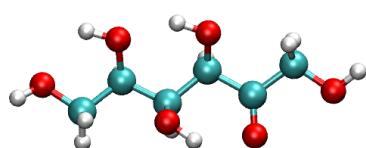
203.048	1215.85	1332.24
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Enantiomers

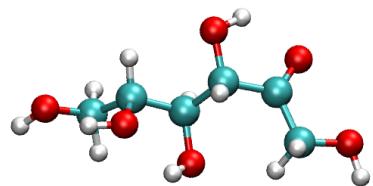


Sugars Número 436

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

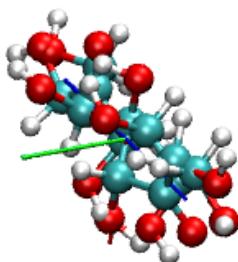
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

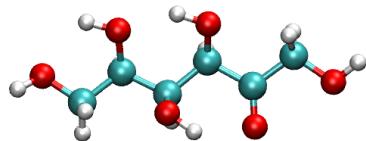
257.845	1154.78	1276.78
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Different

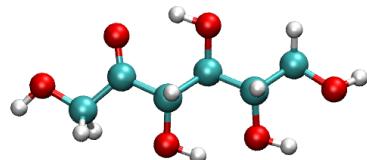


Sugars Número 437

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

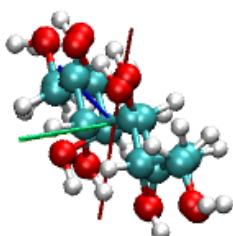
EingenValues - Molecule A

203.032	1215.85	1332.21
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EingenValues - Molecule B

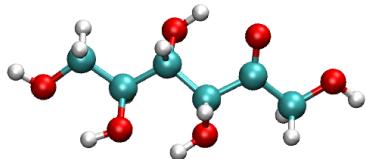
224.041	1180.31	1363.9
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Different

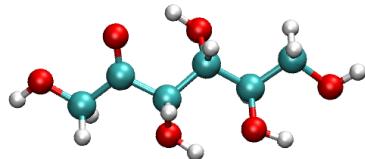


Sugars Número 438

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

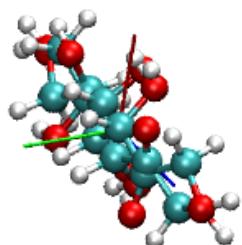
EingenValues - Molecule A

214.698	1187.04	1322.41
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EingenValues - Molecule B

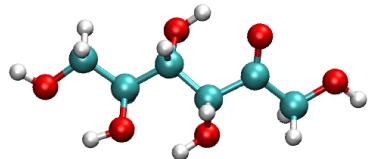
214.739	1186.84	1322.13
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Enantiomers

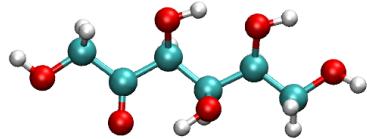


Sugars Número 439

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

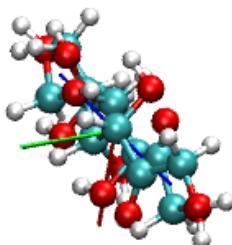
EingenValues - Molecule A

214.698	1187.04	1322.41
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EingenValues - Molecule B

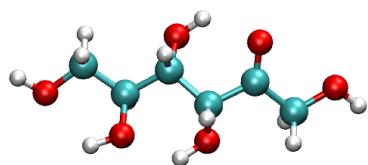
203.048	1215.85	1332.24
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Different

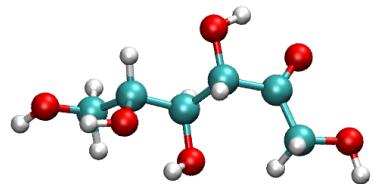


Sugars Número 440

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

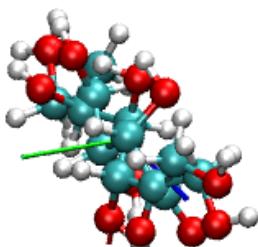
EingenValues - Molecule A

214.698	1187.04	1322.41
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EingenValues - Molecule B

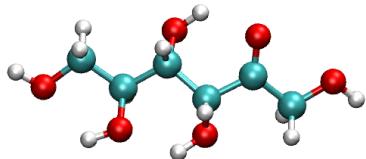
257.845	1154.78	1276.78
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Different

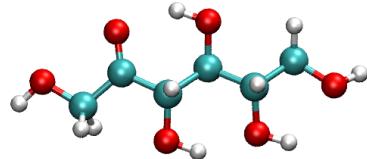


Sugars Número 441

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

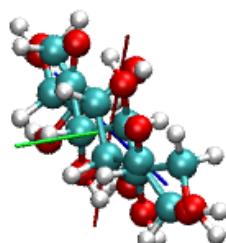
EingenValues - Molecule A

214.698	1187.04	1322.41
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EingenValues - Molecule B

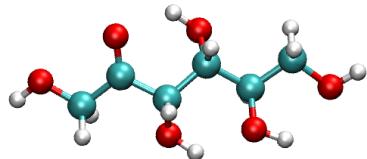
224.041	1180.31	1363.9
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Different

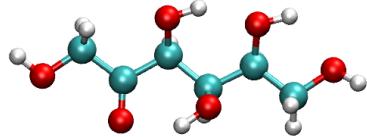


Sugars Número 442

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

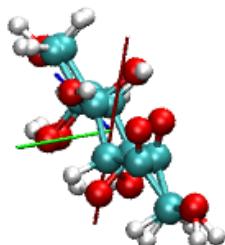
EingenValues - Molecule A

214.739	1186.84	1322.13
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EingenValues - Molecule B

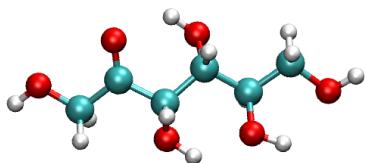
203.048	1215.85	1332.24
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Different

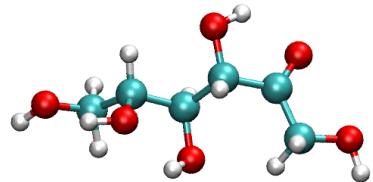


Sugars Número 443

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

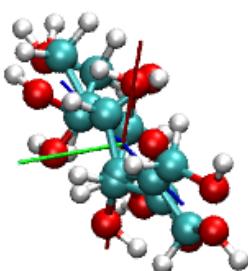
EingenValues - Molecule A

214.739	1186.84	1322.13
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EingenValues - Molecule B

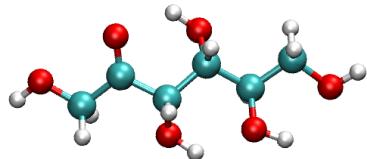
257.845	1154.78	1276.78
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Different

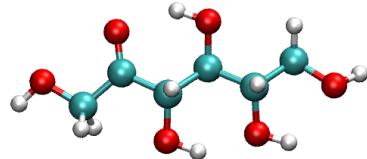


Sugars Número 444

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

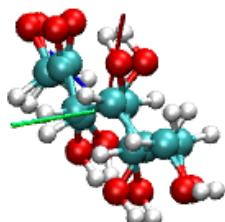
EingenValues - Molecule A

214.739	1186.84	1322.13
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EingenValues - Molecule B

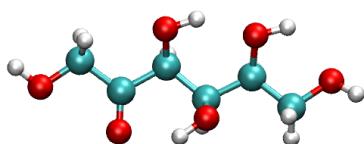
224.041	1180.31	1363.9
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Different

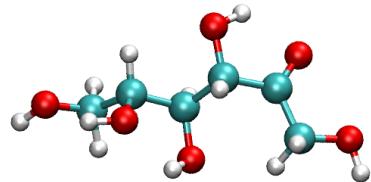


Sugars Número 445

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

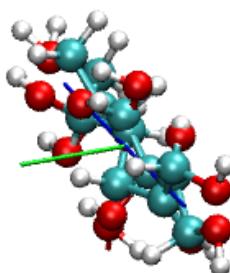
EingenValues - Molecule A

203.048	1215.85	1332.24
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EingenValues - Molecule B

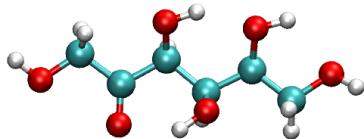
257.845	1154.78	1276.78
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Different

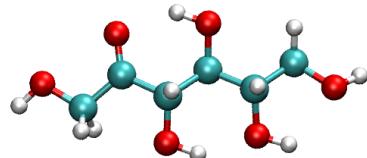


Sugars Número 446

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

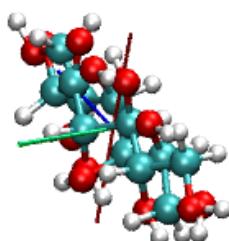
EingenValues - Molecule A

203.048	1215.85	1332.24
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EingenValues - Molecule B

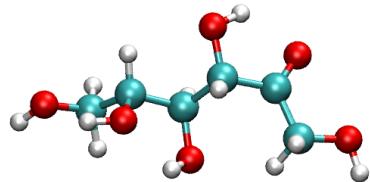
224.041	1180.31	1363.9
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Different

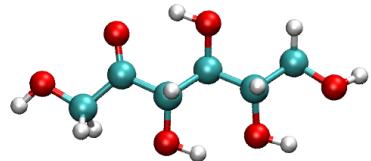


Sugars Número 447

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

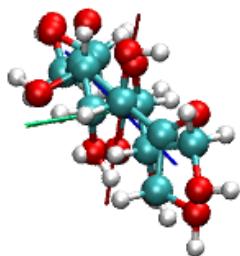
EingenValues - Molecule A

257.845	1154.78	1276.78
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EingenValues - Molecule B

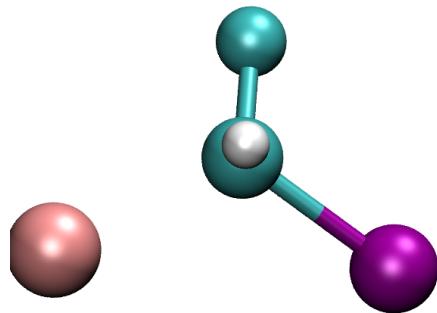
224.041	1180.31	1363.9
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Different



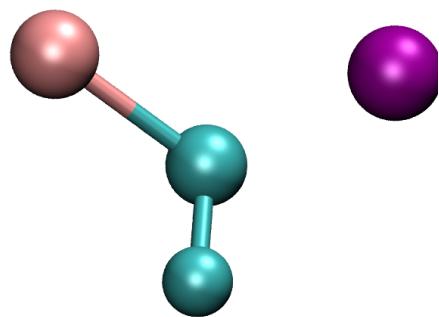
SymmetricEnantiomers Número 448

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

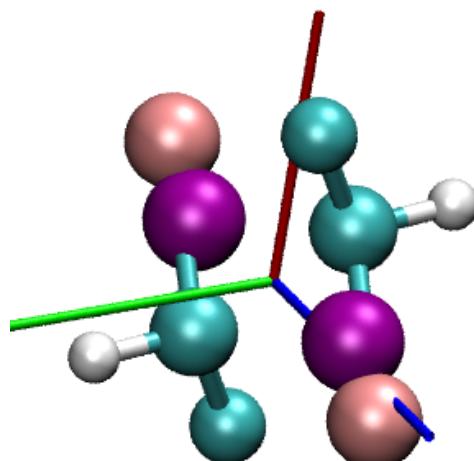
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

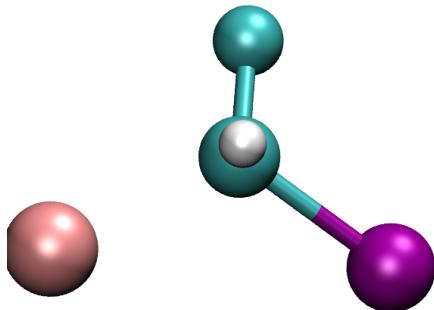
103.739	629.815	722.22
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Enantiomers

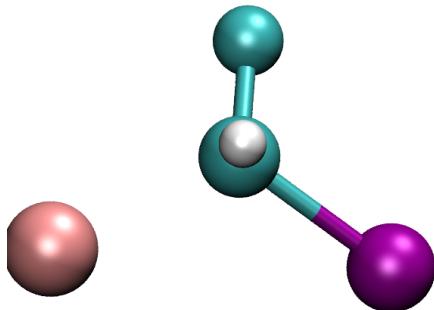


SymmetricEnantiomers Número 449

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

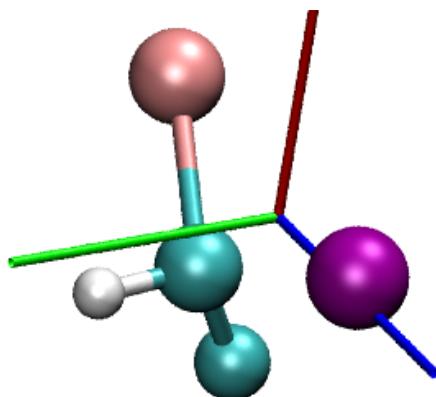
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

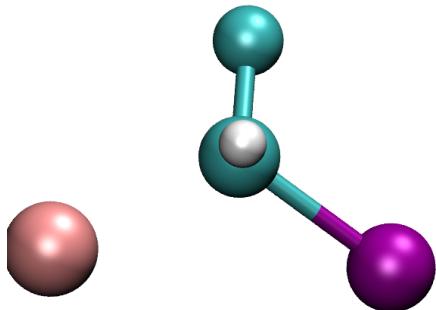
103.739	629.816	722.221
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Equal

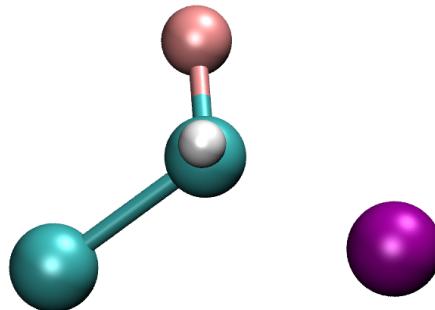


SymmetricEnantiomers Número 450

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

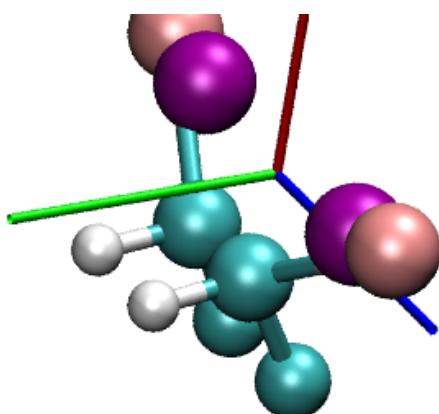
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

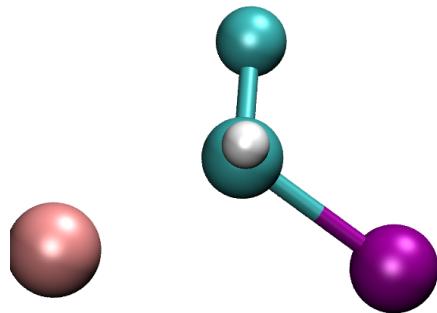
103.701	630.077	722.452
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Enantiomers



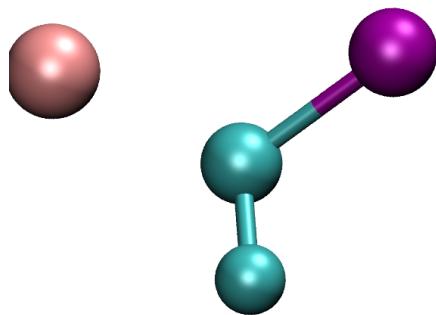
SymmetricEnantiomers Número 451

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

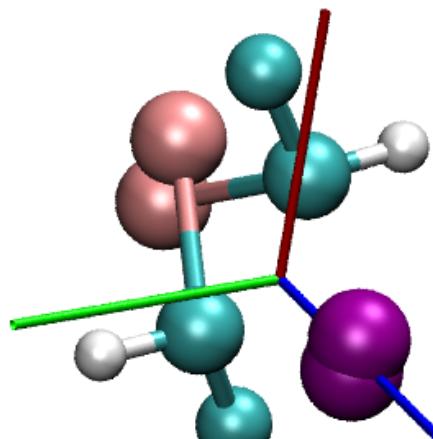
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

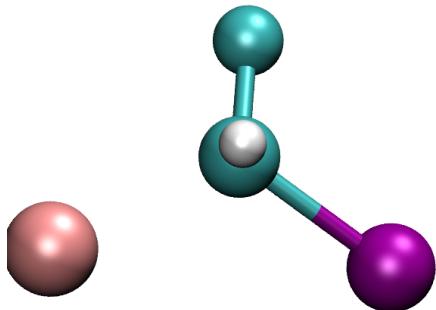
103.7	630.079	722.455
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Equal

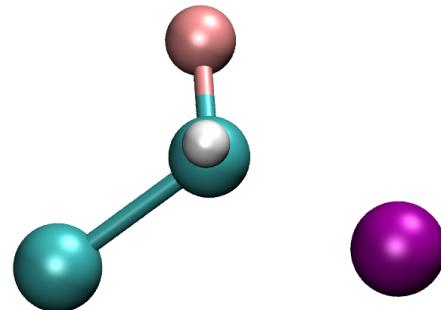


SymmetricEnantiomers Número 452

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

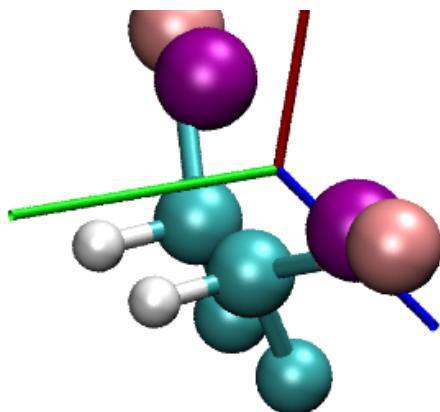
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

103.701	630.077	722.452
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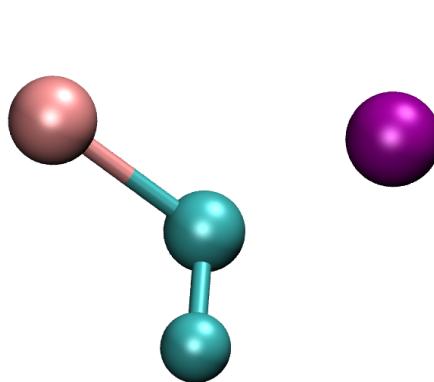
Enantiomers



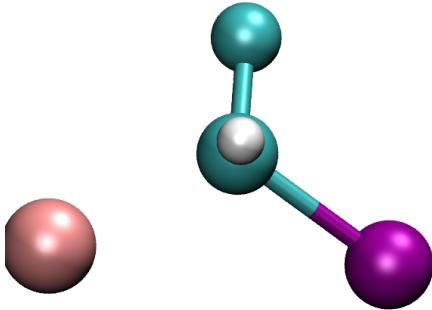
SymmetricEnantiomers Número 453

Molecule A

r-enan_out_G09_inversion_output



Molecule B r-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

Metric	Tensor	Microcar B
103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

EigenVectors - Molecule A

```

Eigenvectors - Molecule 1
-0.999994  0.00286553  0.00169742
-0.00283425 -0.999831   0.018149
 0.00174914  0.0181441   0.999834

```

EigenVectors - Molecule B

-0.999994	0.00286537	0.0016974
-0.00283409	-0.999831	0.0181489
0.00174912	0.018144	0.999834

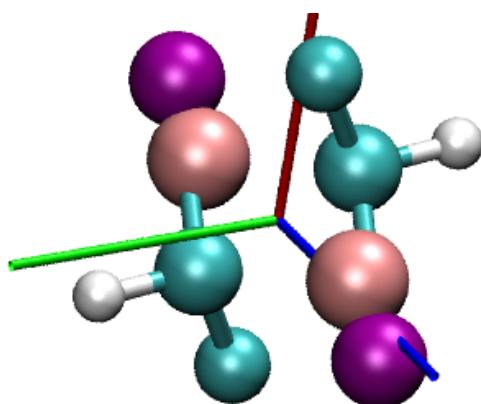
EigenValues - Molecule A

Engenvarde - Microscale II

EigenValues - Molecule B

103.739 629.816 722.221

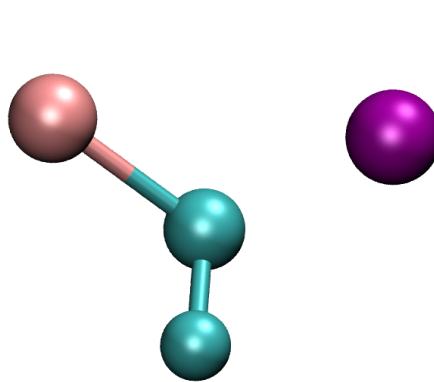
Enantiomers



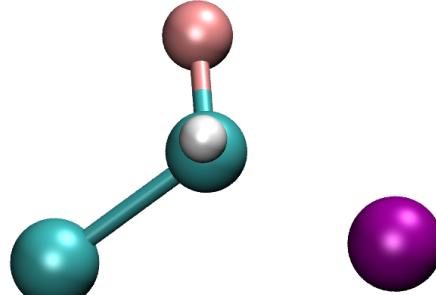
SymmetricEnantiomers Número 454

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

EigenVectors - Molecule A

-0.999994	0.00286553	0.00169742
-0.00283425	-0.999831	0.018149
0.00174914	0.0181441	0.999834

EigenVectors - Molecule B

-0.999994	-0.00286582	-0.00169581
0.0028346	-0.999832	0.018136
-0.0017475	0.0181311	0.999834

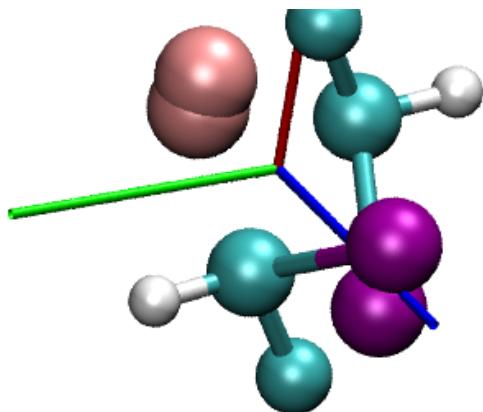
EigenValues - Molecule A

103.739	629.815	722.22
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EigenValues - Molecule B

103.701	630.077	722.452
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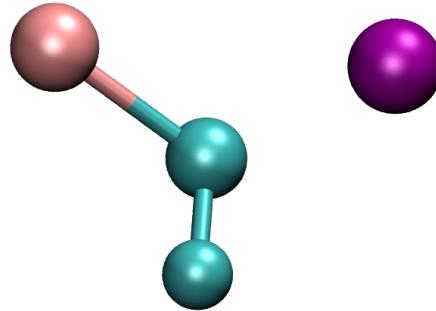
Equal



SymmetricEnantiomers Número 455

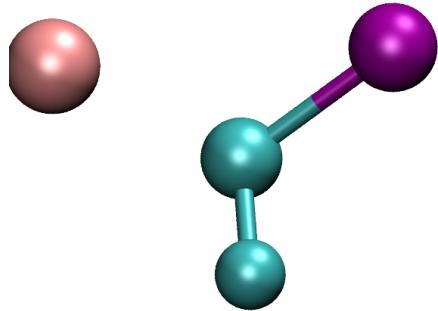
Molecule A

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

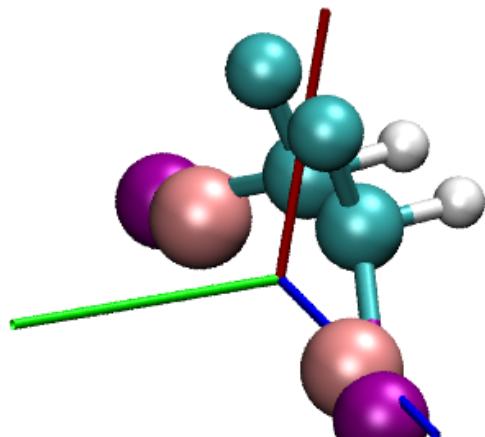
EingenValues - Molecule A

103.739	629.815	722.22
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EingenValues - Molecule B

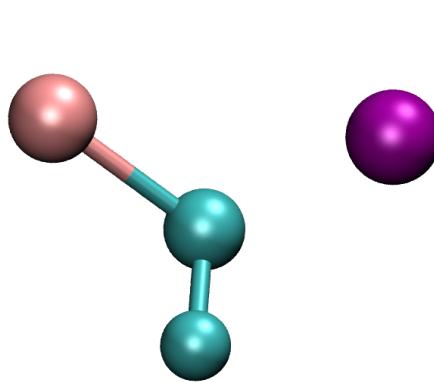
103.7	630.079	722.455
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Enantiomers

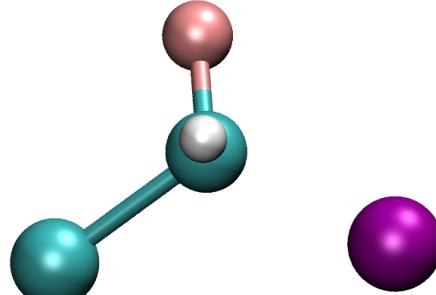


SymmetricEnantiomers Número 456

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

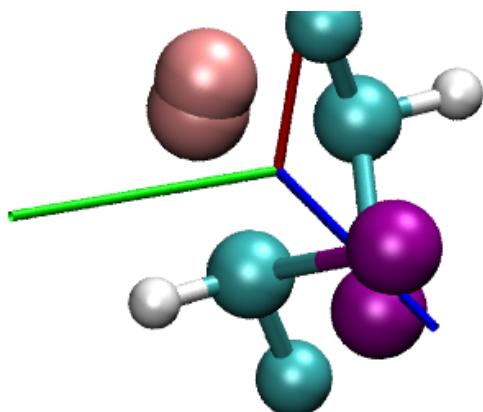
EingenValues - Molecule A

103.739	629.815	722.22
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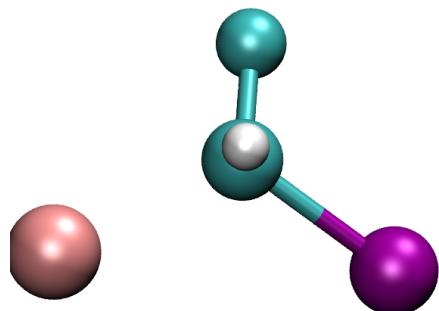
EingenValues - Molecule B

103.701	630.077	722.452
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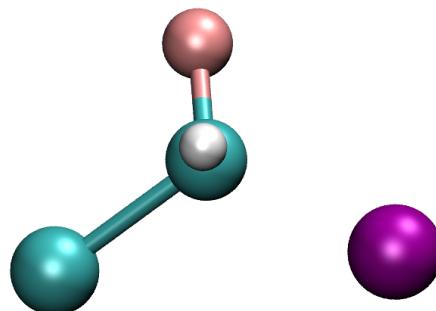
Equal



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

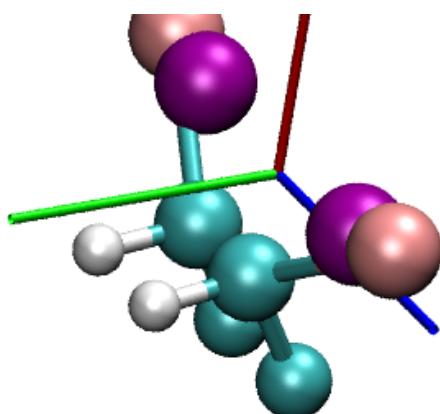
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

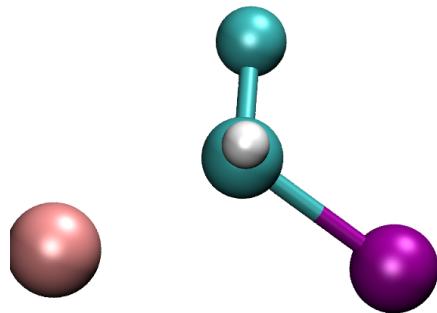
103.701	630.077	722.452
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Enantiomers



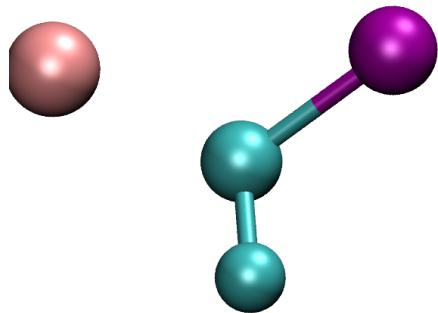
SymmetricEnantiomers Número 458

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

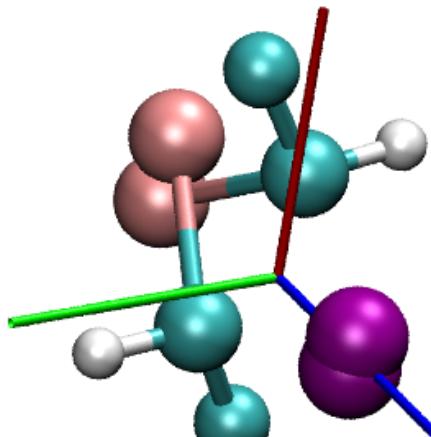
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

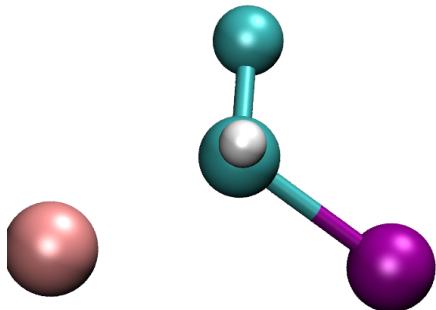
103.7	630.079	722.455
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Equal

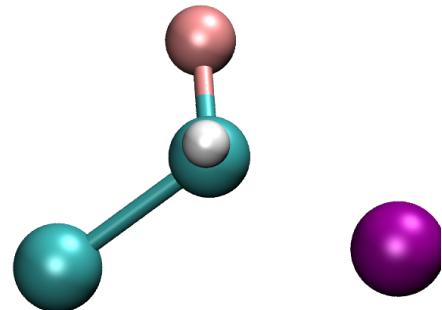


SymmetricEnantiomers Número 459

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

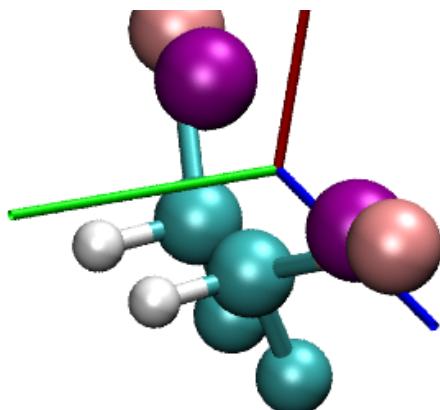
EingenValues - Molecule A

103.739	629.816	722.221
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EingenValues - Molecule B

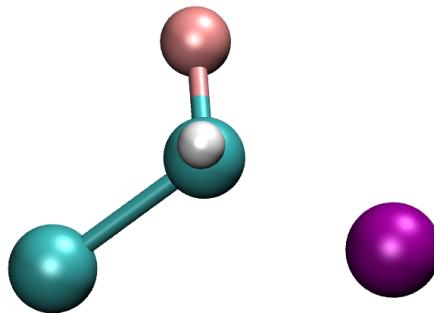
103.701	630.077	722.452
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Enantiomers



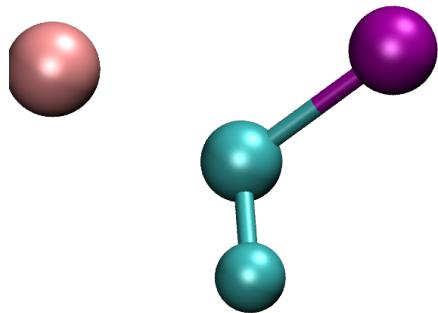
SymmetricEnantiomers Número 460

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

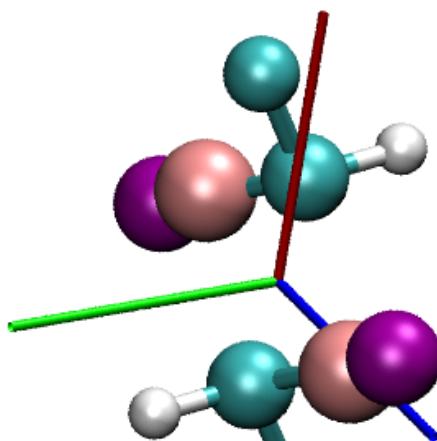
EingenValues - Molecule A

103.701	630.077	722.452
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EingenValues - Molecule B

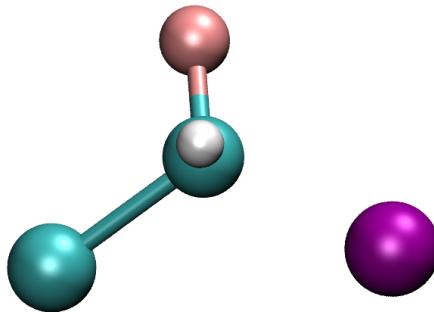
103.7	630.079	722.455
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Enantiomers

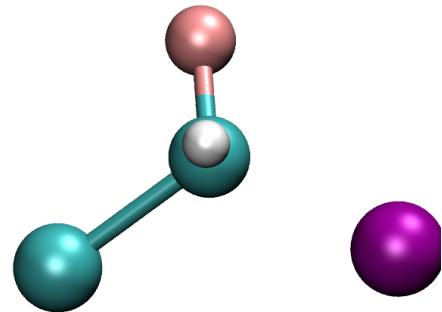


SymmetricEnantiomers Número 461

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

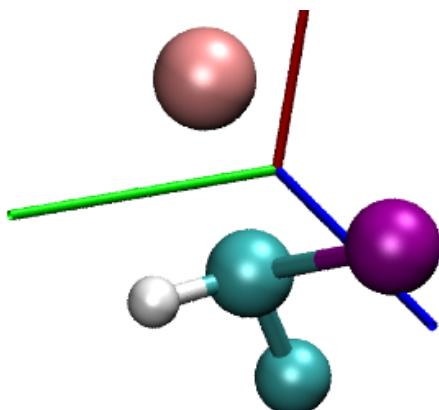
EingenValues - Molecule A

103.701	630.077	722.452
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EingenValues - Molecule B

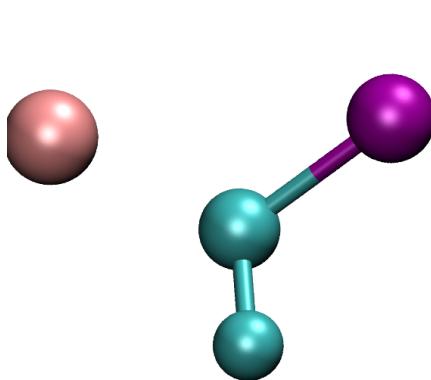
103.701	630.077	722.452
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Equal

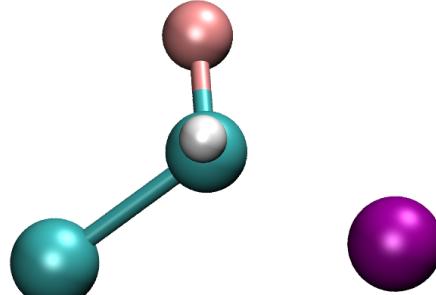


SymmetricEnantiomers Número 462

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

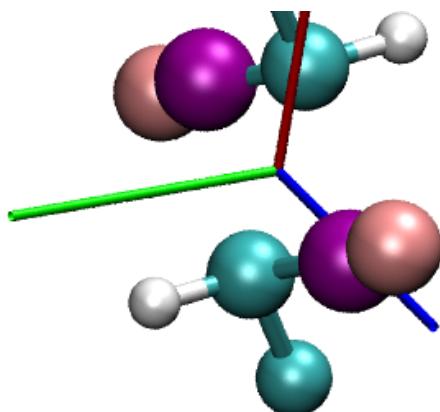
EingenValues - Molecule A

103.7	630.079	722.455
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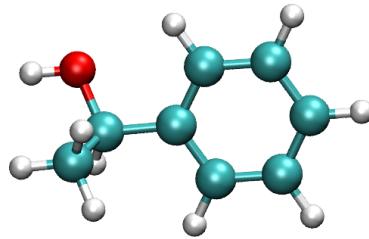
EingenValues - Molecule B

103.701	630.077	722.452
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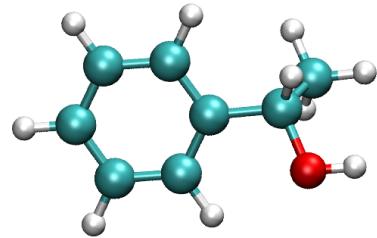
Enantiomers



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

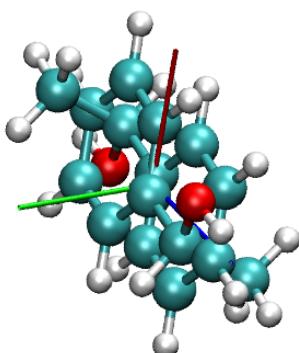
EingenValues - Molecule A

146.173	442.909	530.735
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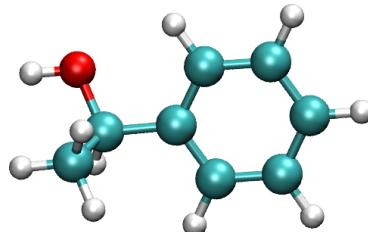
EingenValues - Molecule B

146.173	442.909	530.735
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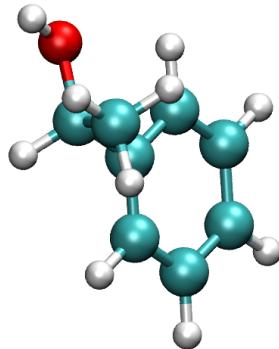
Enantiomers



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

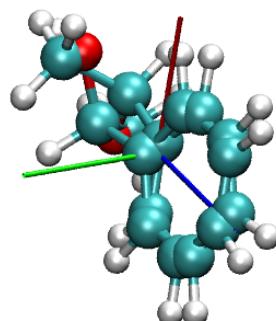
EingenValues - Molecule A

146.173	442.909	530.735
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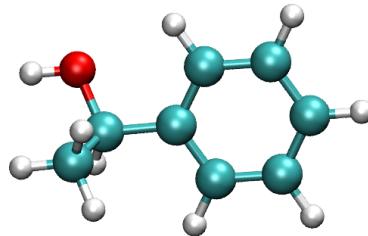
EingenValues - Molecule B

146.173	442.909	530.735
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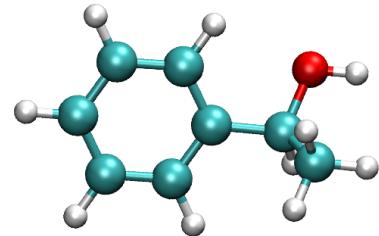
Equal



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

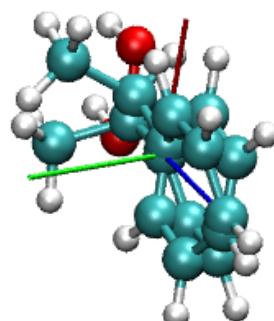
EingenValues - Molecule A

146.173	442.909	530.735
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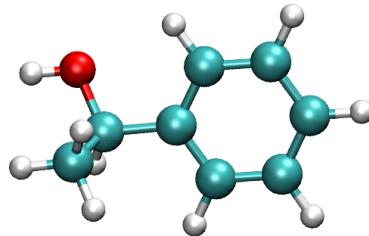
EingenValues - Molecule B

146.173	442.909	530.735
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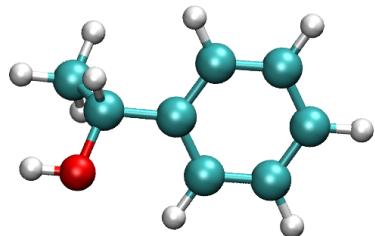
Enantiomers



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

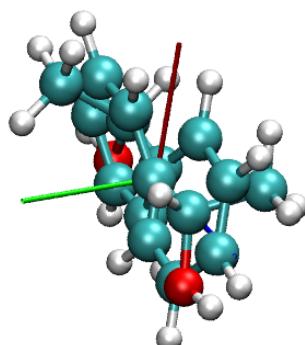
EingenValues - Molecule A

146.173	442.909	530.735
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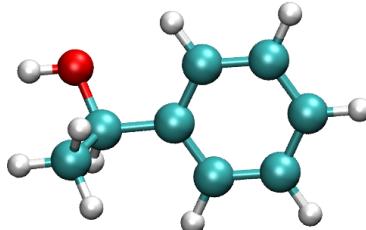
EingenValues - Molecule B

146.173	442.909	530.735
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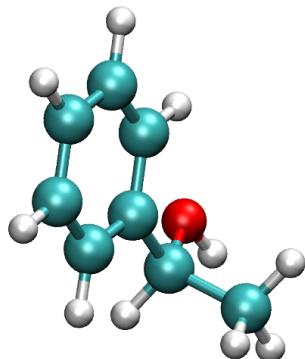
Equal



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

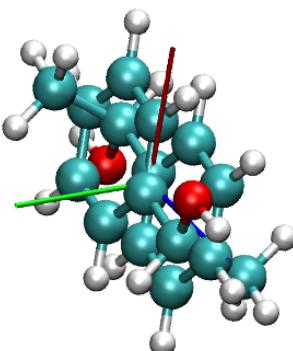
EingenValues - Molecule A

146.173	442.909	530.735
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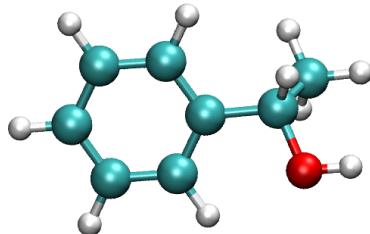
EingenValues - Molecule B

146.173	442.909	530.735
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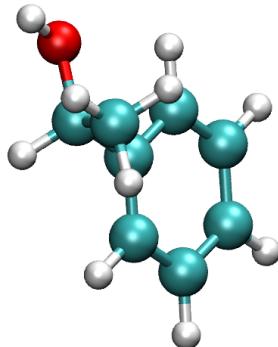
Enantiomers



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

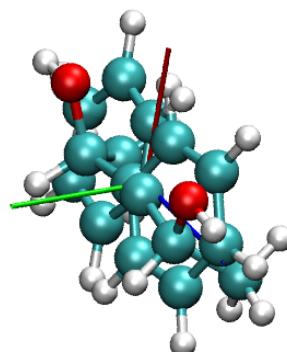
EingenValues - Molecule A

146.173	442.909	530.735
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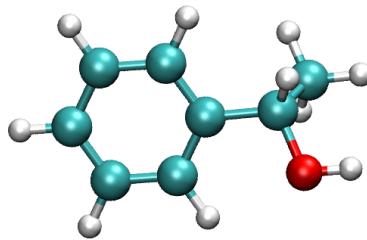
EingenValues - Molecule B

146.173	442.909	530.735
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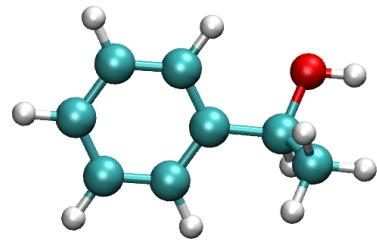
Enantiomers



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

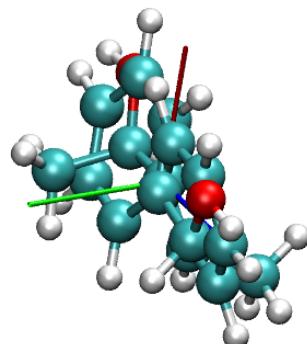
EingenValues - Molecule A

146.173	442.909	530.735
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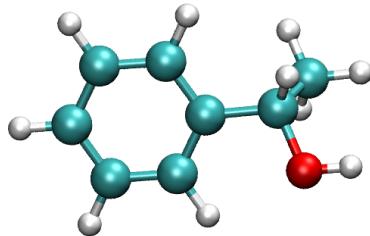
EingenValues - Molecule B

146.173	442.909	530.735
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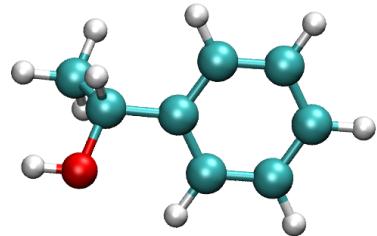
Equal



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

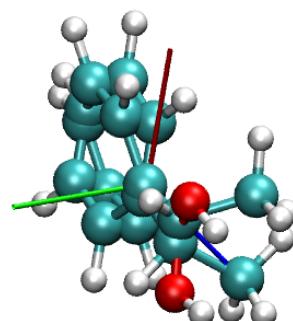
EingenValues - Molecule A

146.173	442.909	530.735
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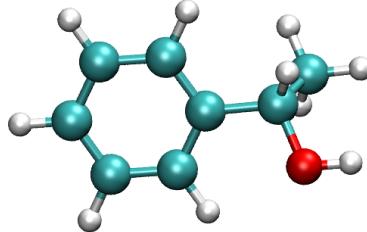
EingenValues - Molecule B

146.173	442.909	530.735
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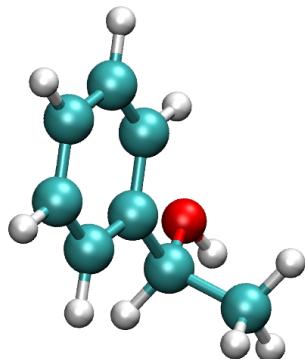
Enantiomers



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

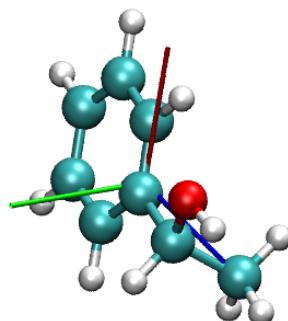
EingenValues - Molecule A

146.173	442.909	530.735
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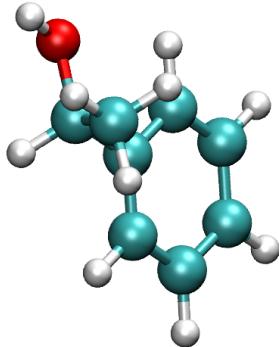
EingenValues - Molecule B

146.173	442.909	530.735
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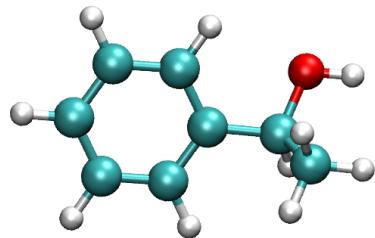
Equal



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

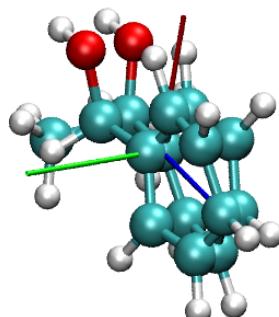
EingenValues - Molecule A

146.173	442.909	530.735
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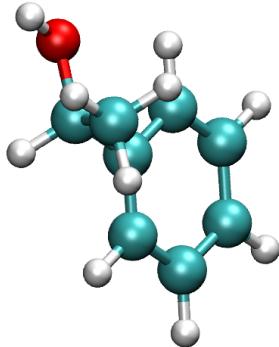
EingenValues - Molecule B

146.173	442.909	530.735
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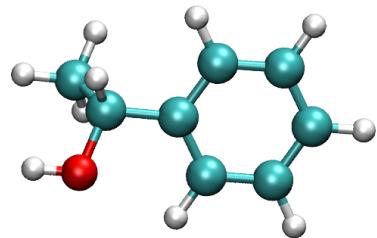
Enantiomers



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

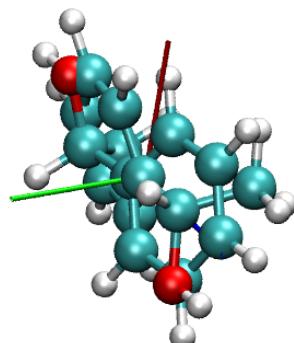
EingenValues - Molecule A

146.173	442.909	530.735
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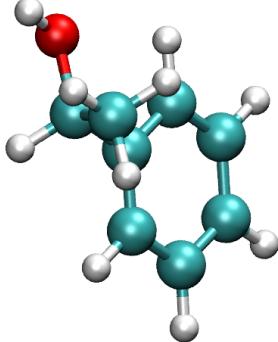
EingenValues - Molecule B

146.173	442.909	530.735
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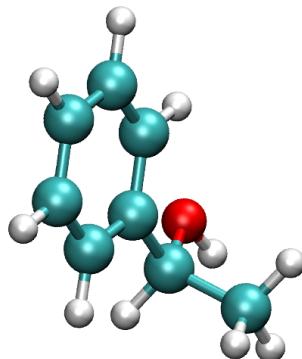
Equal



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

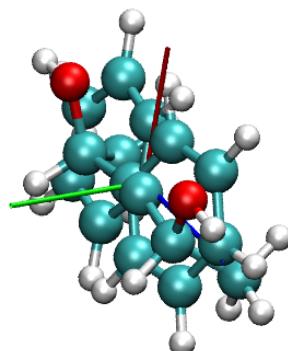
EingenValues - Molecule A

146.173	442.909	530.735
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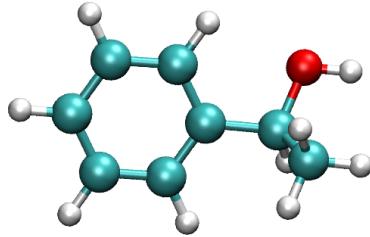
EingenValues - Molecule B

146.173	442.909	530.735
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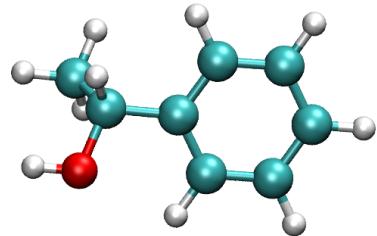
Enantiomers



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

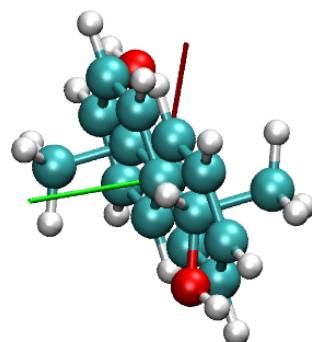
EingenValues - Molecule A

146.173	442.909	530.735
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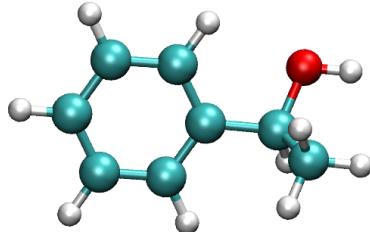
EingenValues - Molecule B

146.173	442.909	530.735
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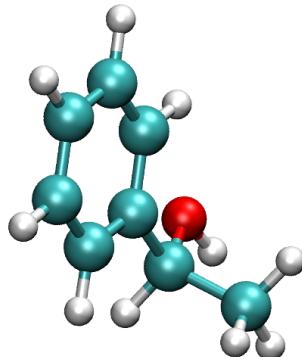
Enantiomers



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

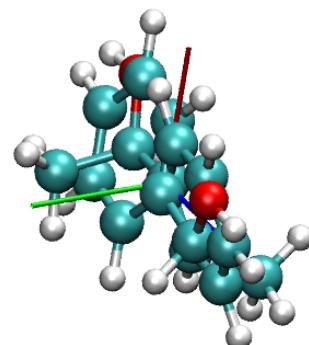
EingenValues - Molecule A

146.173	442.909	530.735
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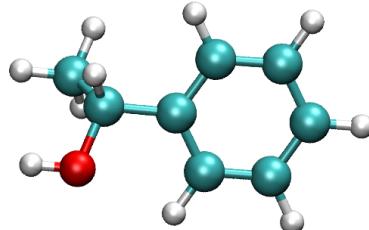
EingenValues - Molecule B

146.173	442.909	530.735
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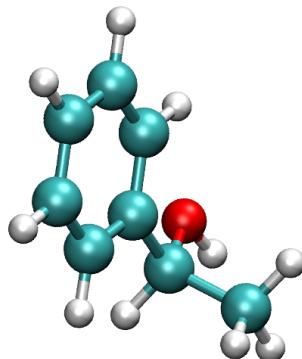
Equal



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

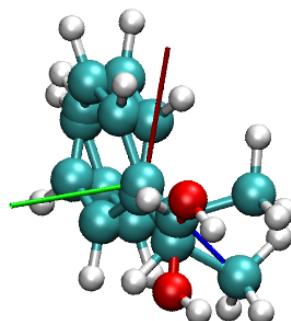
EingenValues - Molecule A

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 RMS = 1.306092E-07
	s-2-chlorobutane_rotated_out_G09 E = -618.057081943 Freq =115.2939		
16	3NFAACa E = No Data Freq =No Data	Equal	Equal RMS = 4.41707E-05
	3NFAACb E = No Data Freq =No Data		
17	3NFAACa E = No Data Freq =No Data	Different	Different RMS = 0.0334016
	3NFAACc E = No Data Freq =No Data		
18	3NFAACa E = No Data Freq =No Data	Different	Different RMS = 0.0888511
	3NFAACd E = No Data Freq =No Data		
19	3NFAACa E = No Data Freq =No Data	Different	Different RMS = 0.162132
	3NFAACE E = No Data Freq =No Data		
20	3NFAACa E = No Data Freq =No Data	Equal	Equal RMS = 0.001455454
	3NFAACf E = No Data Freq =No Data		
21	3NFAACa E = No Data Freq =No Data	Different	Different RMS = 0.0330848
	3NFAACg E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
22	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data	RMS = 0.064417	
23	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data	RMS = 0.0837021	
24	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data	RMS = 0.0903201	
25	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data	RMS = 0.0114116	
26	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data	RMS = 0.0362294	
27	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data	RMS = 0.152833	
28	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data	RMS = 0.157182	

#	Moléculas	Restultado esperado	Resultado programa
29	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data	RMS = 0.219778	
30	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data	RMS = 0.258442	
31	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data	RMS = 0.0186255	
	3NFAACa E = No Data Freq =No Data		
32	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data	RMS = 0.0149078	
	3NFAACa E = No Data Freq =No Data		
33	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data	RMS = 0.0228438	
	3NFAACa E = No Data Freq =No Data		
34	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data	RMS = 0.118302	
	3NFAACa E = No Data Freq =No Data		
35	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.0338585	
	3NFAACa E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
36	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.00146242	
37	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data	RMS = 0.0868356	
38	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data	RMS = 0.0414826	
	3NFAACb E = No Data Freq =No Data	Different	Different
39	3NFAACc E = No Data Freq =No Data	RMS = 0.0881291	
	3NFAACb E = No Data Freq =No Data	Different	Different
40	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACb E = No Data Freq =No Data	RMS = 0.143579	
	3NFAACe E = No Data Freq =No Data	Different	Different
41	3NFAACb E = No Data Freq =No Data	RMS = 0.107404	
	3NFAACf E = No Data Freq =No Data	Equal	Equal
42	3NFAACb E = No Data Freq =No Data	RMS = 0.0004634431	
	3NFAACf E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
43	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data	RMS = 0.0878122	
44	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data	RMS = 0.00968954	
45	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data	RMS = 0.13843	
46	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data	RMS = 0.145048	
47	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACK E = No Data Freq =No Data	RMS = 0.0661391	
48	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data	RMS = 0.018498	
49	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data	RMS = 0.0981054	

#	Moléculas	Restultado esperado	Resultado programa
50	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data	RMS = 0.102455	
51	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data	RMS = 0.274505	
52	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data	RMS = 0.203714	
53	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACC E = No Data Freq =No Data	RMS = 0.036102	
54	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data	RMS = 0.0398197	
55	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data	RMS = 0.0318836	
56	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data	RMS = 0.0635749	

#	Moléculas	Restultado esperado	Resultado programa
57	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.020869	
58	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.0561899	
59	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data	RMS = 0.0321081	
60	3NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data	RMS = 0.0132449	
61	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACd E = No Data Freq =No Data	RMS = 0.0554495	
62	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACe E = No Data Freq =No Data	RMS = 0.195533	
63	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACf E = No Data Freq =No Data	RMS = 0.0879682	

#	Moléculas	Restultado esperado	Resultado programa
64	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data	RMS = 0.000316817	
65	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data	RMS = 0.0978186	
66	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data	RMS = 0.0503005	
67	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data	RMS = 0.0569185	
68	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data	RMS = 0.02199	
69	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data	RMS = 0.069631	
70	3NFAACc E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data	RMS = 0.186234	

#	Moléculas	Restultado esperado	Resultado programa
71	3NFAACc E = No Data Freq =No Data	Enantiomers	Enantiomers RMS = 0.01522269
	3NFAACn E = No Data Freq =No Data		
72	3NFAACc E = No Data Freq =No Data	Different	Different RMS = 0.186376
	4NFAACa E = No Data Freq =No Data		
73	3NFAACc E = No Data Freq =No Data	Different	Different RMS = 0.291844
	4NFAACb E = No Data Freq =No Data		
74	3NFAACc E = No Data Freq =No Data	Different	Different RMS = 0.0520271
	4NFAACc E = No Data Freq =No Data		
75	3NFAACc E = No Data Freq =No Data	Different	Different RMS = 0.0483094
	4NFAACd E = No Data Freq =No Data		
76	3NFAACc E = No Data Freq =No Data	Different	Different RMS = 0.0562454
	4NFAACe E = No Data Freq =No Data		
77	3NFAACc E = No Data Freq =No Data	Different	Different RMS = 0.151704
	4NFAACf E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
78	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.0672601	
79	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.0319392	
80	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data	RMS = 0.120237	
	3NFAACc E = No Data Freq =No Data	Different	Different
81	4NFAACl-3 E = No Data Freq =No Data	Different	Different
	3NFAACc E = No Data Freq =No Data	RMS = 0.0748842	
	4NFAACl-3 E = No Data Freq =No Data		
82	3NFAACd E = No Data Freq =No Data	Equal	Enantiomers
	3NFAACE E = No Data Freq =No Data		
	3NFAACf E = No Data Freq =No Data		
83	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACf E = No Data Freq =No Data	RMS = 0.143418	
	3NFAACd E = No Data Freq =No Data		
84	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data	RMS = 0.0557663	
	3NFAACd E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
85	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data	RMS = 0.153268	
86	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data	RMS = 0.00514902	
87	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data	RMS = 0.00146894	
88	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data	RMS = 0.0774395	
89	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data	RMS = 0.125081	
90	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data	RMS = 0.241684	
91	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data	RMS = 0.246033	

#	Moléculas	Restultado esperado	Resultado programa
92	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data	RMS = 0.130927	
93	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data	RMS = 0.347293	
94	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data	RMS = 0.107477	
	3NFAACd E = No Data Freq =No Data	Different	Different
95	4NFAACd E = No Data Freq =No Data	RMS = 0.103759	
	3NFAACd E = No Data Freq =No Data	Different	Different
96	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data	RMS = 0.111695	
	3NFAACd E = No Data Freq =No Data	Different	Different
97	4NFAACf E = No Data Freq =No Data	RMS = 0.207153	
	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.12271	
98	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.12271	

#	Moléculas	Restultado esperado	Resultado programa
99	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0873887
100	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.175687
101	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.130334
102	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACf E = No Data Freq =No Data		RMS = 0.107565
103	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data		RMS = 0.195216
104	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data		RMS = 0.0977146
105	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.245834

#	Moléculas	Restultado esperado	Resultado programa
106	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.252452
107	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.173543
108	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.125902
109	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.00929873
110	3NFAACe E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.00494937
111	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.381909
112	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.0963103

#	Moléculas	Restultado esperado	Resultado programa
113	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.143506
114	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.147224
115	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.139288
116	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0438293
117	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.128273
118	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.163594
119	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.075296

#	Moléculas	Restultado esperado	Resultado programa
120	3NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.120649
121	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data		RMS = 0.0876514
122	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data		RMS = 0.00985042
123	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.138269
124	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.144887
125	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0659782
126	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.0183372

#	Moléculas	Restultado esperado	Resultado programa
127	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data	RMS = 0.0982663	
128	3NFAACf E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data	RMS = 0.102616	
129	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data	RMS = 0.274344	
	3NFAACf E = No Data Freq =No Data	Different	Different
130	4NFAACb E = No Data Freq =No Data	RMS = 0.203875	
	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACC E = No Data Freq =No Data	RMS = 0.0359411	
131	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data	RMS = 0.0396588	
	3NFAACf E = No Data Freq =No Data	Different	Different
133	4NFAACE E = No Data Freq =No Data	RMS = 0.0317228	
	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		

#	Moléculas	Restultado esperado	Resultado programa
134	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0637358
135	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0207081
136	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.056029
137	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.032269
138	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.013084
139	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACh E = No Data Freq =No Data		RMS = 0.0975018
140	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.0506173

#	Moléculas	Restultado esperado	Resultado programa
141	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.0572353
142	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0216732
143	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.0693142
144	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.185918
145	3NFAACg E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.190267
146	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.186693
147	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.291527

#	Moléculas	Restultado esperado	Resultado programa
148	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.0517103
149	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0479926
150	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.0559286
151	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.151387
152	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0669433
153	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0316224
154	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.11992

#	Moléculas	Restultado esperado	Resultado programa
155	3NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0745674
156	3NFAACH E = No Data Freq =No Data	Different	Different
	3NFAACi E = No Data Freq =No Data		RMS = 0.148119
157	3NFAACH E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.154737
158	3NFAACH E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0758286
159	3NFAACH E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.0281876
160	3NFAACH E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.0884159
161	3NFAACH E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.0927652

#	Moléculas	Restultado esperado	Resultado programa
162	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.284195
163	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.194025
164	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.0457915
165	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0495092
166	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.0415732
167	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0538853
168	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0305585

#	Moléculas	Restultado esperado	Resultado programa
169	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0658794
170	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0224186
171	3NFAACh E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0229344
172	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACj E = No Data Freq =No Data		RMS = 0.00661796
173	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACk E = No Data Freq =No Data		RMS = 0.0722905
174	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.119932
175	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.236535

#	Moléculas	Restultado esperado	Resultado programa
176	3NFAACi E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.240884
177	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.136076
178	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.342144
179	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.102328
180	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0986099
181	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.106546
182	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.202004

#	Moléculas	Restultado esperado	Resultado programa
183	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.117561
184	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0822397
185	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.170538
186	3NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.125185
187	3NFAACj E = No Data Freq =No Data	Different	Different
	3NFAACK E = No Data Freq =No Data		RMS = 0.0789084
188	3NFAACj E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.126549
189	3NFAACj E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.243153

#	Moléculas	Restultado esperado	Resultado programa
190	3NFAACj E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.247502
191	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.129458
192	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.348762
193	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.108946
194	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.105228
195	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.113164
196	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.208622

#	Moléculas	Restultado esperado	Resultado programa
197	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.124179
198	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0888577
199	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.177156
200	3NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.131803
201	3NFAACk E = No Data Freq =No Data	Different	Different
	3NFAACl E = No Data Freq =No Data		RMS = 0.047641
202	3NFAACk E = No Data Freq =No Data	Different	Different
	3NFAACm E = No Data Freq =No Data		RMS = 0.164244
203	3NFAACk E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.168594

#	Moléculas	Restultado esperado	Resultado programa
204	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.208366
205	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.269854
206	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.0300371
207	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.0263194
208	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.0342554
209	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.129714
210	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0452701

#	Moléculas	Restultado esperado	Resultado programa
211	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.00994921
212	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0982472
213	3NFAACk E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0528942
214	3NFAACl E = No Data Freq =No Data	Enantiomers	Equal
	3NFAACm E = No Data Freq =No Data		
215	3NFAACl E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.120953
216	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.256007
217	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.222213

#	Moléculas	Restultado esperado	Resultado programa
218	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data	RMS = 0.0176039	
219	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data	RMS = 0.0213216	
220	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data	RMS = 0.0133856	
221	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data	RMS = 0.0820729	
222	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.00237094	
223	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.0376918	
224	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data	RMS = 0.0506062	

#	Moléculas	Restultado esperado	Resultado programa
225	3NFAACl E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0052532
226	3NFAACm E = No Data Freq =No Data	Different	Different
	3NFAACn E = No Data Freq =No Data		RMS = 0.00434937
227	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.372611
228	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.105609
229	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.134207
230	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.137925
231	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.129989

#	Moléculas	Restultado esperado	Resultado programa
232	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0345305
233	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.118974
234	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.154295
235	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0659973
236	3NFAACm E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.11135
237	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACa E = No Data Freq =No Data		RMS = 0.37696
238	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data		RMS = 0.10126

#	Moléculas	Restultado esperado	Resultado programa
239	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.138557
240	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.142274
241	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.134338
242	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0388799
243	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.123324
244	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.158645
245	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0703467

#	Moléculas	Restultado esperado	Resultado programa
246	3NFAACn E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.1157
247	4NFAACa E = No Data Freq =No Data	Enantiomers	Enantiomers
	4NFAACb E = No Data Freq =No Data		RMS = 0.485443
248	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.238403
249	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.234686
250	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.242622
251	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.33808
252	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.253636

#	Moléculas	Restultado esperado	Resultado programa
253	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.218315
254	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.306613
255	4NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.26126
256	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data		RMS = 0.239816
257	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.243534
258	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.235598
259	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.14014

#	Moléculas	Restultado esperado	Resultado programa
260	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.224583
261	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.259904
262	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.171606
263	4NFAACb E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.216959
264	4NFAACC E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data		RMS = 0.00371771
265	4NFAACC E = No Data Freq =No Data	Different	Different
	4NFAACE E = No Data Freq =No Data		RMS = 0.00421832
266	4NFAACC E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.0996768

#	Moléculas	Restultado esperado	Resultado programa
267	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.015233
268	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0200879
269	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0682101
270	4NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0228571
271	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data		RMS = 0.00793602
272	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data		RMS = 0.103395
273	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0189507

#	Moléculas	Restultado esperado	Resultado programa
274	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.0163702	
275	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data	RMS = 0.0719278	
276	4NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data	RMS = 0.0265748	
277	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data	RMS = 0.0954585	
278	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.0110146	
279	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data	RMS = 0.0243062	
280	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data	RMS = 0.0639918	

#	Moléculas	Restultado esperado	Resultado programa
281	4NFAACe E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0186388
282	4NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data		RMS = 0.0844439
283	4NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.119765
284	4NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0314668
285	4NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.0768197
286	4NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACi E = No Data Freq =No Data		RMS = 0.0353209
287	4NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.0529771

#	Moléculas	Restultado esperado	Resultado programa
288	4NFAACg E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.00762414
289	4NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACj E = No Data Freq =No Data		RMS = 0.088298
290	4NFAACi E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.042945
291	4NFAACj E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data		RMS = 0.045353
292	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 = 0.269312
293	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 = 0.269312
294	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 = 0.0426031

#	Moléculas	Restultado esperado	Resultado programa
295	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 = 0.0778147	
296	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 = 0.766027	
297	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 = 0.766028	
298	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	
299	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	
300	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Equal	Equal
	2,2-dimethyl-butane_out_G09_inversion E = -237.083690318 Freq =92.1843	RMS = 0	
301	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	

#	Moléculas	Restultado esperado	Resultado programa
302	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	
303	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	
304	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	
305	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	
306	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	
307	2,2-dimethyl-butane_out_G09 E = -237.083690318 Freq =92.1843	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752	RMS = 0	
308	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 = 0	

#	Moléculas	Restultado esperado	Resultado programa
309	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
310	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
311	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
312	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
313	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
314	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
315	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

#	Moléculas	Restultado esperado	Resultado programa
316	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	
317	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	
318	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	
319	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	
320	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	
321	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	
322	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	

#	Moléculas	Restultado esperado	Resultado programa
323	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	
324	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	
325	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	
326	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Enantiomers	Enantiomers
	2-methyl-pentane_out_G09_inversion E = -237.084759065 Freq =80.9103		
327	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Different	Different
	3-methyl-pentane_out_G09 E = -237.083213438 Freq =81.4725		
328	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Different	Different
	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725		
329	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752		

#	Moléculas	Restultado esperado	Resultado programa
330	2-methyl-pentane_out_G09 E = -237.084759065 Freq =80.9103	Different	Different
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752	RMS = 0.0426031	
331	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725	Different	Different
	hexane_out_G09 E = -237.085500432 Freq =72.0752	RMS = 0.766028	
332	3-methyl-pentane_out_G09_inversion E = -237.083213438 Freq =81.4725	Different	Different
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752	RMS = 0.766028	
333	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	
334	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	
335	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	
336	hexane_out_G09 E = -237.085500432 Freq =72.0752	Equal	Equal
	hexane_out_G09_inversion E = -237.085500432 Freq =72.0752	RMS = 0	

#	Moléculas	Restultado esperado	Resultado programa
337	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 Warning: Degeneracy	
338	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	RMS = 0.0319157	
339	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	RMS = 0.0319157	
340	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 = 0.0319157	
341	neopentane_out_G09_inversion E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	RMS = 0.390641	
342	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	
343	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 = 0.0670111	

#	Moléculas	Restultado esperado	Resultado programa
344	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 = 0.0670111	
345	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 = 0.0670111	
346	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	
347	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	
348	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	
349	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	
350	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	RMS = 0.0603026	

#	Moléculas	Restultado esperado	Resultado programa
351	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	RMS = 0.0603026	
352	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 = 0.0603026	
353	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	RMS = 0.48286	
354	neopentane_out_G09 E = -197.772988492 Freq =208.9793	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268	RMS = 0.48286	
355	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	
356	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	
357	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	

#	Moléculas	Restultado esperado	Resultado programa
358	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Equal	Equal RMS = 0.0214957 Warning: Degeneracy
	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816		
359	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different RMS = 0.0319051
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777		
360	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different RMS = 0.064439
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777		
361	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different RMS = 0.0319051
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		
362	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different RMS = 0.390652
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268		
363	neopentane_Symmetry_out_G09_inversion E = -197.772988495 Freq =208.9816	Different	Different RMS = 0.390653
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		
364	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = -197.772988495 Freq =208.9816	Equal	Equal RMS = 0.1137 Warning: Degeneracy
	neopentane_out_G09 E = -197.772988492 Freq =208.9793		

#	Moléculas	Restultado esperado	Resultado programa
365	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		RMS = 0.0214849 Warning: Degeneracy
366	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		RMS = 0.120409 Warning: Degeneracy
367	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		RMS = 0.0533989
368	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 = 0.0533989
369	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 = 0.0533989
370	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
371	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

#	Moléculas	Restultado esperado	Resultado programa
372	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	
373	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	
374	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	
375	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	
376	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	
377	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	RMS = 0.0603092	
378	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Different	Different
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	RMS = 0.0603092	

#	Moléculas	Restultado esperado	Resultado programa
379	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 = 0.0603092	
380	neopentane_Symmetry_out_G09 E = -197.772988495 Freq =208.9816	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	RMS = 0.482866	
381	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	
382	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	Equal	Enantiomers
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		
383	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	RMS = 0.102172	
384	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268	RMS = 0.102172	
385	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268	RMS = 0.266281	

#	Moléculas	Restultado esperado	Resultado programa
386	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		RMS = 0.266281
387	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	Equal	Enantiomers
	tert-butylamine_out_G09_inversion E = -213.803110609 Freq =215.0777		RMS = 0.09408316
388	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	Equal	Equal
	tert-butylamine_out_G09_rot_x15_y15_z15 E = -213.803110609 Freq =215.0777		RMS = 1.188653E-12
389	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	Different	Different
	tetramethylsilane_out_G09 E = -449.191777923 Freq =156.0268		RMS = 0.143206
390	tert-butylamine_out_G09 E = -213.803110609 Freq =215.0777	Different	Different
	tetramethylsilane_out_G09_inversion E = -449.191777923 Freq =156.0268		RMS = 0.143206
391	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
392	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596		RMS = 0.117363

#	Moléculas	Restultado esperado	Resultado programa
393	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	RMS = 0.117363	
394	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954	RMS = 0.167859	
395	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954	RMS = 0.167858	
396	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596	RMS = 0.117363	
397	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596	RMS = 0.117363	
398	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Equal	Equal
	Porphin_out_G09_inversion E = -988.182666824 Freq =-3564.4549	RMS = 0	
399	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	RMS = 0.117363	

#	Moléculas	Restultado esperado	Resultado programa
400	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596		RMS = 0.117363
401	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954		RMS = 0.167859
402	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954		RMS = 0.167858
403	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596		RMS = 0.117363
404	Porphin_out_G09 E = -988.182666824 Freq =-3564.4549	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596		RMS = 0.117363
405	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	Equal	Enantiomers
	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954		RMS = 0.0001074955
406	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	Equal	Enantiomers
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954		RMS = 0.0001075617

#	Moléculas	Restultado esperado	Resultado programa
407	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	Equal	Equal RMS = 0
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596		
408	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596	Equal	Equal RMS = 0
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596		
409	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	Equal	Equal RMS = 0
	Tetrabenzoporphyrin_out_G09_inversion E = -1604.15793928 Freq =20.2596		
410	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	Equal	Enantiomers RMS = 0.0001074955
	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954		
411	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	Equal	Enantiomers RMS = 0.0001075617
	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954		
412	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	Equal	Equal RMS = 0
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596		
413	Tetrabenzoporphyrin_out_G09 E = -1604.15793928 Freq =20.2596	Equal	Equal RMS = 0
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596		

#	Moléculas	Restultado esperado	Resultado programa
414	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954	Equal	Enantiomers RMS = 0.0001075617
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596		
415	Tetrabenzoporphyrin_rotated02_out_G09_inversion E = -1604.15788879 Freq =19.3954	Equal	Enantiomers RMS = 0.0001075617
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596		
416	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		
417	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954	Equal	Enantiomers RMS = 0.0001074955
	Tetrabenzoporphyrin_rotated_out_G09 E = -1604.15793928 Freq =20.2596		
418	Tetrabenzoporphyrin_rotated02_out_G09 E = -1604.15788879 Freq =19.3954	Equal	Enantiomers RMS = 0.0001074955
	Tetrabenzoporphyrin_rotated_out_G09_inversion E = -1604.15793928 Freq =20.2596		
419	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		
420	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		

#	Moléculas	Restultado esperado	Resultado programa
421	R-R-R-Fructuose_out_G09 E = -687.366006448 Freq =36.7188	Different	Different
	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257		RMS = 0.274434
422	R-R-R-Fructuose_out_G09 E = -687.366006448 Freq =36.7188	Different	Different
	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064		RMS = 0.404519
423	R-R-R-Fructuose_out_G09 E = -687.366006448 Freq =36.7188	Different	Different
	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777		RMS = 0.299091
424	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
425	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
426	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
427	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

#	Moléculas	Restultado esperado	Resultado programa
428	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
429	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
430	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
431	R-R-S-Fructuose_out_G09 E = -687.367479320 Freq =43.3327	Enantiomers	Enantiomers
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371		
432	R-R-S-Fructuose_out_G09 E = -687.367479320 Freq =43.3327	Different	Different
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992		RMS = 0.0469601
433	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Different	Different
	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064		RMS = 0.130085
434	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Different	Different
	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777		RMS = 0.0246573

#	Moléculas	Restultado esperado	Resultado programa
435	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Enantiomers	Enantiomers RMS = 0.005799255
	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =		
436	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Different	Different RMS = 0.0534457
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371		
437	R-S-R-Fructuose_out_G09 E = -687.362461360 Freq =34.8257	Different	Different RMS = 0.127928
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992		
438	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064	Enantiomers	Enantiomers RMS = 0.0001020726
	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777		
439	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064	Different	Different RMS = 0.134984
	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =		
440	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064	Different	Different RMS = 0.0766398
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371		
441	R-S-S-Fructuose_out_G09 E = -687.363689916 Freq =34.8064	Different	Different RMS = 0.00215791
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992		

#	Moléculas	Restultado esperado	Resultado programa
442	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777	Different	Different
	S-R-S-Fructuose_out_G09 E = -687.362461325 Freq =	RMS = 0.029556	
443	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777	Different	Different
	S-S-R-Fructuose_out_G09 E = -687.367479374 Freq =43.3371	RMS = 0.0287884	
444	S-R-R-Fructuose_out_G09 E = -687.363690093 Freq =34.7777	Different	Different
	S-S-S-Fructuose_out_G09 E = -687.368445846 Freq =30.5992	RMS = 0.10327	
445	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	
446	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	
447	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	
448	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	RMS = 0.01735201	

#	Moléculas	Restultado esperado	Resultado programa
449	r-enan_out_G09_inversion_output E = -9590.12967553 Freq =134.7377	Equal	Equal
	s-enan_out_G09 E = -9590.12967522 Freq =134.6541	RMS = 1.185059E-06	
450	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	RMS = 0.005068578	
451	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	RMS = 1.178757E-06	
452	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers
	r-enan_out_G09_inversion_output E = -9590.12967553 Freq =134.7377	RMS = 0.01735201	
453	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Equal	Equal
	r-enan_rotated_out_G09 E = -9590.12967553 Freq =134.7377	RMS = 0	
454	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Enantiomers	Enantiomers
	s-enan_out_G09 E = -9590.12967522 Freq =134.6541	RMS = 0.00506593	
455	r-enan_out_G09 E = -9590.12967553 Freq =134.7377	Equal	Equal
	s-enan_out_G09_inversion_output E = -9590.12967522 Freq =134.6541	RMS = 3.832848E-06	

#	Moléculas	Restultado esperado	Resultado programa
456	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		
457	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		
458	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		
459	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		
460	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		
461	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		
462	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		

#	Moléculas	Restultado esperado	Resultado programa
463	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		
464	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		
465	test-R_out_G09_inversion E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers RMS = 7.641079E-17
	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428		
466	test-R_out_G09_inversion E = -386.195553794 Freq =38.2428	Equal	Equal RMS = 1.575741E-07
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428		
467	test-R_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers RMS = 0.1189346
	test-S_out_G09 E = -386.195553794 Freq =38.2428		
468	test-R_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	Equal	Equal RMS = 1.229453E-06
	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428		
469	test-R_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers RMS = 0.1261691
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428		

#	Moléculas	Restultado esperado	Resultado programa
470	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
471	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
472	test-R_out_G09 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers
	test-S_out_G09 E = -386.195553794 Freq =38.2428		RMS = 1.273513E-17
473	test-R_out_G09 E = -386.195553794 Freq =38.2428	Equal	Equal
	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428		RMS = 9.494985E-08
474	test-R_out_G09 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428		RMS = 0.2451037
475	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428		RMS = 1.575741E-07
476	test-S_out_G09 E = -386.195553794 Freq =38.2428	Enantiomers	Enantiomers
	test-S_out_G09_inversion E = -386.195553794 Freq =38.2428		RMS = 0.2451035

#	Moléculas	Restultado esperado	Resultado programa
477	test-S_out_G09 E = -386.195553794 Freq =38.2428	Equal	Equal
	test-S_out_G09_rot-45-45-45 E = -386.195553794 Freq =38.2428	RMS = 2.749179E-07	

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.