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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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

EingenValues - Molecule B

112.224	165.623	257.016

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

EingenValues - Molecule B

112.224	165.623	257.016

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

EingenValues - Molecule B

112.224	165.624	257.017

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

EingenValues - Molecule B

112.224	165.624	257.018

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

EingenValues - Molecule B

112.224	165.624	257.017

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

EingenValues - Molecule B

112.224	165.623	257.016

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

EingenValues - Molecule B

112.224	165.624	257.018

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

EingenValues - Molecule B

112.224	165.624	257.017

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

EingenValues - Molecule B

112.224	165.624	257.018

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

EingenValues - Molecule B

112.224	165.624	257.017

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

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

EingenValues - Molecule B

112.224	165.624	257.017

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

EingenValues - Molecule B

112.224	165.624	257.017

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

EingenValues - Molecule B

530.103	915.738	1361.08

Enantiomers

FireTest Número 17

Molecule A 3NFAACa

Molecule B 3NFAACc

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

EingenValues - Molecule B

531.402	913.293	1353.16

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

EingenValues - Molecule B

524.175	935.342	1359.19

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

EingenValues - Molecule B

524.162	935.308	1359.22

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

EingenValues - Molecule B

530.045	915.527	1360.79

Enantiomers

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

530.124	915.807	1361.14

EingenValues - Molecule B

532.89	918.442	1356.93

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

EingenValues - Molecule B

528.663	924.928	1336.12

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

EingenValues - Molecule B

521.475	949.659	1346.18

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

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

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

EingenValues - Molecule A

530.124	915.807	1361.14

EingenValues - Molecule B

533.726	920.137	1348.3

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

EingenValues - Molecule B

534.81	913.339	1353.78

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

EingenValues - Molecule B

531.691	929.434	1355.4

Different

FireTest Número 27

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

EingenValues - Molecule B

531.698	929.417	1355.4

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

EingenValues - Molecule B

531.43	913.309	1353.35

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

EingenValues - Molecule B

479.363	1242.41	1647.39

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

EingenValues - Molecule B

479.308	1242.41	1647.31

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

EingenValues - Molecule B

482.027	1240.32	1647.08

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

EingenValues - Molecule B

491.663	1231.14	1650.13

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

EingenValues - Molecule B

489.011	1233.7	1641.81

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

EingenValues - Molecule B

509.668	1219.11	1681.18

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

530.124	915.807	1361.14

EingenValues - Molecule B

513.751	1208.07	1700.9

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 37

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

EingenValues - Molecule B

509.897	1225.65	1680.83

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 39

Molecule A 3NFAACb

Molecule B 3NFAACc

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

EingenValues - Molecule B

531.402	913.293	1353.16

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

EingenValues - Molecule B

524.175	935.342	1359.19

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

EingenValues - Molecule B

524.162	935.308	1359.22

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

EingenValues - Molecule B

530.045	915.527	1360.79

Enantiomers

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

530.103	915.738	1361.08

EingenValues - Molecule B

532.89	918.442	1356.93

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

EingenValues - Molecule B

528.663	924.928	1336.12

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

EingenValues - Molecule B

521.475	949.659	1346.18

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

530.103	915.738	1361.08

EingenValues - Molecule B

533.726	920.137	1348.3

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

EingenValues - Molecule B

534.81	913.339	1353.78

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

EingenValues - Molecule B

531.691	929.434	1355.4

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

EingenValues - Molecule B

531.698	929.417	1355.4

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

EingenValues - Molecule B

531.43	913.309	1353.35

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

EingenValues - Molecule B

479.363	1242.41	1647.39

Different

FireTest Número 52

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 53

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 54

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 55

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

EingenValues - Molecule B

489.011	1233.7	1641.81

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 57

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 58

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 59

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

EingenValues - Molecule B

509.897	1225.65	1680.83

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 61

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

EingenValues - Molecule B

524.175	935.342	1359.19

Different

FireTest Número 62

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

EingenValues - Molecule B

524.162	935.308	1359.22

Different

FireTest Número 63

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

EingenValues - Molecule B

530.045	915.527	1360.79

Different

FireTest Número 64

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

EingenValues - Molecule B

532.89	918.442	1356.93

Different

FireTest Número 65

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

EingenValues - Molecule B

528.663	924.928	1336.12

Different

FireTest Número 66

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

EingenValues - Molecule B

521.475	949.659	1346.18

Different

FireTest Número 67

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

EingenValues - Molecule B

533.726	920.137	1348.3

Different

FireTest Número 68

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

EingenValues - Molecule B

534.81	913.339	1353.78

Different

FireTest Número 69

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

EingenValues - Molecule B

531.691	929.434	1355.4

Different

FireTest Número 70

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

EingenValues - Molecule B

531.698	929.417	1355.4

Different

FireTest Número 71

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

EingenValues - Molecule B

531.43	913.309	1353.35

Enantiomers

FireTest Número 72

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

EingenValues - Molecule B

479.363	1242.41	1647.39

Different

FireTest Número 73

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 74

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 75

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 76

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 77

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 78

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 79

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

531.402	913.293	1353.16

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 81

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

EingenValues - Molecule B

506.607	1222.36	1678.43

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

EingenValues - Molecule B

524.162	935.308	1359.22

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

EingenValues - Molecule B

530.045	915.527	1360.79

Different

FireTest Número 84

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

EingenValues - Molecule B

532.89	918.442	1356.93

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

EingenValues - Molecule B

528.663	924.928	1336.12

Different

FireTest Número 86

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

EingenValues - Molecule B

521.475	949.659	1346.18

Different

FireTest Número 87

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

EingenValues - Molecule B

533.726	920.137	1348.3

Different

FireTest Número 88

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

EingenValues - Molecule B

534.81	913.339	1353.78

Different

FireTest Número 89

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

EingenValues - Molecule B

531.691	929.434	1355.4

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

EingenValues - Molecule B

531.698	929.417	1355.4

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

EingenValues - Molecule B

531.43	913.309	1353.35

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

EingenValues - Molecule B

479.363	1242.41	1647.39

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

EingenValues - Molecule B

479.308	1242.41	1647.31

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 95

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

EingenValues - Molecule B

491.663	1231.14	1650.13

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 97

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 98

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

EingenValues - Molecule B

513.751	1208.07	1700.9

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

524.175	935.342	1359.19

EingenValues - Molecule B

509.897	1225.65	1680.83

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

EingenValues - Molecule B

506.607	1222.36	1678.43

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

EingenValues - Molecule B

530.045	915.527	1360.79

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

524.162	935.308	1359.22

EingenValues - Molecule B

532.89	918.442	1356.93

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

EingenValues - Molecule B

528.663	924.928	1336.12

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

EingenValues - Molecule B

521.475	949.659	1346.18

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

524.162	935.308	1359.22

EingenValues - Molecule B

533.726	920.137	1348.3

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

EingenValues - Molecule B

534.81	913.339	1353.78

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

EingenValues - Molecule B

531.691	929.434	1355.4

Different

FireTest Número 109

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

EingenValues - Molecule B

531.698	929.417	1355.4

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

EingenValues - Molecule B

531.43	913.309	1353.35

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

EingenValues - Molecule B

479.363	1242.41	1647.39

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 113

Molecule A 3NFAACe

Molecule B 4NFAACc

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 114

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 115

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 116

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 117

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

EingenValues - Molecule B

513.751	1208.07	1700.9

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

524.162	935.308	1359.22

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 120

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

EingenValues - Molecule B

506.607	1222.36	1678.43

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

EingenValues - Molecule B

532.89	918.442	1356.93

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

EingenValues - Molecule B

528.663	924.928	1336.12

Different

FireTest Número 123

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

EingenValues - Molecule B

521.475	949.659	1346.18

Different

FireTest Número 124

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

EingenValues - Molecule B

533.726	920.137	1348.3

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

EingenValues - Molecule B

534.81	913.339	1353.78

Different

FireTest Número 126

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

EingenValues - Molecule B

531.691	929.434	1355.4

Different

FireTest Número 127

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

EingenValues - Molecule B

531.698	929.417	1355.4

Different

FireTest Número 128

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

EingenValues - Molecule B

531.43	913.309	1353.35

Different

FireTest Número 129

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

EingenValues - Molecule B

479.363	1242.41	1647.39

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

EingenValues - Molecule B

479.308	1242.41	1647.31

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

EingenValues - Molecule B

482.027	1240.32	1647.08

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

EingenValues - Molecule B

491.663	1231.14	1650.13

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 134

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

EingenValues - Molecule B

509.668	1219.11	1681.18

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

530.045	915.527	1360.79

EingenValues - Molecule B

513.751	1208.07	1700.9

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

530.045	915.527	1360.79

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 138

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

EingenValues - Molecule B

506.607	1222.36	1678.43

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

EingenValues - Molecule B

528.663	924.928	1336.12

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

EingenValues - Molecule B

521.475	949.659	1346.18

Different

FireTest Número 141

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

EingenValues - Molecule B

533.726	920.137	1348.3

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

EingenValues - Molecule B

534.81	913.339	1353.78

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

532.89	918.442	1356.93

EingenValues - Molecule B

531.691	929.434	1355.4

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

EingenValues - Molecule B

531.698	929.417	1355.4

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

EingenValues - Molecule B

531.43	913.309	1353.35

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

EingenValues - Molecule B

479.363	1242.41	1647.39

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

EingenValues - Molecule B

479.308	1242.41	1647.31

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

EingenValues - Molecule B

482.027	1240.32	1647.08

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

EingenValues - Molecule B

491.663	1231.14	1650.13

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

EingenValues - Molecule B

489.011	1233.7	1641.81

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

EingenValues - Molecule B

509.668	1219.11	1681.18

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

EingenValues - Molecule B

513.751	1208.07	1700.9

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenValues - Molecule B

509.897	1225.65	1680.83

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

EingenValues - Molecule B

506.607	1222.36	1678.43

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

EingenValues - Molecule B

521.475	949.659	1346.18

Different

FireTest Número 157

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

EingenValues - Molecule B

533.726	920.137	1348.3

Different

FireTest Número 158

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

EingenValues - Molecule B

534.81	913.339	1353.78

Different

FireTest Número 159

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

EingenValues - Molecule B

531.691	929.434	1355.4

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

EingenValues - Molecule B

531.698	929.417	1355.4

Different

FireTest Número 161

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

EingenValues - Molecule B

531.43	913.309	1353.35

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

EingenValues - Molecule B

479.363	1242.41	1647.39

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 164

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 165

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 166

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 167

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 168

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 169

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenVectors - Molecule A

0.999942	0.00978475	0.00450803
0.00975199	-0.999926	0.00723269
-0.00457847	0.0071883	0.999964

EingenVectors - Molecule B

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

EingenValues - Molecule A

528.663	924.928	1336.12

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 171

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 172

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

EingenValues - Molecule B

533.726	920.137	1348.3

Different

FireTest Número 173

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

EingenValues - Molecule B

534.81	913.339	1353.78

Different

FireTest Número 174

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

EingenValues - Molecule B

531.691	929.434	1355.4

Different

FireTest Número 175

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

EingenValues - Molecule B

531.698	929.417	1355.4

Different

FireTest Número 176

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

EingenValues - Molecule B

531.43	913.309	1353.35

Different

FireTest Número 177

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

EingenValues - Molecule B

479.363	1242.41	1647.39

Different

FireTest Número 178

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 179

Molecule A 3NFAACi

Molecule B 4NFAACc

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

EingenValues - Molecule B

482.027	1240.32	1647.08

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 181

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 182

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 183

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 184

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 185

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 186

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 187

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

EingenValues - Molecule B

534.81	913.339	1353.78

Different

FireTest Número 188

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

EingenValues - Molecule B

531.691	929.434	1355.4

Different

FireTest Número 189

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

EingenValues - Molecule B

531.698	929.417	1355.4

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

EingenValues - Molecule B

531.43	913.309	1353.35

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

EingenValues - Molecule B

479.363	1242.41	1647.39

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 193

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 194

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

EingenValues - Molecule B

491.663	1231.14	1650.13

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

EingenValues - Molecule B

489.011	1233.7	1641.81

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

EingenValues - Molecule B

509.668	1219.11	1681.18

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

EingenValues - Molecule B

513.751	1208.07	1700.9

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 199

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

EingenValues - Molecule B

509.897	1225.65	1680.83

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

EingenValues - Molecule B

506.607	1222.36	1678.43

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

EingenValues - Molecule B

531.691	929.434	1355.4

Different

FireTest Número 202

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

EingenValues - Molecule B

531.698	929.417	1355.4

Different

FireTest Número 203

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

EingenValues - Molecule B

531.43	913.309	1353.35

Different

FireTest Número 204

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

EingenValues - Molecule B

479.363	1242.41	1647.39

Different

FireTest Número 205

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 206

Molecule A 3NFAACk

Molecule B 4NFAACc

Inertia Tensor - Molecule A

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

Inertia Tensor - Molecule B

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

534.81	913.339	1353.78

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 207

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 208

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 209

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

EingenValues - Molecule B

509.668	1219.11	1681.18

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

EingenValues - Molecule B

513.751	1208.07	1700.9

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 213

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 214

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

EingenValues - Molecule B

531.698	929.417	1355.4

Enantiomers

FireTest Número 215

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

EingenValues - Molecule B

531.43	913.309	1353.35

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

EingenValues - Molecule B

479.363	1242.41	1647.39

Different

FireTest Número 217

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 218

Molecule A 3NFAACl

Molecule B 4NFAACc

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 219

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 220

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 221

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 222

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 223

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 224

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 225

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 226

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

EingenValues - Molecule B

531.43	913.309	1353.35

Different

FireTest Número 227

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

EingenValues - Molecule B

479.363	1242.41	1647.39

Different

FireTest Número 228

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 229

Molecule A 3NFAACm

Molecule B 4NFAACc

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 230

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 231

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 232

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 233

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 234

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 235

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 236

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 237

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

EingenValues - Molecule B

479.363	1242.41	1647.39

Different

FireTest Número 238

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Different

FireTest Número 239

Molecule A 3NFAACn

Molecule B 4NFAACc

Inertia Tensor - Molecule A

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

Inertia Tensor - Molecule B

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

531.43	913.309	1353.35

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 240

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 241

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 242

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 243

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 244

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 246

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 247

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

EingenValues - Molecule B

479.308	1242.41	1647.31

Enantiomers

FireTest Número 248

Molecule A 4NFAACa

Molecule B 4NFAACc

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 249

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 250

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 251

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 252

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 253

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 254

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 255

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 256

Molecule A 4NFAACb

Molecule B 4NFAACc

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

EingenValues - Molecule B

482.027	1240.32	1647.08

Different

FireTest Número 257

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 258

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 259

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

EingenValues - Molecule B

509.668	1219.11	1681.18

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

479.308	1242.41	1647.31

EingenValues - Molecule B

513.751	1208.07	1700.9

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 262

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 263

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 264

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

EingenValues - Molecule B

491.663	1231.14	1650.13

Different

FireTest Número 265

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 266

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 267

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 268

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 269

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 270

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 271

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

EingenValues - Molecule B

489.011	1233.7	1641.81

Different

FireTest Número 272

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 273

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 274

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 275

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 276

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 277

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

EingenValues - Molecule B

509.668	1219.11	1681.18

Different

FireTest Número 278

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 279

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

EingenValues - Molecule B

502.409	1232.26	1676.02

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

489.011	1233.7	1641.81

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 281

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 282

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

EingenValues - Molecule B

513.751	1208.07	1700.9

Different

FireTest Número 283

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 284

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 285

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 286

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

EingenValues - Molecule B

502.409	1232.26	1676.02

Different

FireTest Número 287

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 288

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

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 289

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

EingenValues - Molecule B

509.897	1225.65	1680.83

Different

FireTest Número 290

Molecule A 4NFAACi

Molecule B 4NFAACl-3

Inertia Tensor - Molecule A

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

Inertia Tensor - Molecule B

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

EingenVectors - Molecule A

0.999991	0.000823447	0.00414923
0.000819608	-0.999999	0.00092687
-0.00414999	0.000923461	0.999991

EingenVectors - Molecule B

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

EingenValues - Molecule A

502.409	1232.26	1676.02

EingenValues - Molecule B

506.607	1222.36	1678.43

Different

FireTest Número 291

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

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_invertion

Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

EingenVectors - Molecule A

-0.869274	0.494331	0
0.494331	0.869274	0
0	0	1

EingenVectors - Molecule B

-0.869273	0.494332	0
0.494332	0.869273	0
0	0	1

EingenValues - Molecule A

118.683	204.724	205.419

EingenValues - Molecule B

118.684	204.724	205.419

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

EingenValues - Molecule B

120.611	177.08	272.075

Different

IsomerC6H14 Número 294

Molecule A 2,2-dimethyl-butane_out_G09

Molecule B

2,3-dimethyl-butane_out_G09_invertion

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

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

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_invertion

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

-0.869274	0.494331	0
0.494331	0.869274	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

118.683	204.724	205.419

EingenValues - Molecule B

76.7699	299.061	347.558

Different

IsomerC6H14 Número 297

Molecule A 2,2-dimethyl-butane_out_G09

Molecule B 3-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

$$\begin{vmatrix} 294.318 & 21.9352 & 0 \\ 21.9352 & 302.288 & 0 \\ 0 & 0 & 77.8079 \end{vmatrix}$$

EingenVectors - Molecule A

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

EingenVectors - Molecule B

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.767709 & 0.640799 & 0 \\ 0.640799 & 0.767709 & 0 \end{vmatrix}$$

EingenValues - Molecule A

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

EingenValues - Molecule B

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

Different

IsomerC6H14 Número 298

Molecule A 2,2-dimethyl-butane_out_G09

Molecule B

3-methyl-pentane_out_G09_invertion

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

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

Inertia Tensor - Molecule B

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

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

EingenValues - Molecule B

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

Different

IsomerC6H14 Número 300

Molecule A 2,2-dimethyl-butane_out_G09

Molecule B hexane_out_G09_invertion

Inertia Tensor - Molecule A

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

Inertia Tensor - Molecule B

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

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

EingenValues - Molecule B

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

Different

IsomerC6H14 Número 301

Molecule A

2,2-dimethyl-butane_out_G09_invertion

Molecule B 2,3-dimethyl-butane_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

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

$$\begin{vmatrix} -0.112876 & -0.993609 & 0 \\ 0 & 0 & 1 \\ 0.993609 & -0.112876 & -0 \end{vmatrix}$$

EingenValues - Molecule A

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

EingenValues - Molecule B

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

Different

IsomerC6H14 Número 302

Molecule A

2,2-dimethyl-butane_out_G09_invertion

Molecule B

2,3-dimethyl-butane_out_G09_invertion

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_invertion

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_invertion

Molecule B

2-methyl-pentane_out_G09_invertion

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_invertion

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_invertion

Molecule B

3-methyl-pentane_out_G09_invertion

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_invertion

Molecule B hexane_out_G09

Inertia Tensor - Molecule A

139.709	36.9725	0
36.9725	183.699	0
0	0	205.419

Inertia Tensor - Molecule B

346.244	-179.129	0
-179.129	137.676	0
0	0	465.177

EingenVectors - Molecule A

-0.869273	0.494332	0
0.494332	0.869273	0
0	0	1

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

EingenValues - Molecule A

118.684	204.724	205.419

EingenValues - Molecule B

34.6869	449.234	465.177

Different

IsomerC6H14 Número 308

Molecule A

2,2-dimethyl-butane_out_G09_invertion

Molecule B hexane_out_G09_invertion

Inertia Tensor - Molecule A

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

Inertia Tensor - Molecule B

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

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

EingenValues - Molecule B

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

Different

IsomerC6H14 Número 309

Molecule A 2,3-dimethyl-butane_out_G09

Molecule B

2,3-dimethyl-butane_out_G09_invertion

Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

Inertia Tensor - Molecule B

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

EingenVectors - Molecule A

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

EingenVectors - Molecule B

-0.112875	-0.993609	0
0	0	1
0.993609	-0.112875	-0

EingenValues - Molecule A

120.611	177.08	272.075

EingenValues - Molecule B

120.611	177.08	272.076

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

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_invertion

Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

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

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

EingenVectors - Molecule B

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

EingenValues - Molecule A

120.611	177.08	272.075

EingenValues - Molecule B

76.7699	299.061	347.558

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

EingenValues - Molecule B

77.8079	276.009	320.597

Different

IsomerC6H14 Número 313

Molecule A 2,3-dimethyl-butane_out_G09

Molecule B

3-methyl-pentane_out_G09_invertion

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

-0.112876	-0.993609	0
0	0	1
0.993609	-0.112876	-0

EingenVectors - Molecule B

0	0	1
-0.76771	0.640798	0
0.640798	0.76771	0

EingenValues - Molecule A

120.611	177.08	272.075

EingenValues - Molecule B

77.8081	276.009	320.598

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

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_invertion

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

EingenValues - Molecule B

34.6868	449.234	465.177

Different

IsomerC6H14 Número 316

Molecule A

2,3-dimethyl-butane_out_G09_invertion

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

-0.112875	-0.993609	0
0	0	1
0.993609	-0.112875	-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	272.076

EingenValues - Molecule B

76.7698	299.061	347.558

Different

IsomerC6H14 Número 317

Molecule A

2,3-dimethyl-butane_out_G09_invertion

Molecule B

2-methyl-pentane_out_G09_invertion

Inertia Tensor - Molecule A

270.146	-16.9873	0
-16.9873	122.541	0
0	0	177.08

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

-0.112875	-0.993609	0
0	0	1
0.993609	-0.112875	-0

EingenVectors - Molecule B

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

EingenValues - Molecule A

120.611	177.08	272.076

EingenValues - Molecule B

76.7699	299.061	347.558

Different

IsomerC6H14 Número 318

Molecule A

2,3-dimethyl-butane_out_G09_invertion

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

EingenValues - Molecule B

77.8079	276.009	320.597

Different

IsomerC6H14 Número 319

Molecule A

2,3-dimethyl-butane_out_G09_invertion

Molecule B

3-methyl-pentane_out_G09_invertion

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_invertion

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

-0.112875	-0.993609	0
0	0	1
0.993609	-0.112875	-0

EingenVectors - Molecule B

-0.498436	-0.866927	0
0.866927	-0.498436	-0
0	0	1

EingenValues - Molecule A

120.611	177.08	272.076

EingenValues - Molecule B

34.6869	449.234	465.177

Different

IsomerC6H14 Número 321

Molecule A

2,3-dimethyl-butane_out_G09_invertion

Molecule B hexane_out_G09_invertion

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_invertion

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

EingenValues - Molecule B

76.7699	299.061	347.558

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

EingenValues - Molecule B

77.8079	276.009	320.597

Different

IsomerC6H14 Número 324

Molecule A 2-methyl-pentane_out_G09

Molecule B

3-methyl-pentane_out_G09_invertion

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	21.9353	0
21.9353	302.289	0
0	0	77.8081

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
-0.76771	0.640798	0
0.640798	0.76771	0

EingenValues - Molecule A

76.7698	299.061	347.558

EingenValues - Molecule B

77.8081	276.009	320.598

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

EingenValues - Molecule B

34.6869	449.234	465.177

Different

IsomerC6H14 Número 326

Molecule A 2-methyl-pentane_out_G09

Molecule B hexane_out_G09_invertion

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

EingenValues - Molecule B

34.6868	449.234	465.177

Different

IsomerC6H14 Número 327

Molecule A

2-methyl-pentane_out_G09_invertion

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

EingenValues - Molecule B

77.8079	276.009	320.597

Different

IsomerC6H14 Número 328

Molecule A

2-methyl-pentane_out_G09_invertion

Molecule B

3-methyl-pentane_out_G09_invertion

Inertia Tensor - Molecule A

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

Inertia Tensor - Molecule B

294.318	21.9353	0
21.9353	302.289	0
0	0	77.8081

EingenVectors - Molecule A

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

EingenVectors - Molecule B

0	0	1
-0.76771	0.640798	0
0.640798	0.76771	0

EingenValues - Molecule A

76.7699	299.061	347.558

EingenValues - Molecule B

77.8081	276.009	320.598

Different

IsomerC6H14 Número 329

Molecule A

2-methyl-pentane_out_G09_invertion

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_invertion

Molecule B hexane_out_G09_invertion

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_invertion

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

EingenValues - Molecule B

34.6869	449.234	465.177

Different

IsomerC6H14 Número 333

Molecule A 3-methyl-pentane_out_G09

Molecule B hexane_out_G09_invertion

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

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

EingenVectors - Molecule A

$$\begin{vmatrix} 0 & 0 & 1 \\ -0.767709 & 0.640799 & 0 \\ 0.640799 & 0.767709 & 0 \end{vmatrix}$$

EingenVectors - Molecule B

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

EingenValues - Molecule A

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

EingenValues - Molecule B

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

Different

IsomerC6H14 Número 334

Molecule A

3-methyl-pentane_out_G09_invertion

Molecule B hexane_out_G09

Inertia Tensor - Molecule A

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

Inertia Tensor - Molecule B

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

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

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

EingenValues - Molecule B

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

Different

IsomerC6H14 Número 335

Molecule A

3-methyl-pentane_out_G09_invertion

Molecule B hexane_out_G09_invertion

Inertia Tensor - Molecule A

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

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

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

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

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_invertion

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

NeoConformation Número 337

Molecule A neopentane_Symmetry_out_G09

Molecule B

neopentane_Symmetry_out_G09_invertion

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

Enantiomers

NeoConformation Número 338

Molecule A neopentane_Symmetry_out_G09

Molecule B neopentane_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

Enantiomers

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

Enantiomers

NeoConformation Número 340

Molecule A neopentane_Symmetry_out_G09

Molecule B neopentane_out_G09_invertion

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

Enantiomers

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

Enantiomers

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_invertion

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_invertion

Different

NeoConformation Número 347

Molecule A

neopentane_Symmetry_out_G09_invertion

Molecule B neopentane_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_invertion

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

Enantiomers

NeoConformation Número 349

Molecule A

neopentane_Symmetry_out_G09_invertion

Molecule B neopentane_out_G09_invertion

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

Enantiomers

NeoConformation Número 350

Molecule A

neopentane_Symmetry_out_G09_invertion

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

Enantiomers

NeoConformation Número 351

Molecule A

neopentane_Symmetry_out_G09_invertion

Molecule B

tert-butylamine_out_G09

Different

NeoConformation Número 352

Molecule A

neopentane_Symmetry_out_G09_invertion

Molecule B

tert-butylamine_out_G09_invertion

Different

NeoConformation Número 353

Molecule A

neopentane_Symmetry_out_G09_invertion

Molecule B

tert-butylamine_out_G09_rot_x15_y15_z15

Different

NeoConformation Número 354

Molecule A

neopentane_Symmetry_out_G09_invertion

Molecule B

tetramethylsilane_out_G09

Different

NeoConformation Número 355

Molecule A

neopentane_Symmetry_out_G09_invertion

Molecule B

tetramethylsilane_out_G09_invertion

Different

NeoConformation Número 356

Molecule A neopentane_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

EingenValues - Molecule B

114.662	114.667	114.672

Enantiomers

NeoConformation Número 357

Molecule A neopentane_Symmetry_out_G09_rot_x45_y45_z60

Molecule B neopentane_out_G09_invertion

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

Enantiomers

NeoConformation Número 358

Molecule A neopentane_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	0.00148446	0.00262579
0.00148446	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

Enantiomers

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_invertion

Different

NeoConformation Número 361

Molecule A

neopentane_Symmetry_out_G09_rot_x45_y45_z60

Molecule B

tert-butylamine_out_G09_rot_x15_y15_z15

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_invertion

Different

NeoConformation Número 364

Molecule A neopentane_out_G09

Molecule B neopentane_out_G09_invertion

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

EingenValues - Molecule B

114.662	114.667	114.672

Enantiomers

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	0.00148446	0.00262579
0.00148446	114.666	0.000207396
0.00262579	0.000207396	114.671

EingenVectors - Molecule A

-0.999133	0.0364989	0.020046
-0.0375297	-0.997851	-0.053713
0.0180425	-0.0544187	0.998355

EingenVectors - Molecule B

0.919257	-0.288184	-0.268173
-0.236481	-0.948878	0.209061
0.314712	0.128763	0.940413

EingenValues - Molecule A

114.662	114.667	114.672

EingenValues - Molecule B

114.662	114.667	114.672

Enantiomers

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_invertion

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_invertion

Different

NeoConformation Número 371

Molecule A neopentane_out_G09_invertion

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

Enantiomers

NeoConformation Número 372

Molecule A

neopentane_out_G09_invertion

Molecule B

tert-butylamine_out_G09

Different

NeoConformation Número 373

Molecule A

neopentane_out_G09_invertion

Molecule B

tert-butylamine_out_G09_invertion

Different

NeoConformation Número 374

Molecule A

neopentane_out_G09_invertion

Molecule B

tert-butylamine_out_G09_rot_x15_y15_z15

Different

NeoConformation Número 375

Molecule A

neopentane_out_G09_invertion

Molecule B

tetramethylsilane_out_G09

Different

NeoConformation Número 376

Molecule A

neopentane_out_G09_invertion

Molecule B

tetramethylsilane_out_G09_invertion

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_invertion

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_invertion

Different

NeoConformation Número 382

Molecule A tert-butylamine_out_G09

Molecule B

tert-butylamine_out_G09_invertion

Inertia Tensor - Molecule A

110.655	-1.46159e-05	4.47474e-05
-1.46159e-05	111.529	0.82631
4.47474e-05	0.82631	113.378

Inertia Tensor - Molecule B

110.655	-4.00493e-05	5.05193e-05
-4.00493e-05	111.529	0.826271
5.05193e-05	0.826271	113.378

EingenVectors - Molecule A

-1	-4.53031e-05	3.01901e-05
5.30915e-05	-0.934229	0.356674
1.2046e-05	0.356674	0.934229

EingenVectors - Molecule B

-1	-8.8937e-05	4.55534e-05
9.93354e-05	-0.934224	0.356687
1.08344e-05	0.356687	0.934224

EingenValues - Molecule A

110.655	111.213	113.693

EingenValues - Molecule B

110.655	111.213	113.693

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

tert-butylamine_out_G09

Molecule B

tetramethylsilane_out_G09

Different

NeoConformation Número 385

Molecule A

tert-butylamine_out_G09

Molecule B

tetramethylsilane_out_G09_invertion

Different

NeoConformation Número 386

Molecule A

tert-butylamine_out_G09_invertion

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_invertion

Molecule B

tetramethylsilane_out_G09

Different

NeoConformation Número 388

Molecule A

tert-butylamine_out_G09_invertion

Molecule B

tetramethylsilane_out_G09_invertion

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_invertion

Different

NeoConformation Número 391

Molecule A tetramethylsilane_out_G09

Molecule B

tetramethylsilane_out_G09_invertion

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_invertion

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

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

Enantiomers

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_invertion

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_invertion

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_invertion

Different

RotationSameMolecule Número 399

Molecule A

Porphin_out_G09_invertion

Molecule B

Tetrabenzoporphyrin_out_G09

Different

RotationSameMolecule Número 400

Molecule A

Porphin_out_G09_invertion

Molecule B

Tetrabenzoporphyrin_out_G09_invertion

Different

RotationSameMolecule Número 401

Molecule A

Porphin_out_G09_invertion

Molecule B

Tetrabenzoporphyrin_rotated02_out_G09

Different

RotationSameMolecule Número 402

Molecule A

Porphin_out_G09_invertion

Molecule B

Tetrabenzoporphyrin_rotated02_out_G09_invertion

Different

RotationSameMolecule Número 403

Molecule A

Porphin_out_G09_invertion

Molecule B

Tetrabenzoporphyrin_rotated_out_G09

Different

RotationSameMolecule Número 404

Molecule A

Porphin_out_G09_invertion

Molecule B

Tetrabenzoporphyrin_rotated_out_G09_invertion

Different

RotationSameMolecule Número 405

Molecule A Tetrabenzoporphyrin_out_G09

Molecule B

Tetrabenzoporphyrin_out_G09_invertion

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

RotationSameMolecule Número 407

Molecule A Tetrabenzoporphyrin_out_G09

Molecule B Tetrabenzopor-phyrin_rotated02_out_G09_invertion

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 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_invertion

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 410

Molecule A

Tetrabenzoporphyrin_out_G09_invertion

Molecule B

Tetrabenzoporphyrin_rotated02_out_G09

Inertia Tensor - Molecule A

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

Inertia Tensor - Molecule B

$$\begin{vmatrix} 7791.57 & 2641.52 & -788.168 \\ 2641.52 & 9673.67 & -1103.82 \\ -788.168 & -1103.82 & 6265.27 \end{vmatrix}$$

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

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

EingenValues - Molecule B

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

Enantiomers

RotationSameMolecule Número 411

Molecule A

Tetrabenzoporphyrin_out_G09_invertion

Molecule B Tetrabenzoporphyrin_rotated02_out_G09_invertion

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

Tetrabenzoporphyrin_out_G09_invertion

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 413

Molecule A

Tetrabenzoporphyrin_out_G09_invertion

Molecule B Tetrabenzoporphyrin_rotated_out_G09_invertion

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_invertion

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

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 416

Molecule A

Tetrabenzoporphyrin_rotated02_out_G09

Molecule B Tetrabenzoporphyrin_rotated_out_G09_invertion

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_invertion

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

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 418

Molecule A Tetrabenzoporphyrin_rotated02_out_G09_invertion

Molecule B Tetrabenzoporphyrin_rotated_out_G09_invertion

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_invertion

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

EingenValues - Molecule B

257.858	1154.77	1276.75

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

EingenValues - Molecule B

203.032	1215.85	1332.21

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

EingenValues - Molecule B

214.698	1187.04	1322.41

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

EingenValues - Molecule B

214.739	1186.84	1322.13

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

EingenValues - Molecule B

203.048	1215.85	1332.24

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

EingenValues - Molecule B

257.845	1154.78	1276.78

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

EingenValues - Molecule B

224.041	1180.31	1363.9

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

EingenValues - Molecule B

203.032	1215.85	1332.21

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

EingenValues - Molecule B

214.698	1187.04	1322.41

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

EingenValues - Molecule B

214.739	1186.84	1322.13

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

EingenValues - Molecule B

203.048	1215.85	1332.24

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

EingenValues - Molecule B

257.845	1154.78	1276.78

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

EingenValues - Molecule B

224.041	1180.31	1363.9

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

EingenValues - Molecule B

214.698	1187.04	1322.41

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

EingenValues - Molecule B

214.739	1186.84	1322.13

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

EingenValues - Molecule B

203.048	1215.85	1332.24

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

EingenValues - Molecule B

257.845	1154.78	1276.78

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

EingenValues - Molecule B

224.041	1180.31	1363.9

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

EingenValues - Molecule B

214.739	1186.84	1322.13

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

EingenValues - Molecule B

203.048	1215.85	1332.24

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

EingenValues - Molecule B

257.845	1154.78	1276.78

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

EingenValues - Molecule B

224.041	1180.31	1363.9

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

EingenValues - Molecule B

203.048	1215.85	1332.24

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

EingenValues - Molecule B

257.845	1154.78	1276.78

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

EingenValues - Molecule B

224.041	1180.31	1363.9

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

EingenValues - Molecule B

257.845	1154.78	1276.78

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

EingenValues - Molecule B

224.041	1180.31	1363.9

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

EingenValues - Molecule B

224.041	1180.31	1363.9

Different

SymmetricEnantiomers Número 448

Molecule A r-enan_out_G09

Molecule B

r-enan_out_G09_invertion_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

EingenValues - Molecule B

103.739	629.815	722.22

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

EingenValues - Molecule B

103.739	629.816	722.221

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

EingenValues - Molecule B

103.701	630.077	722.452

Enantiomers

SymmetricEnantiomers Número 451

Molecule A r-enan_out_G09

Molecule B

s-enan_out_G09_invertion_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

EingenValues - Molecule B

103.7	630.079	722.455

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

EingenValues - Molecule B

103.701	630.077	722.452

Enantiomers

SymmetricEnantiomers Número 453

Molecule A

r-enan_out_G09_invertion_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

103.745	1.51033	1.05456
1.51033	629.842	1.67376
1.05456	1.67376	722.189

EingenVectors - Molecule A

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

EingenVectors - Molecule B

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

EingenValues - Molecule A

103.739	629.815	722.22

EingenValues - Molecule B

103.739	629.816	722.221

Enantiomers

SymmetricEnantiomers Número 454

Molecule A

r-enan_out_G09_invertion_output

Molecule B s-enan_out_G09

Inertia Tensor - Molecule A

$$\begin{vmatrix} 103.745 & 1.51041 & 1.05457 \\ 1.51041 & 629.841 & 1.67376 \\ 1.05457 & 1.67376 & 722.187 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 103.707 & -1.51142 & -1.05403 \\ -1.51142 & 630.103 & 1.67204 \\ -1.05403 & 1.67204 & 722.42 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.999994 & 0.00286553 & 0.00169742 \\ -0.00283425 & -0.999831 & 0.018149 \\ 0.00174914 & 0.0181441 & 0.999834 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999994 & -0.00286582 & -0.00169581 \\ 0.0028346 & -0.999832 & 0.018136 \\ -0.0017475 & 0.0181311 & 0.999834 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 103.739 & 629.815 & 722.22 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 103.701 & 630.077 & 722.452 \end{vmatrix}$$

Equal

SymmetricEnantiomers Número 455

Molecule A

r-enan_out_G09_invertion_output

Molecule B

s-enan_out_G09_invertion_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

EingenValues - Molecule B

103.7	630.079	722.455

Enantiomers

SymmetricEnantiomers Número 456

Molecule A

r-enan_out_G09_invertion_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

EingenValues - Molecule B

103.701	630.077	722.452

Equal

SymmetricEnantiomers Número 457

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

EingenValues - Molecule B

103.701	630.077	722.452

Enantiomers

SymmetricEnantiomers Número 458

Molecule A r-enan_rotated_out_G09

Molecule B

s-enan_out_G09_invertion_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

EingenValues - Molecule B

103.7	630.079	722.455

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

EingenValues - Molecule B

103.701	630.077	722.452

Enantiomers

SymmetricEnantiomers Número 460

Molecule A s-enan_out_G09

Molecule B

s-enan_out_G09_invertion_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

EingenValues - Molecule B

103.7	630.079	722.455

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

EingenValues - Molecule B

103.701	630.077	722.452

Equal

SymmetricEnantiomers Número 462

Molecule A

s-enan_out_G09_invertion_output

Molecule B s-enan_rotated_out_G09

Inertia Tensor - Molecule A

$$\begin{vmatrix} 103.707 & -1.51147 & -1.05403 \\ -1.51147 & 630.105 & 1.67201 \\ -1.05403 & 1.67201 & 722.422 \end{vmatrix}$$

Inertia Tensor - Molecule B

$$\begin{vmatrix} 103.707 & -1.51138 & -1.05403 \\ -1.51138 & 630.103 & 1.67204 \\ -1.05403 & 1.67204 & 722.42 \end{vmatrix}$$

EingenVectors - Molecule A

$$\begin{vmatrix} -0.999994 & -0.0028659 & -0.0016958 \\ 0.00283468 & -0.999832 & 0.0181359 \\ -0.00174749 & 0.018131 & 0.999834 \end{vmatrix}$$

EingenVectors - Molecule B

$$\begin{vmatrix} -0.999994 & -0.00286575 & -0.00169582 \\ 0.00283453 & -0.999832 & 0.018136 \\ -0.0017475 & 0.0181311 & 0.999834 \end{vmatrix}$$

EingenValues - Molecule A

$$\begin{vmatrix} 103.7 & 630.079 & 722.455 \end{vmatrix}$$

EingenValues - Molecule B

$$\begin{vmatrix} 103.701 & 630.077 & 722.452 \end{vmatrix}$$

Enantiomers

TesisExample Número 463

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

EingenValues - Molecule B

146.173	442.909	530.735

Enantiomers

#	Moléculas	Restultado esperado	Resultado programa
1	r-2-chlorobutane_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	r-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	RMS = 0.02719433	
2	r-2-chlorobutane_out_G09 E = No Data Freq =No Data	Equal	Equal
	r-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	RMS = 1.236488E-09	
3	r-2-chlorobutane_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-2-chlorobutane_out_G09 E = No Data Freq =No Data	RMS = 0.2294273	
4	r-2-chlorobutane_out_G09 E = No Data Freq =No Data	Equal	Equal
	s-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	RMS = 4.044324E-06	
5	r-2-chlorobutane_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.2294272	
6	r-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	Enantiomers	Enantiomers
	r-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.02719433	
7	r-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	Equal	Equal
	s-2-chlorobutane_out_G09 E = No Data Freq =No Data	RMS = 4.366941E-07	

#	Moléculas	Restultado esperado	Resultado programa
8	r-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	RMS = 0.2294318	
9	r-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	Equal	Equal
	s-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	RMS = 5.673033E-07	
10	r-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-2-chlorobutane_out_G09 E = No Data Freq =No Data	RMS = 0.2294273	
11	r-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	Equal	Equal
	s-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	RMS = 4.043088E-06	
12	r-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.2294272	
13	s-2-chlorobutane_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	RMS = 0.02719881	
14	s-2-chlorobutane_out_G09 E = No Data Freq =No Data	Equal	Equal
	s-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	RMS = 1.306092E-07	

#	Moléculas	Restultado esperado	Resultado programa
15	s-2-chlorobutane_out_G09_inversion E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-2-chlorobutane_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.02719894	
16	3NFAACa E = No Data Freq =No Data	**Equal**	**Enantiomers**
	3NFAACb E = No Data Freq =No Data	RMS = 0.02603601	
17	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACc E = No Data Freq =No Data	RMS = 0.0334016	
18	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACd E = No Data Freq =No Data	RMS = 0.0888511	
19	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACe E = No Data Freq =No Data	RMS = 0.162132	
20	3NFAACa E = No Data Freq =No Data	**Equal**	**Enantiomers**
	3NFAACf E = No Data Freq =No Data	RMS = 0.02649945	
21	3NFAACa E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data	RMS = 0.0330848	

#	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	
32	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data	RMS = 0.0149078	
33	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data	RMS = 0.0228438	
34	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data	RMS = 0.118302	
35	3NFAACa E = No Data Freq =No Data	Different	Different
	4NFAACg E = No Data Freq =No Data	RMS = 0.0338585	

#	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	
39	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACc E = No Data Freq =No Data	RMS = 0.0881291	
40	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACd E = No Data Freq =No Data	RMS = 0.143579	
41	3NFAACb E = No Data Freq =No Data	Different	Different
	3NFAACe E = No Data Freq =No Data	RMS = 0.107404	
42	3NFAACb E = No Data Freq =No Data	**Equal**	**Enantiomers**
	3NFAACf E = No Data Freq =No Data	RMS = 0.0004634431	

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

#	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	
81	3NFAACc E = No Data Freq =No Data	Different	Different
	4NFAACl-3 E = No Data Freq =No Data	RMS = 0.0748842	
82	3NFAACd E = No Data Freq =No Data	**Equal**	**Enantiomers**
	3NFAACe E = No Data Freq =No Data	RMS = 0.0004675477	
83	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACf E = No Data Freq =No Data	RMS = 0.143418	
84	3NFAACd E = No Data Freq =No Data	Different	Different
	3NFAACg E = No Data Freq =No Data	RMS = 0.0557663	

#	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	
95	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data	RMS = 0.103759	
96	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data	RMS = 0.111695	
97	3NFAACd E = No Data Freq =No Data	Different	Different
	4NFAACf E = No Data Freq =No Data	RMS = 0.207153	
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	
130	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACb E = No Data Freq =No Data	RMS = 0.203875	
131	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACc E = No Data Freq =No Data	RMS = 0.0359411	
132	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACd E = No Data Freq =No Data	RMS = 0.0396588	
133	3NFAACf E = No Data Freq =No Data	Different	Different
	4NFAACe E = No Data Freq =No Data	RMS = 0.0317228	

#	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	Enantiomers
	3NFAACm E = No Data Freq =No Data	RMS = 0.02978757	
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 E = No Data Freq =No Data	Equal	Equal
	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	RMS = 0	
293	2,2-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	RMS = 0.269312	
294	2,2-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.269312	

#	Moléculas	Restultado esperado	Resultado programa
295	2,2-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	2-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.0426031	
296	2,2-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0778147	
297	2,2-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.766027	
298	2,2-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.766028	
299	2,2-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	hexane_out_G09 E = No Data Freq =No Data	RMS = 0	
300	2,2-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0	
301	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	RMS = 0.269312	

#	Moléculas	Restultado esperado	Resultado programa
302	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.269312	
303	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	2-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.0426031	
304	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0778147	
305	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.766027	
306	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.766028	
307	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	hexane_out_G09 E = No Data Freq =No Data	RMS = 0	
308	2,2-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0	

#	Moléculas	Restultado esperado	Resultado programa
309	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	Equal	Equal
	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	RMS = 1.773561E-07	
310	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	2-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.311916	
311	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.191498	
312	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.496715	
313	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.496715	
314	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	hexane_out_G09 E = No Data Freq =No Data	RMS = 0.269312	
315	2,3-dimethyl-butane_out_G09 E = No Data Freq =No Data	Different	Different
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.269312	

#	Moléculas	Restultado esperado	Resultado programa
316	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	2-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.311915	
317	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.191497	
318	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.496715	
319	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.496716	
320	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	hexane_out_G09 E = No Data Freq =No Data	RMS = 0.269312	
321	2,3-dimethyl-butane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.269312	
322	2-methyl-pentane_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.1203334	

#	Moléculas	Restultado esperado	Resultado programa
323	2-methyl-pentane_out_G09 E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.80863	
324	2-methyl-pentane_out_G09 E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.808631	
325	2-methyl-pentane_out_G09 E = No Data Freq =No Data	Different	Different
	hexane_out_G09 E = No Data Freq =No Data	RMS = 0.0426031	
326	2-methyl-pentane_out_G09 E = No Data Freq =No Data	Different	Different
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0426031	
327	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09 E = No Data Freq =No Data	RMS = 0.688213	
328	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.688213	
329	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	hexane_out_G09 E = No Data Freq =No Data	RMS = 0.0778147	

#	Moléculas	Restultado esperado	Resultado programa
330	2-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0778147	
331	3-methyl-pentane_out_G09 E = No Data Freq =No Data	Equal	Equal
	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	RMS = 2.333815E-07	
332	3-methyl-pentane_out_G09 E = No Data Freq =No Data	Different	Different
	hexane_out_G09 E = No Data Freq =No Data	RMS = 0.766027	
333	3-methyl-pentane_out_G09 E = No Data Freq =No Data	Different	Different
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.766027	
334	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	hexane_out_G09 E = No Data Freq =No Data	RMS = 0.766028	
335	3-methyl-pentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.766028	
336	hexane_out_G09 E = No Data Freq =No Data	Equal	Equal
	hexane_out_G09_invertion E = No Data Freq =No Data	RMS = 0	

#	Moléculas	Restultado esperado	Resultado programa
337	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	RMS = 0.08661368	
338	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	RMS = 0.002619224	
339	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09 E = No Data Freq =No Data	RMS = 0.0005811388	
340	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.08655257	
341	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	RMS = 0.002335402	
342	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09 E = No Data Freq =No Data	RMS = 0.0603092	
343	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0603092	

#	Moléculas	Restultado esperado	Resultado programa
344	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	**Equal**	**Different**
	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	RMS = 0.0603092	
345	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.0587334	
346	neopentane_Symmetry_out_G09 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0587334	
347	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	Equal	Equal
	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	RMS = 3.444809E-09	
348	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09 E = No Data Freq =No Data	RMS = 0.08719482	
349	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_invertion E = No Data Freq =No Data	RMS = 6.111066E-05	
350	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	RMS = 0.08894908	

#	Moléculas	Restultado esperado	Resultado programa
351	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09 E = No Data Freq =No Data	RMS = 0.0319051	
352	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0319051	
353	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Different**
	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	RMS = 0.0319051	
354	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.150948	
355	neopentane_Symmetry_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.150948	
356	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09 E = No Data Freq =No Data	RMS = 0.002038085	
357	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0891718	

#	Moléculas	Restultado esperado	Resultado programa
358	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	RMS = 0.000283822	
359	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09 E = No Data Freq =No Data	RMS = 0.0533989	
360	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0533989	
361	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	RMS = 0.0533989	
362	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.172441	
363	neopentane_Symmetry_out_G09_rot_x45_y45_z60 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.172441	
364	neopentane_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.08713371	

#	Moléculas	Restultado esperado	Resultado programa
365	neopentane_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	RMS = 0.001754263	
366	neopentane_out_G09 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09 E = No Data Freq =No Data	RMS = 0.0603026	
367	neopentane_out_G09 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0603026	
368	neopentane_out_G09 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	RMS = 0.0603026	
369	neopentane_out_G09 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.0587399	
370	neopentane_out_G09 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0587399	
371	neopentane_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	RMS = 0.08888797	

#	Moléculas	Restultado esperado	Resultado programa
372	neopentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09 E = No Data Freq =No Data	RMS = 0.0319157	
373	neopentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0319157	
374	neopentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	RMS = 0.0319157	
375	neopentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.150958	
376	neopentane_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.150958	
377	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09 E = No Data Freq =No Data	RMS = 0.0670111	
378	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0670111	

#	Moléculas	Restultado esperado	Resultado programa
379	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	Different	Different
	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	RMS = 0.0670111	
380	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.0520314	
381	neopentane_out_G09_rot_x15-y15-z15 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0520314	
382	tert-butylamine_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	RMS = 0.09408316	
383	tert-butylamine_out_G09 E = No Data Freq =No Data	Equal	Equal
	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	RMS = 1.188653E-12	
384	tert-butylamine_out_G09 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.415062	
385	tert-butylamine_out_G09 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.415063	

#	Moléculas	Restultado esperado	Resultado programa
386	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	RMS = 0.09408316	
387	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.456096	
388	tert-butylamine_out_G09_invertion E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.456097	
389	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09 E = No Data Freq =No Data	RMS = 0.291987	
390	tert-butylamine_out_G09_rot_x15_y15_z15 E = No Data Freq =No Data	Different	Different
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0.291987	
391	tetramethylsilane_out_G09 E = No Data Freq =No Data	Equal	Equal
	tetramethylsilane_out_G09_invertion E = No Data Freq =No Data	RMS = 0	
392	Porphin_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Porphin_out_G09_invertion E = No Data Freq =No Data	RMS = 0	

#	Moléculas	Restultado esperado	Resultado programa
393	Porphin_out_G09 E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_out_G09 E = No Data Freq =No Data	RMS = 0.117363	
394	Porphin_out_G09 E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_out_G09_invertion E = No Data Freq =No Data	RMS = 0.117363	
395	Porphin_out_G09 E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09 E = No Data Freq =No Data	RMS = 0.167859	
396	Porphin_out_G09 E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09_invertion E = No Data Freq =No Data	RMS = 0.167858	
397	Porphin_out_G09 E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.117363	
398	Porphin_out_G09 E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09_invertion E = No Data Freq =No Data	RMS = 0.117363	
399	Porphin_out_G09_invertion E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_out_G09 E = No Data Freq =No Data	RMS = 0.117363	

#	Moléculas	Restultado esperado	Resultado programa
400	Porphin_out_G09_invertion E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_out_G09_invertion E = No Data Freq =No Data	RMS = 0.117363	
401	Porphin_out_G09_invertion E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09 E = No Data Freq =No Data	RMS = 0.167859	
402	Porphin_out_G09_invertion E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_rotated02_out_G09_invertion E = No Data Freq =No Data	RMS = 0.167858	
403	Porphin_out_G09_invertion E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.117363	
404	Porphin_out_G09_invertion E = No Data Freq =No Data	Different	Different
	Tetrabenzoporphyrin_rotated_out_G09_invertion E = No Data Freq =No Data	RMS = 0.117363	
405	Tetrabenzoporphyrin_out_G09 E = No Data Freq =No Data	Equal	Equal
	Tetrabenzoporphyrin_out_G09_invertion E = No Data Freq =No Data	RMS = 0	
406	Tetrabenzoporphyrin_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Tetrabenzoporphyrin_rotated02_out_G09 E = No Data Freq =No Data	RMS = 0.0001074955	

#	Moléculas	Restultado esperado	Resultado programa
407	Tetrabenzoporphyrin_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Tetrabenzoporphyrin_rotated02_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0001075617	
408	Tetrabenzoporphyrin_out_G09 E = No Data Freq =No Data	Equal	Equal
	Tetrabenzoporphyrin_rotated_out_G09 E = No Data Freq =No Data	RMS = 0	
409	Tetrabenzoporphyrin_out_G09 E = No Data Freq =No Data	Equal	Equal
	Tetrabenzoporphyrin_rotated_out_G09_invertion E = No Data Freq =No Data	RMS = 0	
410	Tetrabenzoporphyrin_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Tetrabenzoporphyrin_rotated02_out_G09 E = No Data Freq =No Data	RMS = 0.0001074955	
411	Tetrabenzoporphyrin_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Tetrabenzoporphyrin_rotated02_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0001075617	
412	Tetrabenzoporphyrin_out_G09_invertion E = No Data Freq =No Data	Equal	Equal
	Tetrabenzoporphyrin_rotated_out_G09 E = No Data Freq =No Data	RMS = 0	
413	Tetrabenzoporphyrin_out_G09_invertion E = No Data Freq =No Data	Equal	Equal
	Tetrabenzoporphyrin_rotated_out_G09_invertion E = No Data Freq =No Data	RMS = 0	

#	Moléculas	Restultado esperado	Resultado programa
414	Tetrabenzoporphyrin_rotated02_out_G09 E = No Data Freq =No Data	Equal	Equal
	Tetrabenzoporphyrin_rotated02_out_G09_invertion E = No Data Freq =No Data	RMS = 6.620476E-08	
415	Tetrabenzoporphyrin_rotated02_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Tetrabenzoporphyrin_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.0001074955	
416	Tetrabenzoporphyrin_rotated02_out_G09 E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Tetrabenzoporphyrin_rotated_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0001074955	
417	Tetrabenzoporphyrin_rotated02_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Tetrabenzoporphyrin_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.0001075617	
418	Tetrabenzoporphyrin_rotated02_out_G09_invertion E = No Data Freq =No Data	**Equal**	**Enantiomers**
	Tetrabenzoporphyrin_rotated_out_G09_invertion E = No Data Freq =No Data	RMS = 0.0001075617	
419	Tetrabenzoporphyrin_rotated_out_G09 E = No Data Freq =No Data	Equal	Equal
	Tetrabenzoporphyrin_rotated_out_G09_invertion E = No Data Freq =No Data	RMS = 0	
420	R-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	R-R-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.449321	

#	Moléculas	Restultado esperado	Resultado programa
421	R-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	R-S-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.274434	
422	R-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	R-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.404519	
423	R-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-R-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.299091	
424	R-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-R-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.269535	
425	R-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.327879	
426	R-R-R-Fructuose_out_G09 E = No Data Freq =No Data	**Enantiomers**	**Different**
	S-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.402361	
427	R-R-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	R-S-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.174888	

#	Moléculas	Restultado esperado	Resultado programa
428	R-R-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	R-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0448022	
429	R-R-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-R-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.15023	
430	R-R-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-R-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.179786	
431	R-R-S-Fructuose_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	S-S-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0005551068	
432	R-R-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0469601	
433	R-S-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	R-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.130085	
434	R-S-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-R-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0246573	

#	Moléculas	Restultado esperado	Resultado programa
435	R-S-R-Fructuose_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	S-R-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.005799255	
436	R-S-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0534457	
437	R-S-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.127928	
438	R-S-S-Fructuose_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	S-R-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0001020726	
439	R-S-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-R-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.134984	
440	R-S-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0766398	
441	R-S-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.00215791	

#	Moléculas	Restultado esperado	Resultado programa
442	S-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-R-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.029556	
443	S-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0287884	
444	S-R-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.10327	
445	S-R-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-R-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0583444	
446	S-R-S-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.132826	
447	S-S-R-Fructuose_out_G09 E = No Data Freq =No Data	Different	Different
	S-S-S-Fructuose_out_G09 E = No Data Freq =No Data	RMS = 0.0744819	
448	r-enan_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	r-enan_out_G09_invertion_output E = No Data Freq =No Data	RMS = 0.01735201	

#	Moléculas	Restultado esperado	Resultado programa
449	r-enan_out_G09 E = No Data Freq =No Data	Equal	Equal
	r-enan_rotated_out_G09 E = No Data Freq =No Data	RMS = 0	
450	r-enan_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-enan_out_G09 E = No Data Freq =No Data	RMS = 0.00506593	
451	r-enan_out_G09 E = No Data Freq =No Data	Equal	Equal
	s-enan_out_G09_invertion_output E = No Data Freq =No Data	RMS = 3.832848E-06	
452	r-enan_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-enan_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.005065924	
453	r-enan_out_G09_invertion_output E = No Data Freq =No Data	Enantiomers	Enantiomers
	r-enan_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.01735201	
454	r-enan_out_G09_invertion_output E = No Data Freq =No Data	Equal	Equal
	s-enan_out_G09 E = No Data Freq =No Data	RMS = 1.185059E-06	
455	r-enan_out_G09_invertion_output E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-enan_out_G09_invertion_output E = No Data Freq =No Data	RMS = 0.005068578	

#	Moléculas	Restultado esperado	Resultado programa
456	r-enan_out_G09_invertion_output E = No Data Freq =No Data	Equal	Equal
	s-enan_rotated_out_G09 E = No Data Freq =No Data	RMS = 1.178757E-06	
457	r-enan_rotated_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-enan_out_G09 E = No Data Freq =No Data	RMS = 0.00506593	
458	r-enan_rotated_out_G09 E = No Data Freq =No Data	Equal	Equal
	s-enan_out_G09_invertion_output E = No Data Freq =No Data	RMS = 3.832848E-06	
459	r-enan_rotated_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-enan_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.005065924	
460	s-enan_out_G09 E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-enan_out_G09_invertion_output E = No Data Freq =No Data	RMS = 0.01734936	
461	s-enan_out_G09 E = No Data Freq =No Data	Equal	Equal
	s-enan_rotated_out_G09 E = No Data Freq =No Data	RMS = 6.301958E-09	
462	s-enan_out_G09_invertion_output E = No Data Freq =No Data	Enantiomers	Enantiomers
	s-enan_rotated_out_G09 E = No Data Freq =No Data	RMS = 0.01734936	

<table>
<tr><th>#</th><th>Moléculas</th><th>Restultado esperado</th><th>Resultado programa</th></tr>
<tr><td rowspan="2">463</td><td>test-R_out_G09
E = No Data Freq =No Data</td><td rowspan="2">Enantiomers</td><td rowspan="2">Enantiomers</td></tr>
<tr><td>test-S_out_G09
E = No Data Freq =No Data</td></tr>
<tr><td></td><td></td><td colspan="2">RMS = 1.273513E-17</td></tr>
</table>

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 repositiorio del programa.