

SUPPORTING INFORMATION

Electron transport through the ruthenium-based extended metal atom chain (EMACS), $\text{Ru}_3(\text{dpa})_4\text{X}_2$.

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Figure S1 Zero-bias transmission spectra for ‘hollow’, ‘on-top’ and ‘tilted’ contact geometries.

Figure S2 Correlation of Ru-X bond length (and also energy) with angle in $\text{Ru}_3(\text{dpa})_4\text{Cl}_2$
and $\text{Ru}_3(\text{dpa})_4(\text{CN})_2$

Figure S3 Comparison of transmission spectra for (a) linear $\text{Ru}_3(\text{dpa})_4(\text{NCS})_2$, unrestricted (b)
linear $\text{Ru}_3(\text{dpa})_4(\text{NCS})_2$, restricted (i.e. singlet) and (c) bent $\text{Ru}_3(\text{dpa})_4(\text{NCS})_2$ (restricted
and unrestricted calculations converge to the same closed-shell density).

Table S1 Full Cartesian coordinates for all stationary points.

Table S2 Full Cartesian coordinates for scattering regions in the transport calculations.

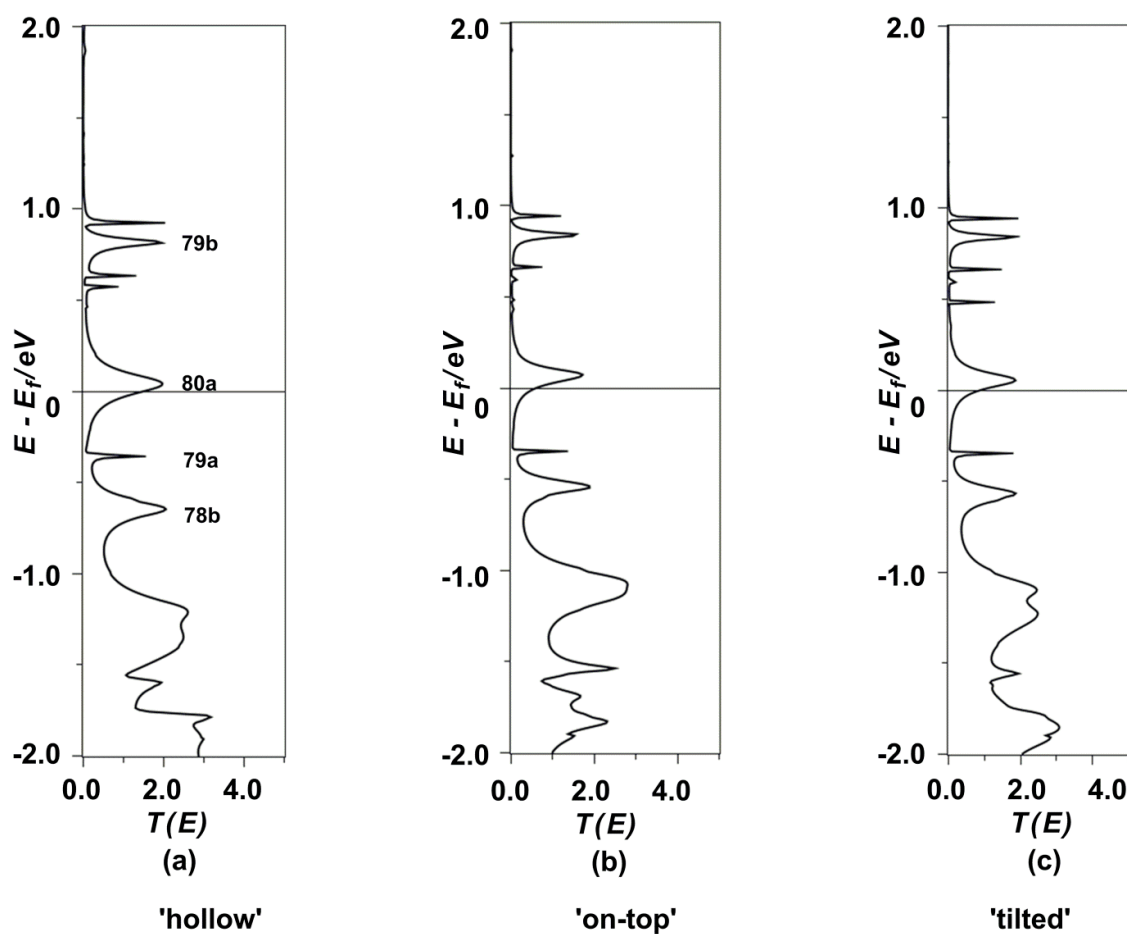


Figure S1 Zero-bias transmission spectra for 'hollow', 'on-top' and 'tilted' contact geometries.

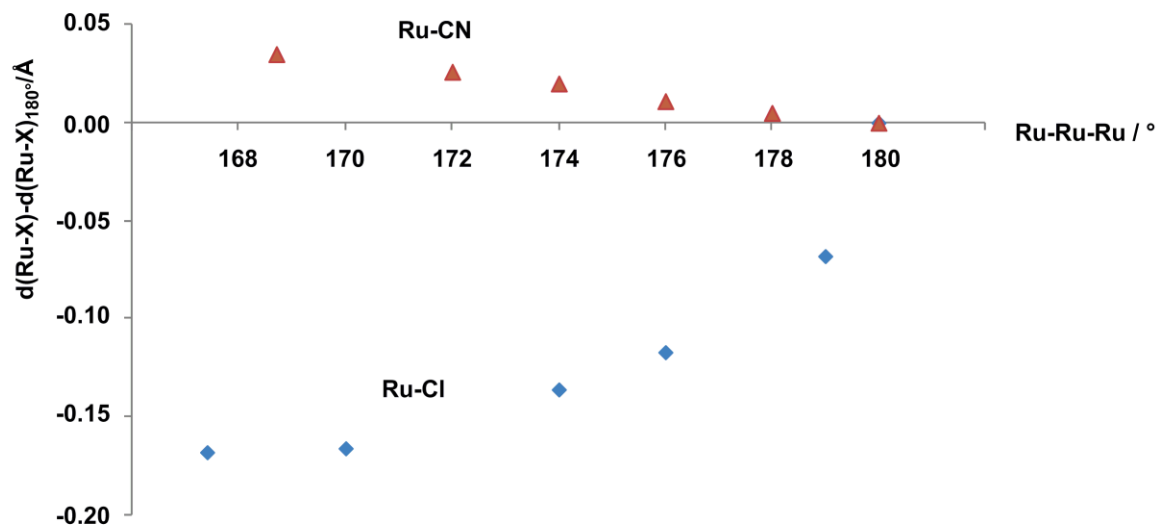


Figure S2 Correlation of Ru-X bond length (and also energy) with angle in $\text{Ru}_3(\text{dpa})_4\text{Cl}_2$ and $\text{Ru}_3(\text{dpa})_4(\text{CN})_2$

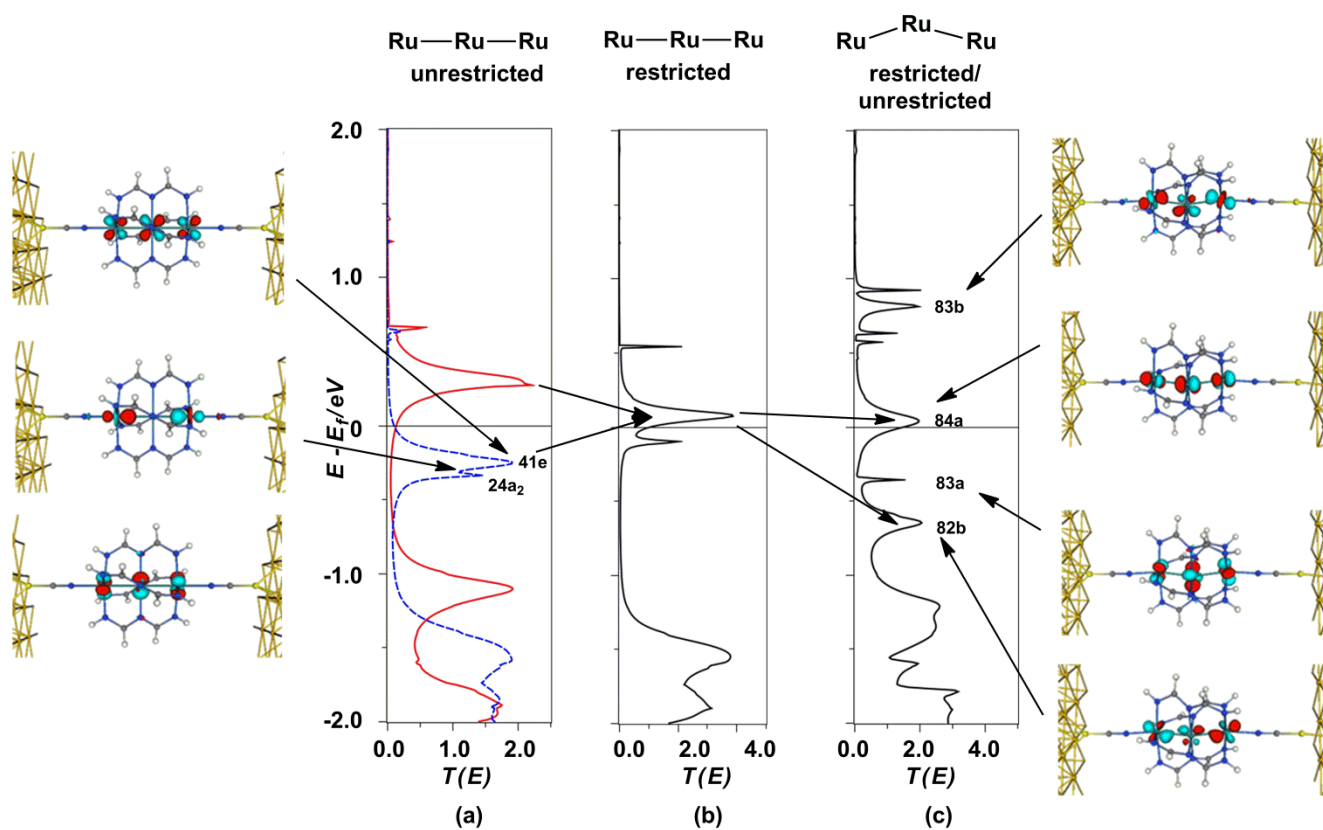


Figure S3 Comparison of transmission spectra for (a) linear Ru₃(dpa)₄(NCS)₂, unrestricted (b) linear Ru₃(dpa)₄(NCS)₂, restricted (i.e. singlet) and (c) bent Ru₃(dpa)₄(NCS)₂ (restricted and unrestricted calculations converge to the same closed-shell density).

Table S1 Coordinates of optimized geometries:

Ru₃(dpa)₄Cl₂:

¹A₁:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.300312
Cl	0.000000	0.000000	4.966419
N	-0.920641	-1.927378	2.212146
N	-1.479112	1.479112	0.000000
N	-1.927378	0.920641	2.212146
N	1.927378	-0.920641	2.212146
N	1.479112	-1.479112	0.000000
N	0.920641	1.927378	2.212146
C	-0.862501	-2.766895	3.270452
C	-1.370272	-4.053706	3.242405
C	-1.926516	-4.521685	2.048336
C	-1.981147	-3.684728	0.951607
C	-1.498520	-2.362709	1.042736
C	-2.362709	1.498520	1.042736
C	-3.684728	1.981147	0.951607
C	-4.521685	1.926516	2.048336
C	-4.053706	1.370272	3.242405
C	-2.766895	0.862501	3.270452
C	2.766895	-0.862501	3.270452
C	4.053706	-1.370272	3.242405
C	4.521685	-1.926516	2.048336
C	3.684728	-1.981147	0.951607
C	2.362709	-1.498520	1.042736
C	1.498520	-2.362709	-1.042736
C	1.981147	-3.684728	-0.951607
C	1.926516	-4.521685	-2.048336
C	1.370272	-4.053706	-3.242405
C	0.862501	2.766895	3.270452
H	-0.399675	-2.344393	4.163218
H	-1.308750	-4.677663	4.133258
H	-2.293175	-5.546489	1.967349
H	-2.356998	-4.042175	-0.006263
H	-4.042175	2.356998	-0.006263
H	-5.546489	2.293175	1.967349
H	-4.677663	1.308750	4.133258
H	-2.344393	0.399675	4.163218
H	2.344393	-0.399675	4.163218
H	4.677663	-1.308750	4.133258
H	5.546489	-2.293175	1.967349
H	4.042175	-2.356998	-0.006263
H	2.356998	-4.042175	0.006263
H	2.293175	-5.546489	-1.967349
H	1.308750	-4.677663	-4.133258
H	0.399675	2.344393	4.163218
N	-1.479112	-1.479112	0.000000
Ru	0.000000	0.000000	-2.300312
Cl	0.000000	0.000000	-4.966419
N	-0.920641	1.927378	-2.212146
C	-0.862501	2.766895	-3.270452
C	-1.370272	4.053706	-3.242405
C	-1.926516	4.521685	-2.048336
C	-1.981147	3.684728	-0.951607

C	-1.498520	2.362709	-1.042736
C	1.498520	2.362709	1.042736
N	1.479112	1.479112	0.000000
C	2.362709	1.498520	-1.042736
N	1.927378	0.920641	-2.212146
N	-1.927378	-0.920641	-2.212146
C	-2.362709	-1.498520	-1.042736
C	-3.684728	-1.981147	-0.951607
C	-4.521685	-1.926516	-2.048336
C	-4.053706	-1.370272	-3.242405
C	-2.766895	-0.862501	-3.270452
H	-2.344393	-0.399675	-4.163218
H	-4.677663	-1.308750	-4.133258
H	-5.546489	-2.293175	-1.967349
H	-4.042175	-2.356998	0.006263
N	0.920641	-1.927378	-2.212146
C	0.862501	-2.766895	-3.270452
H	0.399675	-2.344393	-4.163218
C	2.766895	0.862501	-3.270452
C	4.053706	1.370272	-3.242405
C	4.521685	1.926516	-2.048336
C	3.684728	1.981147	-0.951607
H	4.042175	2.356998	0.006263
H	5.546489	2.293175	-1.967349
H	4.677663	1.308750	-4.133258
H	2.344393	0.399675	-4.163218
C	1.981147	3.684728	0.951607
C	1.926516	4.521685	2.048336
C	1.370272	4.053706	3.242405
H	1.308750	4.677663	4.133258
H	2.293175	5.546489	1.967349
H	2.356998	4.042175	-0.006263
H	-2.356998	4.042175	0.006263
H	-2.293175	5.546489	-1.967349
H	-1.308750	4.677663	-4.133258
H	-0.399675	2.344393	-4.163218

Total Energy: -602.96900501 eV

³A₂:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.354199
Cl	0.000000	0.000000	4.765295
N	-0.853946	-1.946199	2.204072
N	-1.458677	1.458677	0.000000
N	-1.946199	0.853946	2.204072
N	1.946199	-0.853946	2.204072
N	1.458677	-1.458677	0.000000
N	0.853946	1.946199	2.204072
C	-0.733081	-2.834435	3.217294
C	-1.203615	-4.133643	3.155320
C	-1.802880	-4.566749	1.968309
C	-1.918816	-3.686110	0.911668
C	-1.453786	-2.359882	1.030049
C	-2.359882	1.453786	1.030049
C	-3.686110	1.918816	0.911668
C	-4.566749	1.802880	1.968309
C	-4.133643	1.203615	3.155320

C	-2.834435	0.733081	3.217294
C	2.834435	-0.733081	3.217294
C	4.133643	-1.203615	3.155320
C	4.566749	-1.802880	1.968309
C	3.686110	-1.918816	0.911668
C	2.359882	-1.453786	1.030049
C	1.453786	-2.359882	-1.030049
C	1.918816	-3.686110	-0.911668
C	1.802880	-4.566749	-1.968309
C	1.203615	-4.133643	-3.155320
C	0.733081	2.834435	3.217294
H	-0.246300	-2.446648	4.110893
H	-1.083615	-4.792827	4.014313
H	-2.154206	-5.594414	1.861885
H	-2.328197	-4.011307	-0.044319
H	-4.011307	2.328197	-0.044319
H	-5.594414	2.154206	1.861885
H	-4.792827	1.083615	4.014313
H	-2.446648	0.246300	4.110893
H	2.446648	-0.246300	4.110893
H	4.792827	-1.083615	4.014313
H	5.594414	-2.154206	1.861885
H	4.011307	-2.328197	-0.044319
H	2.328197	-4.011307	0.044319
H	2.154206	-5.594414	-1.861885
H	1.083615	-4.792827	-4.014313
H	0.246300	2.446648	4.110893
N	-1.458677	-1.458677	0.000000
Ru	0.000000	0.000000	-2.354199
Cl	0.000000	0.000000	-4.765295
N	-0.853946	1.946199	-2.204072
C	-0.733081	2.834435	-3.217294
C	-1.203615	4.133643	-3.155320
C	-1.802880	4.566749	-1.968309
C	-1.918816	3.686110	-0.911668
C	-1.453786	2.359882	-1.030049
C	1.453786	2.359882	1.030049
N	1.458677	1.458677	0.000000
C	2.359882	1.453786	-1.030049
N	1.946199	0.853946	-2.204072
N	-1.946199	-0.853946	-2.204072
C	-2.359882	-1.453786	-1.030049
C	-3.686110	-1.918816	-0.911668
C	-4.566749	-1.802880	-1.968309
C	-4.133643	-1.203615	-3.155320
C	-2.834435	-0.733081	-3.217294
H	-2.446648	-0.246300	-4.110893
H	-4.792827	-1.083615	-4.014313
H	-5.594414	-2.154206	-1.861885
H	-4.011307	-2.328197	0.044319
N	0.853946	-1.946199	-2.204072
C	0.733081	-2.834435	-3.217294
H	0.246300	-2.446648	-4.110893
C	2.834435	0.733081	-3.217294
C	4.133643	1.203615	-3.155320
C	4.566749	1.802880	-1.968309
C	3.686110	1.918816	-0.911668
H	4.011307	2.328197	0.044319
H	5.594414	2.154206	-1.861885

H	4.792827	1.083615	-4.014313
H	2.446648	0.246300	-4.110893
C	1.918816	3.686110	0.911668
C	1.802880	4.566749	1.968309
C	1.203615	4.133643	3.155320
H	1.083615	4.792827	4.014313
H	2.154206	5.594414	1.861885
H	2.328197	4.011307	-0.044319
H	-2.328197	4.011307	0.044319
H	-2.154206	5.594414	-1.861885
H	-1.083615	4.792827	-4.014313
H	-0.246300	2.446648	-4.110893

Total Energy: -603.00497627 eV

³A₂:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.410517
Cl	0.000000	0.000000	5.172974
N	-1.041034	-1.816152	2.278137
N	-1.445782	1.445782	0.000000
N	-1.816152	1.041034	2.278137
N	1.816152	-1.041034	2.278137
N	1.445782	-1.445782	0.000000
N	1.041034	1.816152	2.278137
C	-1.098336	-2.621064	3.370706
C	-1.603055	-3.906223	3.335476
C	-2.045615	-4.419424	2.111264
C	-2.011791	-3.612660	0.992936
C	-1.543192	-2.285243	1.086589
C	-2.285243	1.543192	1.086589
C	-3.612660	2.011791	0.992936
C	-4.419424	2.045615	2.111264
C	-3.906223	1.603055	3.335476
C	-2.621064	1.098336	3.370706
C	2.621064	-1.098336	3.370706
C	3.906223	-1.603055	3.335476
C	4.419424	-2.045615	2.111264
C	3.612660	-2.011791	0.992936
C	2.285243	-1.543192	1.086589
C	1.543192	-2.285243	-1.086589
C	2.011791	-3.612660	-0.992936
C	2.045615	-4.419424	-2.111264
C	1.603055	-3.906223	-3.335476
C	1.098336	2.621064	3.370706
H	-0.709524	-2.166009	4.284920
H	-1.621075	-4.501313	4.248358
H	-2.394462	-5.450113	2.028994
H	-2.305572	-3.998764	0.017861
H	-3.998764	2.305572	0.017861
H	-5.450113	2.394462	2.028994
H	-4.501313	1.621075	4.248358
H	-2.166009	0.709524	4.284920
H	2.166009	-0.709524	4.284920
H	4.501313	-1.621075	4.248358
H	5.450113	-2.394462	2.028994
H	3.998764	-2.305572	0.017861
H	2.305572	-3.998764	-0.017861

H	2.394462	-5.450113	-2.028994
H	1.621075	-4.501313	-4.248358
H	0.709524	2.166009	4.284920
N	-1.445782	-1.445782	0.000000
Ru	0.000000	0.000000	-2.410517
Cl	0.000000	0.000000	-5.172974
N	-1.041034	1.816152	-2.278137
C	-1.098336	2.621064	-3.370706
C	-1.603055	3.906223	-3.335476
C	-2.045615	4.419424	-2.111264
C	-2.011791	3.612660	-0.992936
C	-1.543192	2.285243	-1.086589
C	1.543192	2.285243	1.086589
N	1.445782	1.445782	0.000000
C	2.285243	1.543192	-1.086589
N	1.816152	1.041034	-2.278137
N	-1.816152	-1.041034	-2.278137
C	-2.285243	-1.543192	-1.086589
C	-3.612660	-2.011791	-0.992936
C	-4.419424	-2.045615	-2.111264
C	-3.906223	-1.603055	-3.335476
C	-2.621064	-1.098336	-3.370706
H	-2.166009	-0.709524	-4.284920
H	-4.501313	-1.621075	-4.248358
H	-5.450113	-2.394462	-2.028994
H	-3.998764	-2.305572	-0.017861
N	1.041034	-1.816152	-2.278137
C	1.098336	-2.621064	-3.370706
H	0.709524	-2.166009	-4.284920
C	2.621064	1.098336	-3.370706
C	3.906223	1.603055	-3.335476
C	4.419424	2.045615	-2.111264
C	3.612660	2.011791	-0.992936
H	3.998764	2.305572	-0.017861
H	5.450113	2.394462	-2.028994
H	4.501313	1.621075	-4.248358
H	2.166009	0.709524	-4.284920
C	2.011791	3.612660	0.992936
C	2.045615	4.419424	2.111264
C	1.603055	3.906223	3.335476
H	1.621075	4.501313	4.248358
H	2.394462	5.450113	2.028994
H	2.305572	3.998764	0.017861
H	-2.305572	3.998764	-0.017861
H	-2.394462	5.450113	-2.028994
H	-1.621075	4.501313	-4.248358
H	-0.709524	2.166009	-4.284920

Total Energy: -602.45476501 eV

³E:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.331868
Cl	0.000000	0.000000	4.851590
N	-0.886407	-1.940410	2.206404
N	-1.468601	1.468601	0.000000
N	-1.940410	0.886407	2.206404
N	1.940410	-0.886407	2.206404

N	1.468601	-1.468601	0.000000
N	0.886407	1.940410	2.206404
C	-0.792774	-2.808767	3.239333
C	-1.274051	-4.104982	3.190980
C	-1.853379	-4.552635	1.999990
C	-1.945955	-3.688313	0.927113
C	-1.474861	-2.363002	1.034765
C	-2.363002	1.474861	1.034765
C	-3.688313	1.945955	0.927113
C	-4.552635	1.853379	1.999990
C	-4.104982	1.274051	3.190980
C	-2.808767	0.792774	3.239333
C	2.808767	-0.792774	3.239333
C	4.104982	-1.274051	3.190980
C	4.552635	-1.853379	1.999990
C	3.688313	-1.945955	0.927113
C	2.363002	-1.474861	1.034765
C	1.474861	-2.363002	-1.034765
C	1.945955	-3.688313	-0.927113
C	1.853379	-4.552635	-1.999990
C	1.274051	-4.104982	-3.190980
C	0.792774	2.808767	3.239333
H	-0.317501	-2.405779	4.133499
H	-1.176207	-4.750745	4.062883
H	-2.206245	-5.581277	1.902111
H	-2.338473	-4.027931	-0.031020
H	-4.027931	2.338473	-0.031020
H	-5.581277	2.206245	1.902111
H	-4.750745	1.176207	4.062883
H	-2.405779	0.317501	4.133499
H	2.405779	-0.317501	4.133499
H	4.750745	-1.176207	4.062883
H	5.581277	-2.206245	1.902111
H	4.027931	-2.338473	-0.031020
H	2.338473	-4.027931	0.031020
H	2.206245	-5.581277	-1.902111
H	1.176207	-4.750745	-4.062883
H	0.317501	2.405779	4.133499
N	-1.468601	-1.468601	0.000000
Ru	0.000000	0.000000	-2.331868
Cl	0.000000	0.000000	-4.851590
N	-0.886407	1.940410	-2.206404
C	-0.792774	2.808767	-3.239333
C	-1.274051	4.104982	-3.190980
C	-1.853379	4.552635	-1.999990
C	-1.945955	3.688313	-0.927113
C	-1.474861	2.363002	-1.034765
C	1.474861	2.363002	1.034765
N	1.468601	1.468601	0.000000
C	2.363002	1.474861	-1.034765
N	1.940410	0.886407	-2.206404
N	-1.940410	-0.886407	-2.206404
C	-2.363002	-1.474861	-1.034765
C	-3.688313	-1.945955	-0.927113
C	-4.552635	-1.853379	-1.999990
C	-4.104982	-1.274051	-3.190980
C	-2.808767	-0.792774	-3.239333
H	-2.405779	-0.317501	-4.133499
H	-4.750745	-1.176207	-4.062883

H	-5.581277	-2.206245	-1.902111
H	-4.027931	-2.338473	0.031020
N	0.886407	-1.940410	-2.206404
C	0.792774	-2.808767	-3.239333
H	0.317501	-2.405779	-4.133499
C	2.808767	0.792774	-3.239333
C	4.104982	1.274051	-3.190980
C	4.552635	1.853379	-1.999990
C	3.688313	1.945955	-0.927113
H	4.027931	2.338473	0.031020
H	5.581277	2.206245	-1.902111
H	4.750745	1.176207	-4.062883
H	2.405779	0.317501	-4.133499
C	1.945955	3.688313	0.927113
C	1.853379	4.552635	1.999990
C	1.274051	4.104982	3.190980
H	1.176207	4.750745	4.062883
H	2.206245	5.581277	1.902111
H	2.338473	4.027931	-0.031020
H	-2.338473	4.027931	0.031020
H	-2.206245	5.581277	-1.902111
H	-1.176207	4.750745	-4.062883
H	-0.317501	2.405779	-4.133499

Total Energy: -603.03482869 eV

⁵B₂:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.390800
Cl	0.000000	0.000000	4.945352
N	-0.951326	-1.887805	2.245705
N	-1.452794	1.452794	0.000000
N	-1.887805	0.951326	2.245705
N	1.887805	-0.951326	2.245705
N	1.452794	-1.452794	0.000000
N	0.951326	1.887805	2.245705
C	-0.926040	-2.738041	3.300861
C	-1.419818	-4.028068	3.250864
C	-1.937254	-4.496601	2.039209
C	-1.968076	-3.650268	0.949482
C	-1.499300	-2.325005	1.060224
C	-2.325005	1.499300	1.060224
C	-3.650268	1.968076	0.949482
C	-4.496601	1.937254	2.039209
C	-4.028068	1.419818	3.250864
C	-2.738041	0.926040	3.300861
C	2.738041	-0.926040	3.300861
C	4.028068	-1.419818	3.250864
C	4.496601	-1.937254	2.039209
C	3.650268	-1.968076	0.949482
C	2.325005	-1.499300	1.060224
C	1.499300	-2.325005	-1.060224
C	1.968076	-3.650268	-0.949482
C	1.937254	-4.496601	-2.039209
C	1.419818	-4.028068	-3.250864
C	0.926040	2.738041	3.300861
H	-0.490249	-2.320670	4.208756
H	-1.374738	-4.656904	4.139535

H	-2.290191	-5.524502	1.940541
H	-2.314219	-4.003255	-0.021139
H	-4.003255	2.314219	-0.021139
H	-5.524502	2.290191	1.940541
H	-4.656904	1.374738	4.139535
H	-2.320670	0.490249	4.208756
H	2.320670	-0.490249	4.208756
H	4.656904	-1.374738	4.139535
H	5.524502	-2.290191	1.940541
H	4.003255	-2.314219	-0.021139
H	2.314219	-4.003255	0.021139
H	2.290191	-5.524502	-1.940541
H	1.374738	-4.656904	-4.139535
H	0.490249	2.320670	4.208756
N	-1.452794	-1.452794	0.000000
Ru	0.000000	0.000000	-2.390800
Cl	0.000000	0.000000	-4.945352
N	-0.951326	1.887805	-2.245705
C	-0.926040	2.738041	-3.300861
C	-1.419818	4.028068	-3.250864
C	-1.937254	4.496601	-2.039209
C	-1.968076	3.650268	-0.949482
C	-1.499300	2.325005	-1.060224
C	1.499300	2.325005	1.060224
N	1.452794	1.452794	0.000000
C	2.325005	1.499300	-1.060224
N	1.887805	0.951326	-2.245705
N	-1.887805	-0.951326	-2.245705
C	-2.325005	-1.499300	-1.060224
C	-3.650268	-1.968076	-0.949482
C	-4.496601	-1.937254	-2.039209
C	-4.028068	-1.419818	-3.250864
C	-2.738041	-0.926040	-3.300861
H	-2.320670	-0.490249	-4.208756
H	-4.656904	-1.374738	-4.139535
H	-5.524502	-2.290191	-1.940541
H	-4.003255	-2.314219	0.021139
N	0.951326	-1.887805	-2.245705
C	0.926040	-2.738041	-3.300861
H	0.490249	-2.320670	-4.208756
C	2.738041	0.926040	-3.300861
C	4.028068	1.419818	-3.250864
C	4.496601	1.937254	-2.039209
C	3.650268	1.968076	-0.949482
H	4.003255	2.314219	0.021139
H	5.524502	2.290191	-1.940541
H	4.656904	1.374738	-4.139535
H	2.320670	0.490249	-4.208756
C	1.968076	3.650268	0.949482
C	1.937254	4.496601	2.039209
C	1.419818	4.028068	3.250864
H	1.374738	4.656904	4.139535
H	2.290191	5.524502	1.940541
H	2.314219	4.003255	-0.021139
H	-2.314219	4.003255	0.021139
H	-2.290191	5.524502	-1.940541
H	-1.374738	4.656904	-4.139535
H	-0.490249	2.320670	-4.208756

Total Energy: -603.28625170 eV

¹A:

Ru	0.000000	0.000000	0.201819
Ru	1.953369	-1.208193	-0.079370
Cl	4.042395	-2.594809	0.060170
N	2.908837	0.459782	-0.901727
N	-0.767969	-1.245874	-1.377155
N	1.409859	-1.837625	-1.962138
N	2.351407	-0.397413	1.953204
N	0.776868	1.264463	1.577189
N	0.779556	-2.820956	0.824567
C	4.247494	0.644853	-0.821408
C	4.875674	1.788203	-1.277497
C	4.086397	2.817973	-1.802882
C	2.717255	2.656739	-1.866467
C	2.119560	1.457141	-1.426401
C	0.083294	-1.739245	-2.322590
C	-0.288162	-2.048991	-3.650176
C	0.656021	-2.481038	-4.559307
C	1.994130	-2.596454	-4.166187
C	2.325732	-2.247017	-2.871223
C	3.206654	-1.034891	2.782283
C	3.502498	-0.594530	4.062219
C	2.863592	0.552220	4.537914
C	1.965326	1.209761	3.719132
C	1.716735	0.731234	2.420239
C	0.410718	2.577887	1.478347
C	1.204470	3.652032	1.926632
C	0.773133	4.953291	1.757609
C	-0.449225	5.190455	1.125300
C	1.173805	-4.103170	0.666261
H	4.798221	-0.187588	-0.384229
H	5.959125	1.875177	-1.203635
H	4.539906	3.754175	-2.133474
H	2.072768	3.463092	-2.216095
H	-1.324025	-1.901248	-3.953636
H	0.356319	-2.706255	-5.584343
H	2.769518	-2.935705	-4.851673
H	3.346501	-2.307211	-2.494913
H	3.676126	-1.923427	2.361006
H	4.210237	-1.153213	4.674154
H	3.042949	0.913632	5.552013
H	1.399954	2.068069	4.080562
H	2.178582	3.439527	2.364900
H	1.397589	5.781654	2.096870
H	-0.832330	6.198374	0.969858
H	2.129403	-4.229501	0.158421
N	0.767969	1.245874	-1.377155
Ru	-1.953369	1.208193	-0.079370
Cl	-4.042395	2.594809	0.060170
N	-2.908837	-0.459782	-0.901727
C	-4.247494	-0.644853	-0.821408
C	-4.875674	-1.788203	-1.277497
C	-4.086397	-2.817973	-1.802882
C	-2.717255	-2.656739	-1.866467
C	-2.119560	-1.457141	-1.426401
C	-0.410718	-2.577887	1.478347

N	-0.776868	-1.264463	1.577189
C	-1.716735	-0.731234	2.420239
N	-2.351407	0.397413	1.953204
N	-1.409859	1.837625	-1.962138
C	-0.083294	1.739245	-2.322590
C	0.288162	2.048991	-3.650176
C	-0.656021	2.481038	-4.559307
C	-1.994130	2.596454	-4.166187
C	-2.325732	2.247017	-2.871223
H	-3.346501	2.307211	-2.494913
H	-2.769518	2.935705	-4.851673
H	-0.356319	2.706255	-5.584343
H	1.324025	1.901248	-3.953636
N	-0.779556	2.820956	0.824567
C	-1.173805	4.103170	0.666261
H	-2.129403	4.229501	0.158421
C	-3.206654	1.034891	2.782283
C	-3.502498	0.594530	4.062219
C	-2.863592	-0.552220	4.537914
C	-1.965326	-1.209761	3.719132
H	-1.399954	-2.068069	4.080562
H	-3.042949	-0.913632	5.552013
H	-4.210237	1.153213	4.674154
H	-3.676126	1.923427	2.361006
C	-1.204470	-3.652032	1.926632
C	-0.773133	-4.953291	1.757609
C	0.449225	-5.190455	1.125300
H	0.832330	-6.198374	0.969858
H	-1.397589	-5.781654	2.096870
H	-2.178582	-3.439527	2.364900
H	-2.072768	-3.463092	-2.216095
H	-4.539906	-3.754175	-2.133474
H	-5.959125	-1.875177	-1.203635
H	-4.798221	0.187588	-0.384229

Total Energy: -603.43686072 eV

³A:

Ru	0.000000	0.000000	0.191393
Ru	1.995614	-1.246155	-0.090975
Cl	4.105222	-2.616160	0.033459
N	2.911023	0.414562	-0.938716
N	-0.760264	-1.246884	-1.347102
N	1.403027	-1.927004	-1.929692
N	2.398752	-0.371890	1.890985
N	0.760305	1.259159	1.555948
N	0.840315	-2.806206	0.853490
C	4.255999	0.586414	-0.904430
C	4.878345	1.748473	-1.317700
C	4.083967	2.813583	-1.757325
C	2.712121	2.660822	-1.788143
C	2.120561	1.441219	-1.402018
C	0.076635	-1.797207	-2.281198
C	-0.321533	-2.134656	-3.594178
C	0.593147	-2.634770	-4.498215
C	1.930791	-2.787247	-4.112590
C	2.291067	-2.407059	-2.835373
C	3.282200	-0.985489	2.711859

C	3.567585	-0.550860	3.995269
C	2.893979	0.568067	4.488196
C	1.976011	1.207005	3.676653
C	1.739548	0.738002	2.372411
C	0.356233	2.569448	1.497457
C	1.143840	3.645498	1.951658
C	0.704448	4.945245	1.793701
C	-0.525148	5.176972	1.172302
C	1.246611	-4.089696	0.712389
H	4.812572	-0.270483	-0.524967
H	5.964480	1.822814	-1.271678
H	4.533710	3.765472	-2.044528
H	2.061383	3.487187	-2.073588
H	-1.355314	-1.960768	-3.889882
H	0.273861	-2.882890	-5.511792
H	2.685561	-3.177921	-4.794031
H	3.313325	-2.490266	-2.466834
H	3.775486	-1.855901	2.279674
H	4.293806	-1.095735	4.598214
H	3.062224	0.922035	5.506704
H	1.384588	2.042392	4.049378
H	2.123797	3.438109	2.378541
H	1.327169	5.775069	2.132001
H	-0.915693	6.183456	1.025073
H	2.207385	-4.209895	0.212941
N	0.760264	1.246884	-1.347102
Ru	-1.995614	1.246155	-0.090975
Cl	-4.105222	2.616160	0.033459
N	-2.911023	-0.414562	-0.938716
C	-4.255999	-0.586414	-0.904430
C	-4.878345	-1.748473	-1.317700
C	-4.083967	-2.813583	-1.757325
C	-2.712121	-2.660822	-1.788143
C	-2.120561	-1.441219	-1.402018
C	-0.356233	-2.569448	1.497457
N	-0.760305	-1.259159	1.555948
C	-1.739548	-0.738002	2.372411
N	-2.398752	0.371890	1.890985
N	-1.403027	1.927004	-1.929692
C	-0.076635	1.797207	-2.281198
C	0.321533	2.134656	-3.594178
C	-0.593147	2.634770	-4.498215
C	-1.930791	2.787247	-4.112590
C	-2.291067	2.407059	-2.835373
H	-3.313325	2.490266	-2.466834
H	-2.685561	3.177921	-4.794031
H	-0.273861	2.882890	-5.511792
H	1.355314	1.960768	-3.889882
N	-0.840315	2.806206	0.853490
C	-1.246611	4.089696	0.712389
H	-2.207385	4.209895	0.212941
C	-3.282200	0.985489	2.711859
C	-3.567585	0.550860	3.995269
C	-2.893979	-0.568067	4.488196
C	-1.976011	-1.207005	3.676653
H	-1.384588	-2.042392	4.049378
H	-3.062224	-0.922035	5.506704
H	-4.293806	1.095735	4.598214
H	-3.775486	1.855901	2.279674

C	-1.143840	-3.645498	1.951658
C	-0.704448	-4.945245	1.793701
C	0.525148	-5.176972	1.172302
H	0.915693	-6.183456	1.025073
H	-1.327169	-5.775069	2.132001
H	-2.123797	-3.438109	2.378541
H	-2.061383	-3.487187	-2.073588
H	-4.533710	-3.765472	-2.044528
H	-5.964480	-1.822814	-1.271678
H	-4.812572	0.270483	-0.524967

Total Energy: -603.38258934 eV

⁵A:

Ru	0.000000	0.000000	0.191393
Ru	1.995614	-1.246155	-0.090975
Cl	4.105222	-2.616160	0.033459
N	2.911023	0.414562	-0.938716
N	-0.760264	-1.246884	-1.347102
N	1.403027	-1.927004	-1.929692
N	2.398752	-0.371890	1.890985
N	0.760305	1.259159	1.555948
N	0.840315	-2.806206	0.853490
C	4.255999	0.586414	-0.904430
C	4.878345	1.748473	-1.317700
C	4.083967	2.813583	-1.757325
C	2.712121	2.660822	-1.788143
C	2.120561	1.441219	-1.402018
C	0.076635	-1.797207	-2.281198
C	-0.321533	-2.134656	-3.594178
C	0.593147	-2.634770	-4.498215
C	1.930791	-2.787247	-4.112590
C	2.291067	-2.407059	-2.835373
C	3.282200	-0.985489	2.711859
C	3.567585	-0.550860	3.995269
C	2.893979	0.568067	4.488196
C	1.976011	1.207005	3.676653
C	1.739548	0.738002	2.372411
C	0.356233	2.569448	1.497457
C	1.143840	3.645498	1.951658
C	0.704448	4.945245	1.793701
C	-0.525148	5.176972	1.172302
C	1.246611	-4.089696	0.712389
H	4.812572	-0.270483	-0.524967
H	5.964480	1.822814	-1.271678
H	4.533710	3.765472	-2.044528
H	2.061383	3.487187	-2.073588
H	-1.355314	-1.960768	-3.889882
H	0.273861	-2.882890	-5.511792
H	2.685561	-3.177921	-4.794031
H	3.313325	-2.490266	-2.466834
H	3.775486	-1.855901	2.279674
H	4.293806	-1.095735	4.598214
H	3.062224	0.922035	5.506704
H	1.384588	2.042392	4.049378
H	2.123797	3.438109	2.378541
H	1.327169	5.775069	2.132001

H	-0.915693	6.183456	1.025073
H	2.207385	-4.209895	0.212941
N	0.760264	1.246884	-1.347102
Ru	-1.995614	1.246155	-0.090975
Cl	-4.105222	2.616160	0.033459
N	-2.911023	-0.414562	-0.938716
C	-4.255999	-0.586414	-0.904430
C	-4.878345	-1.748473	-1.317700
C	-4.083967	-2.813583	-1.757325
C	-2.712121	-2.660822	-1.788143
C	-2.120561	-1.441219	-1.402018
C	-0.356233	-2.569448	1.497457
N	-0.760305	-1.259159	1.555948
C	-1.739548	-0.738002	2.372411
N	-2.398752	0.371890	1.890985
N	-1.403027	1.927004	-1.929692
C	-0.076635	1.797207	-2.281198
C	0.321533	2.134656	-3.594178
C	-0.593147	2.634770	-4.498215
C	-1.930791	2.787247	-4.112590
C	-2.291067	2.407059	-2.835373
H	-3.313325	2.490266	-2.466834
H	-2.685561	3.177921	-4.794031
H	-0.273861	2.882890	-5.511792
H	1.355314	1.960768	-3.889882
N	-0.840315	2.806206	0.853490
C	-1.246611	4.089696	0.712389
H	-2.207385	4.209895	0.212941
C	-3.282200	0.985489	2.711859
C	-3.567585	0.550860	3.995269
C	-2.893979	-0.568067	4.488196
C	-1.976011	-1.207005	3.676653
H	-1.384588	-2.042392	4.049378
H	-3.062224	-0.922035	5.506704
H	-4.293806	1.095735	4.598214
H	-3.775486	1.855901	2.279674
C	-1.143840	-3.645498	1.951658
C	-0.704448	-4.945245	1.793701
C	0.525148	-5.176972	1.172302
H	0.915693	-6.183456	1.025073
H	-1.327169	-5.775069	2.132001
H	-2.123797	-3.438109	2.378541
H	-2.061383	-3.487187	-2.073588
H	-4.533710	-3.765472	-2.044528
H	-5.964480	-1.822814	-1.271678
H	-4.812572	0.270483	-0.524967

Total Energy: -603.28142745 eV

Ru₃(dpa)₄(NCS)₂:

¹A₁:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.309145
N	-0.941163	-1.912291	2.222218
N	-1.479595	1.479595	0.000000
N	-1.912291	0.941163	2.222218
N	1.912291	-0.941163	2.222218
N	1.479595	-1.479595	0.000000
N	0.941163	1.912291	2.222218
C	-0.898217	-2.740970	3.288289
C	-1.407202	-4.026899	3.269829
C	-1.949151	-4.505302	2.072638
C	-1.990816	-3.678792	0.967055
C	-1.509460	-2.355045	1.049570
C	-2.355045	1.509460	1.049570
C	-3.678792	1.990816	0.967055
C	-4.505302	1.949151	2.072638
C	-4.026899	1.407202	3.269829
C	-2.740970	0.898217	3.288289
C	2.740970	-0.898217	3.288289
C	4.026899	-1.407202	3.269829
C	4.505302	-1.949151	2.072638
C	3.678792	-1.990816	0.967055
C	2.355045	-1.509460	1.049570
C	1.509460	-2.355045	-1.049570
C	1.990816	-3.678792	-0.967055
C	1.949151	-4.505302	-2.072638
C	1.407202	-4.026899	-3.269829
C	0.898217	2.740970	3.288289
H	-0.437036	-2.318543	4.179740
H	-1.356332	-4.641823	4.167383
H	-2.315210	-5.530896	1.997570
H	-2.357215	-4.046200	0.009285
H	-4.046200	2.357215	0.009285
H	-5.530896	2.315210	1.997570
H	-4.641823	1.356332	4.167383
H	-2.318543	0.437036	4.179740
H	2.318543	-0.437036	4.179740
H	4.641823	-1.356332	4.167383
H	5.530896	-2.315210	1.997570
H	4.046200	-2.357215	0.009285
H	2.357215	-4.046200	-0.009285
H	2.315210	-5.530896	-1.997570
H	1.356332	-4.641823	-4.167383
H	0.437036	2.318543	4.179740
N	-1.479595	-1.479595	0.000000
Ru	0.000000	0.000000	-2.309145
N	-0.941163	1.912291	-2.222218
C	-0.898217	2.740970	-3.288289
C	-1.407202	4.026899	-3.269829
C	-1.949151	4.505302	-2.072638

C	-1.990816	3.678792	-0.967055
C	-1.509460	2.355045	-1.049570
C	1.509460	2.355045	1.049570
N	1.479595	1.479595	0.000000
C	2.355045	1.509460	-1.049570
N	1.912291	0.941163	-2.222218
N	-1.912291	-0.941163	-2.222218
C	-2.355045	-1.509460	-1.049570
C	-3.678792	-1.990816	-0.967055
C	-4.505302	-1.949151	-2.072638
C	-4.026899	-1.407202	-3.269829
C	-2.740970	-0.898217	-3.288289
H	-2.318543	-0.437036	-4.179740
H	-4.641823	-1.356332	-4.167383
H	-5.530896	-2.315210	-1.997570
H	-4.046200	-2.357215	-0.009285
N	0.941163	-1.912291	-2.222218
C	0.898217	-2.740970	-3.288289
H	0.437036	-2.318543	-4.179740
C	2.740970	0.898217	-3.288289
C	4.026899	1.407202	-3.269829
C	4.505302	1.949151	-2.072638
C	3.678792	1.990816	-0.967055
H	4.046200	2.357215	-0.009285
H	5.530896	2.315210	-1.997570
H	4.641823	1.356332	-4.167383
H	2.318543	0.437036	-4.179740
C	1.990816	3.678792	0.967055
C	1.949151	4.505302	2.072638
C	1.407202	4.026899	3.269829
H	1.356332	4.641823	4.167383
H	2.315210	5.530896	1.997570
H	2.357215	4.046200	0.009285
H	-2.357215	4.046200	-0.009285
H	-2.315210	5.530896	-1.997570
H	-1.356332	4.641823	-4.167383
H	-0.437036	2.318543	-4.179740
N	0.000000	0.000000	4.587379
N	0.000000	0.000000	-4.587379
C	0.000000	0.000000	-5.788354
C	0.000000	0.000000	5.788354
S	0.000000	0.000000	7.404164
S	0.000000	0.000000	-7.404164

Total Energy: -638.20326436 eV

³A₂:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.361830
N	-0.915887	-1.913029	2.231353
N	-1.463894	1.463894	0.000000
N	-1.913029	0.915887	2.231353
N	1.913029	-0.915887	2.231353
N	1.463894	-1.463894	0.000000
N	0.915887	1.913029	2.231353
C	-0.854035	-2.766167	3.278248
C	-1.351829	-4.055214	3.242774
C	-1.912177	-4.513733	2.046074

C	-1.971498	-3.666230	0.958320
C	-1.490716	-2.343013	1.050796
C	-2.343013	1.490716	1.050796
C	-3.666230	1.971498	0.958320
C	-4.513733	1.912177	2.046074
C	-4.055214	1.351829	3.242774
C	-2.766167	0.854035	3.278248
C	2.766167	-0.854035	3.278248
C	4.055214	-1.351829	3.242774
C	4.513733	-1.912177	2.046074
C	3.666230	-1.971498	0.958320
C	2.343013	-1.490716	1.050796
C	1.490716	-2.343013	-1.050796
C	1.971498	-3.666230	-0.958320
C	1.912177	-4.513733	-2.046074
C	1.351829	-4.055214	-3.242774
C	0.854035	2.766167	3.278248
H	-0.385441	-2.363722	4.173493
H	-1.279540	-4.687055	4.127008
H	-2.276163	-5.538645	1.957016
H	-2.349324	-4.018611	-0.000623
H	-4.018611	2.349324	-0.000623
H	-5.538645	2.276163	1.957016
H	-4.687055	1.279540	4.127008
H	-2.363722	0.385441	4.173493
H	2.363722	-0.385441	4.173493
H	4.687055	-1.279540	4.127008
H	5.538645	-2.276163	1.957016
H	4.018611	-2.349324	-0.000623
H	2.349324	-4.018611	0.000623
H	2.276163	-5.538645	-1.957016
H	1.279540	-4.687055	-4.127008
H	0.385441	2.363722	4.173493
N	-1.463894	-1.463894	0.000000
Ru	0.000000	0.000000	-2.361830
N	-0.915887	1.913029	-2.231353
C	-0.854035	2.766167	-3.278248
C	-1.351829	4.055214	-3.242774
C	-1.912177	4.513733	-2.046074
C	-1.971498	3.666230	-0.958320
C	-1.490716	2.343013	-1.050796
C	1.490716	2.343013	1.050796
N	1.463894	1.463894	0.000000
C	2.343013	1.490716	-1.050796
N	1.913029	0.915887	-2.231353
N	-1.913029	-0.915887	-2.231353
C	-2.343013	-1.490716	-1.050796
C	-3.666230	-1.971498	-0.958320
C	-4.513733	-1.912177	-2.046074
C	-4.055214	-1.351829	-3.242774
C	-2.766167	-0.854035	-3.278248
H	-2.363722	-0.385441	-4.173493
H	-4.687055	-1.279540	-4.127008
H	-5.538645	-2.276163	-1.957016
H	-4.018611	-2.349324	0.000623
N	0.915887	-1.913029	-2.231353
C	0.854035	-2.766167	-3.278248
H	0.385441	-2.363722	-4.173493
C	2.766167	0.854035	-3.278248

C	4.055214	1.351829	-3.242774
C	4.513733	1.912177	-2.046074
C	3.666230	1.971498	-0.958320
H	4.018611	2.349324	0.000623
H	5.538645	2.276163	-1.957016
H	4.687055	1.279540	-4.127008
H	2.363722	0.385441	-4.173493
C	1.971498	3.666230	0.958320
C	1.912177	4.513733	2.046074
C	1.351829	4.055214	3.242774
H	1.279540	4.687055	4.127008
H	2.276163	5.538645	1.957016
H	2.349324	4.018611	-0.000623
H	-2.349324	4.018611	0.000623
H	-2.276163	5.538645	-1.957016
H	-1.279540	4.687055	-4.127008
H	-0.385441	2.363722	-4.173493
N	0.000000	0.000000	4.363226
N	0.000000	0.000000	-4.363226
C	0.000000	0.000000	-5.562543
C	0.000000	0.000000	5.562543
S	0.000000	0.000000	7.178240
S	0.000000	0.000000	-7.178240

Total Energy: -638.56343371 eV

³A₂:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.417455
N	-1.052924	-1.807859	2.282857
N	-1.445144	1.445144	0.000000
N	-1.807859	1.052924	2.282857
N	1.807859	-1.052924	2.282857
N	1.445144	-1.445144	0.000000
N	1.052924	1.807859	2.282857
C	-1.124498	-2.605401	3.377979
C	-1.634437	-3.887744	3.349641
C	-2.066584	-4.407164	2.123836
C	-2.017587	-3.608740	1.000142
C	-1.547456	-2.281370	1.088986
C	-2.281370	1.547456	1.088986
C	-3.608740	2.017587	1.000142
C	-4.407164	2.066584	2.123836
C	-3.887744	1.634437	3.349641
C	-2.605401	1.124498	3.377979
C	2.605401	-1.124498	3.377979
C	3.887744	-1.634437	3.349641
C	4.407164	-2.066584	2.123836
C	3.608740	-2.017587	1.000142
C	2.281370	-1.547456	1.088986
C	1.547456	-2.281370	-1.088986
C	2.017587	-3.608740	-1.000142
C	2.066584	-4.407164	-2.123836
C	1.634437	-3.887744	-3.349641
C	1.124498	2.605401	3.377979
H	-0.735645	-2.153933	4.290151
H	-1.664230	-4.475303	4.266452
H	-2.419387	-5.436778	2.045965

H	-2.303927	-4.000607	0.025222
H	-4.000607	2.303927	0.025222
H	-5.436778	2.419387	2.045965
H	-4.475303	1.664230	4.266452
H	-2.153933	0.735645	4.290151
H	2.153933	-0.735645	4.290151
H	4.475303	-1.664230	4.266452
H	5.436778	-2.419387	2.045965
H	4.000607	-2.303927	0.025222
H	2.303927	-4.000607	-0.025222
H	2.419387	-5.436778	-2.045965
H	1.664230	-4.475303	-4.266452
H	0.735645	2.153933	4.290151
N	-1.445144	-1.445144	0.000000
Ru	0.000000	0.000000	-2.417455
N	-1.052924	1.807859	-2.282857
C	-1.124498	2.605401	-3.377979
C	-1.634437	3.887744	-3.349641
C	-2.066584	4.407164	-2.123836
C	-2.017587	3.608740	-1.000142
C	-1.547456	2.281370	-1.088986
C	1.547456	2.281370	1.088986
N	1.445144	1.445144	0.000000
C	2.281370	1.547456	-1.088986
N	1.807859	1.052924	-2.282857
N	-1.807859	-1.052924	-2.282857
C	-2.281370	-1.547456	-1.088986
C	-3.608740	-2.017587	-1.000142
C	-4.407164	-2.066584	-2.123836
C	-3.887744	-1.634437	-3.349641
C	-2.605401	-1.124498	-3.377979
H	-2.153933	-0.735645	-4.290151
H	-4.475303	-1.664230	-4.266452
H	-5.436778	-2.419387	-2.045965
H	-4.000607	-2.303927	-0.025222
N	1.052924	-1.807859	-2.282857
C	1.124498	-2.605401	-3.377979
H	0.735645	-2.153933	-4.290151
C	2.605401	1.124498	-3.377979
C	3.887744	1.634437	-3.349641
C	4.407164	2.066584	-2.123836
C	3.608740	2.017587	-1.000142
H	4.000607	2.303927	-0.025222
H	5.436778	2.419387	-2.045965
H	4.475303	1.664230	-4.266452
H	2.153933	0.735645	-4.290151
C	2.017587	3.608740	1.000142
C	2.066584	4.407164	2.123836
C	1.634437	3.887744	3.349641
H	1.664230	4.475303	4.266452
H	2.419387	5.436778	2.045965
H	2.303927	4.000607	0.025222
H	-2.303927	4.000607	-0.025222
H	-2.419387	5.436778	-2.045965
H	-1.664230	4.475303	-4.266452
H	-0.735645	2.153933	-4.290151
N	0.000000	0.000000	4.736846
N	0.000000	0.000000	-4.736846
C	0.000000	0.000000	-5.937117

C	0.000000	0.000000	5.937117
S	0.000000	0.000000	7.559328
S	0.000000	0.000000	-7.559328

Total Energy: -637.70368900 eV

³E:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.344300
N	-0.920867	-1.918363	2.222968
N	-1.470386	1.470386	0.000000
N	-1.918363	0.920867	2.222968
N	1.918363	-0.920867	2.222968
N	1.470386	-1.470386	0.000000
N	0.920867	1.918363	2.222968
C	-0.864937	-2.763910	3.275524
C	-1.366910	-4.051974	3.245570
C	-1.921141	-4.516559	2.048413
C	-1.974542	-3.675541	0.954953
C	-1.494374	-2.351802	1.046392
C	-2.351802	1.494374	1.046392
C	-3.675541	1.974542	0.954953
C	-4.516559	1.921141	2.048413
C	-4.051974	1.366910	3.245570
C	-2.763910	0.864937	3.275524
C	2.763910	-0.864937	3.275524
C	4.051974	-1.366910	3.245570
C	4.516559	-1.921141	2.048413
C	3.675541	-1.974542	0.954953
C	2.351802	-1.494374	1.046392
C	1.494374	-2.351802	-1.046392
C	1.974542	-3.675541	-0.954953
C	1.921141	-4.516559	-2.048413
C	1.366910	-4.051974	-3.245570
C	0.864937	2.763910	3.275524
H	-0.398207	-2.355177	4.169311
H	-1.302295	-4.678491	4.134310
H	-2.285567	-5.541724	1.963761
H	-2.348671	-4.031827	-0.004022
H	-4.031827	2.348671	-0.004022
H	-5.541724	2.285567	1.963761
H	-4.678491	1.302295	4.134310
H	-2.355177	0.398207	4.169311
H	2.355177	-0.398207	4.169311
H	4.678491	-1.302295	4.134310
H	5.541724	-2.285567	1.963761
H	4.031827	-2.348671	-0.004022
H	2.348671	-4.031827	0.004022
H	2.285567	-5.541724	-1.963761
H	1.302295	-4.678491	-4.134310
H	0.398207	2.355177	4.169311
N	-1.470386	-1.470386	0.000000
Ru	0.000000	0.000000	-2.344300
N	-0.920867	1.918363	-2.222968
C	-0.864937	2.763910	-3.275524
C	-1.366910	4.051974	-3.245570
C	-1.921141	4.516559	-2.048413
C	-1.974542	3.675541	-0.954953

C	-1.494374	2.351802	-1.046392
C	1.494374	2.351802	1.046392
N	1.470386	1.470386	0.000000
C	2.351802	1.494374	-1.046392
N	1.918363	0.920867	-2.222968
N	-1.918363	-0.920867	-2.222968
C	-2.351802	-1.494374	-1.046392
C	-3.675541	-1.974542	-0.954953
C	-4.516559	-1.921141	-2.048413
C	-4.051974	-1.366910	-3.245570
C	-2.763910	-0.864937	-3.275524
H	-2.355177	-0.398207	-4.169311
H	-4.678491	-1.302295	-4.134310
H	-5.541724	-2.285567	-1.963761
H	-4.031827	-2.348671	0.004022
N	0.920867	-1.918363	-2.222968
C	0.864937	-2.763910	-3.275524
H	0.398207	-2.355177	-4.169311
C	2.763910	0.864937	-3.275524
C	4.051974	1.366910	-3.245570
C	4.516559	1.921141	-2.048413
C	3.675541	1.974542	-0.954953
H	4.031827	2.348671	0.004022
H	5.541724	2.285567	-1.963761
H	4.678491	1.302295	-4.134310
H	2.355177	0.398207	-4.169311
C	1.974542	3.675541	0.954953
C	1.921141	4.516559	2.048413
C	1.366910	4.051974	3.245570
H	1.302295	4.678491	4.134310
H	2.285567	5.541724	1.963761
H	2.348671	4.031827	-0.004022
H	-2.348671	4.031827	0.004022
H	-2.285567	5.541724	-1.963761
H	-1.302295	4.678491	-4.134310
H	-0.398207	2.355177	-4.169311
N	0.000000	0.000000	4.455247
N	0.000000	0.000000	-4.455247
C	0.000000	0.000000	-5.656137
C	0.000000	0.000000	5.656137
S	0.000000	0.000000	7.270263
S	0.000000	0.000000	-7.270263

Total Energy: -638.44368007 eV

³E:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.369045
N	-0.984969	-1.870014	2.250040
N	-1.460755	1.460755	0.000000
N	-1.870014	0.984969	2.250040
N	1.870014	-0.984969	2.250040
N	1.460755	-1.460755	0.000000
N	0.984969	1.870014	2.250040
C	-0.993548	-2.688984	3.327655
C	-1.505715	-3.972341	3.300845
C	-1.999447	-4.464566	2.088106
C	-1.998586	-3.646742	0.975887

C	-1.520814	-2.322765	1.066385
C	-2.322765	1.520814	1.066385
C	-3.646742	1.998586	0.975887
C	-4.464566	1.999447	2.088106
C	-3.972341	1.505715	3.300845
C	-2.688984	0.993548	3.327655
C	2.688984	-0.993548	3.327655
C	3.972341	-1.505715	3.300845
C	4.464566	-1.999447	2.088106
C	3.646742	-1.998586	0.975887
C	2.322765	-1.520814	1.066385
C	1.520814	-2.322765	-1.066385
C	1.998586	-3.646742	-0.975887
C	1.999447	-4.464566	-2.088106
C	1.505715	-3.972341	-3.300845
C	0.993548	2.688984	3.327655
H	-0.565020	-2.257431	4.231189
H	-1.491775	-4.577986	4.206322
H	-2.361742	-5.490916	2.008257
H	-2.329653	-4.021376	0.008146
H	-4.021376	2.329653	0.008146
H	-5.490916	2.361742	2.008257
H	-4.577986	1.491775	4.206322
H	-2.257431	0.565020	4.231189
H	2.257431	-0.565020	4.231189
H	4.577986	-1.491775	4.206322
H	5.490916	-2.361742	2.008257
H	4.021376	-2.329653	0.008146
H	2.329653	-4.021376	-0.008146
H	2.361742	-5.490916	-2.008257
H	1.491775	-4.577986	-4.206322
H	0.565020	2.257431	4.231189
N	-1.460755	-1.460755	0.000000
Ru	0.000000	0.000000	-2.369045
N	-0.984969	1.870014	-2.250040
C	-0.993548	2.688984	-3.327655
C	-1.505715	3.972341	-3.300845
C	-1.999447	4.464566	-2.088106
C	-1.998586	3.646742	-0.975887
C	-1.520814	2.322765	-1.066385
C	1.520814	2.322765	1.066385
N	1.460755	1.460755	0.000000
C	2.322765	1.520814	-1.066385
N	1.870014	0.984969	-2.250040
N	-1.870014	-0.984969	-2.250040
C	-2.322765	-1.520814	-1.066385
C	-3.646742	-1.998586	-0.975887
C	-4.464566	-1.999447	-2.088106
C	-3.972341	-1.505715	-3.300845
C	-2.688984	-0.993548	-3.327655
H	-2.257431	-0.565020	-4.231189
H	-4.577986	-1.491775	-4.206322
H	-5.490916	-2.361742	-2.008257
H	-4.021376	-2.329653	-0.008146
N	0.984969	-1.870014	-2.250040
C	0.993548	-2.688984	-3.327655
H	0.565020	-2.257431	-4.231189
C	2.688984	0.993548	-3.327655
C	3.972341	1.505715	-3.300845

C	4.464566	1.999447	-2.088106
C	3.646742	1.998586	-0.975887
H	4.021376	2.329653	-0.008146
H	5.490916	2.361742	-2.008257
H	4.577986	1.491775	-4.206322
H	2.257431	0.565020	-4.231189
C	1.998586	3.646742	0.975887
C	1.999447	4.464566	2.088106
C	1.505715	3.972341	3.300845
H	1.491775	4.577986	4.206322
H	2.361742	5.490916	2.008257
H	2.329653	4.021376	0.008146
H	-2.329653	4.021376	-0.008146
H	-2.361742	5.490916	-2.008257
H	-1.491775	4.577986	-4.206322
H	-0.565020	2.257431	-4.231189
N	0.000000	0.000000	4.661757
N	0.000000	0.000000	-4.661757
C	0.000000	0.000000	-5.862372
C	0.000000	0.000000	5.862372
S	0.000000	0.000000	7.481602
S	0.000000	0.000000	-7.481602

Total Energy: -638.07908787 eV

⁵B₂:

Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	2.397184
N	-0.968825	-1.876241	2.253358
N	-1.453536	1.453536	0.000000
N	-1.876241	0.968825	2.253358
N	1.876241	-0.968825	2.253358
N	1.453536	-1.453536	0.000000
N	0.968825	1.876241	2.253358
C	-0.959974	-2.712649	3.317862
C	-1.458048	-4.000724	3.278030
C	-1.961592	-4.479770	2.064286
C	-1.977929	-3.645770	0.964394
C	-1.507724	-2.320254	1.065393
C	-2.320254	1.507724	1.065393
C	-3.645770	1.977929	0.964394
C	-4.479770	1.961592	2.064286
C	-4.000724	1.458048	3.278030
C	-2.712649	0.959974	3.317862
C	2.712649	-0.959974	3.317862
C	4.000724	-1.458048	3.278030
C	4.479770	-1.961592	2.064286
C	3.645770	-1.977929	0.964394
C	2.320254	-1.507724	1.065393
C	1.507724	-2.320254	-1.065393
C	1.977929	-3.645770	-0.964394
C	1.961592	-4.479770	-2.064286
C	1.458048	-4.000724	-3.278030
C	0.959974	2.712649	3.317862
H	-0.528011	-2.292391	4.224143
H	-1.426656	-4.619265	4.174145
H	-2.316806	-5.507673	1.973456
H	-2.315829	-4.009333	-0.005205

H	-4.009333	2.315829	-0.005205
H	-5.507673	2.316806	1.973456
H	-4.619265	1.426656	4.174145
H	-2.292391	0.528011	4.224143
H	2.292391	-0.528011	4.224143
H	4.619265	-1.426656	4.174145
H	5.507673	-2.316806	1.973456
H	4.009333	-2.315829	-0.005205
H	2.315829	-4.009333	0.005205
H	2.316806	-5.507673	-1.973456
H	1.426656	-4.619265	-4.174145
H	0.528011	2.292391	4.224143
N	-1.453536	-1.453536	0.000000
Ru	0.000000	0.000000	-2.397184
N	-0.968825	1.876241	-2.253358
C	-0.959974	2.712649	-3.317862
C	-1.458048	4.000724	-3.278030
C	-1.961592	4.479770	-2.064286
C	-1.977929	3.645770	-0.964394
C	-1.507724	2.320254	-1.065393
C	1.507724	2.320254	1.065393
N	1.453536	1.453536	0.000000
C	2.320254	1.507724	-1.065393
N	1.876241	0.968825	-2.253358
N	-1.876241	-0.968825	-2.253358
C	-2.320254	-1.507724	-1.065393
C	-3.645770	-1.977929	-0.964394
C	-4.479770	-1.961592	-2.064286
C	-4.000724	-1.458048	-3.278030
C	-2.712649	-0.959974	-3.317862
H	-2.292391	-0.528011	-4.224143
H	-4.619265	-1.426656	-4.174145
H	-5.507673	-2.316806	-1.973456
H	-4.009333	-2.315829	0.005205
N	0.968825	-1.876241	-2.253358
C	0.959974	-2.712649	-3.317862
H	0.528011	-2.292391	-4.224143
C	2.712649	0.959974	-3.317862
C	4.000724	1.458048	-3.278030
C	4.479770	1.961592	-2.064286
C	3.645770	1.977929	-0.964394
H	4.009333	2.315829	0.005205
H	5.507673	2.316806	-1.973456
H	4.619265	1.426656	-4.174145
H	2.292391	0.528011	-4.224143
C	1.977929	3.645770	0.964394
C	1.961592	4.479770	2.064286
C	1.458048	4.000724	3.278030
H	1.426656	4.619265	4.174145
H	2.316806	5.507673	1.973456
H	2.315829	4.009333	-0.005205
H	-2.315829	4.009333	0.005205
H	-2.316806	5.507673	-1.973456
H	-1.426656	4.619265	-4.174145
H	-0.528011	2.292391	-4.224143
N	0.000000	0.000000	4.528069
N	0.000000	0.000000	-4.528069
C	0.000000	0.000000	-5.728151
C	0.000000	0.000000	5.728151

S	0.000000	0.000000	7.346851
S	0.000000	0.000000	-7.346851

Total Energy: -638.66383174 eV

¹A:

Ru	0.000000	0.000000	0.211707
Ru	1.969714	-1.201722	-0.078161
N	2.907157	0.443145	-0.938964
N	-0.760777	-1.245224	-1.376678
N	1.421339	-1.846131	-1.950988
N	2.366907	-0.371483	1.942329
N	0.764043	1.269041	1.586691
N	0.819772	-2.809476	0.852793
C	4.250327	0.601793	-0.912638
C	4.884587	1.714251	-1.429887
C	4.094508	2.741469	-1.960854
C	2.720621	2.607802	-1.968786
C	2.114319	1.435677	-1.468462
C	0.099727	-1.722451	-2.324404
C	-0.253010	-1.986473	-3.667842
C	0.696150	-2.417651	-4.572306
C	2.024642	-2.577699	-4.159533
C	2.340862	-2.260253	-2.853199
C	3.240325	-0.999059	2.758599
C	3.539630	-0.564961	4.039444
C	2.883684	0.567156	4.528114
C	1.968849	1.216620	3.721096
C	1.717371	0.744409	2.420298
C	0.374847	2.577457	1.503354
C	1.149019	3.661542	1.962973
C	0.690117	4.956340	1.816562
C	-0.540175	5.179789	1.193844
C	1.240871	-4.085041	0.717201
H	4.800608	-0.223981	-0.464801
H	5.971323	1.780887	-1.399464
H	4.553832	3.655082	-2.341876
H	2.081747	3.414990	-2.325734
H	-1.279099	-1.806907	-3.986631
H	0.409170	-2.608026	-5.607938
H	2.803437	-2.922395	-4.838214
H	3.356290	-2.338882	-2.468992
H	3.715105	-1.881998	2.338309
H	4.261328	-1.117192	4.640508
H	3.064250	0.922973	5.543888
H	1.392400	2.062305	4.094273
H	2.130368	3.463348	2.391627
H	1.299687	5.791692	2.164945
H	-0.945837	6.181141	1.057098
H	2.190295	-4.208047	0.200859
N	0.760777	1.245224	-1.376678
Ru	-1.969714	1.201722	-0.078161
N	-2.907157	-0.443145	-0.938964
C	-4.250327	-0.601793	-0.912638
C	-4.884587	-1.714251	-1.429887
C	-4.094508	-2.741469	-1.960854
C	-2.720621	-2.607802	-1.968786
C	-2.114319	-1.435677	-1.468462

C	-0.374847	-2.577457	1.503354
N	-0.764043	-1.269041	1.586691
C	-1.717371	-0.744409	2.420298
N	-2.366907	0.371483	1.942329
N	-1.421339	1.846131	-1.950988
C	-0.099727	1.722451	-2.324404
C	0.253010	1.986473	-3.667842
C	-0.696150	2.417651	-4.572306
C	-2.024642	2.577699	-4.159533
C	-2.340862	2.260253	-2.853199
H	-3.356290	2.338882	-2.468992
H	-2.803437	2.922395	-4.838214
H	-0.409170	2.608026	-5.607938
H	1.279099	1.806907	-3.986631
N	-0.819772	2.809476	0.852793
C	-1.240871	4.085041	0.717201
H	-2.190295	4.208047	0.200859
C	-3.240325	0.999059	2.758599
C	-3.539630	0.564961	4.039444
C	-2.883684	-0.567156	4.528114
C	-1.968849	-1.216620	3.721096
H	-1.392400	-2.062305	4.094273
H	-3.064250	-0.922973	5.543888
H	-4.261328	1.117192	4.640508
H	-3.715105	1.881998	2.338309
C	-1.149019	-3.661542	1.962973
C	-0.690117	-4.956340	1.816562
C	0.540175	-5.179789	1.193844
H	0.945837	-6.181141	1.057098
H	-1.299687	-5.791692	2.164945
H	-2.130368	-3.463348	2.391627
H	-2.081747	-3.414990	-2.325734
H	-4.553832	-3.655082	-2.341876
H	-5.971323	-1.780887	-1.399464
H	-4.800608	0.223981	-0.464801
N	3.718746	-2.334481	0.077757
N	-3.718746	2.334481	0.077757
C	4.609025	-3.116479	0.262396
C	-4.609025	3.116479	0.262396
S	-5.809951	4.166145	0.510646
S	5.809951	-4.166145	0.510646

Total Energy: -638.88267628 eV

³A:

Ru	0.000000	0.000000	-0.012562
Ru	2.028413	-1.282257	-0.012719
N	2.907077	0.372182	-0.994083
N	-0.775724	-1.227280	-1.465016
N	1.385573	-2.034140	-1.881506
N	2.433874	-0.377733	1.854898
N	0.777297	1.228073	1.438996
N	0.909782	-2.786102	0.967342
C	4.254411	0.504803	-1.001269
C	4.908731	1.612295	-1.506030
C	4.138740	2.671000	-1.997578
C	2.762631	2.559764	-1.998265
C	2.140102	1.386187	-1.525756

C	0.095792	-1.847103	-2.329367
C	-0.240151	-2.188431	-3.655553
C	0.694612	-2.773916	-4.485967
C	1.985362	-3.009013	-4.001961
C	2.285930	-2.607320	-2.714454
C	3.339379	-0.943951	2.687096
C	3.576967	-0.497015	3.972805
C	2.813423	0.570388	4.455753
C	1.882124	1.162329	3.626165
C	1.713521	0.708724	2.301804
C	0.335970	2.529015	1.497579
C	1.129704	3.595729	1.966852
C	0.638997	4.886150	1.966840
C	-0.649033	5.126430	1.478310
C	1.368852	-4.059704	0.975048
H	4.797658	-0.336719	-0.575906
H	5.997281	1.650045	-1.488115
H	4.611512	3.586786	-2.356341
H	2.136870	3.387715	-2.329002
H	-1.237592	-1.948357	-4.021508
H	0.428402	-3.025756	-5.513897
H	2.756800	-3.471921	-4.616224
H	3.280997	-2.734330	-2.292561
H	3.879090	-1.789822	2.265881
H	4.326896	-0.994504	4.586675
H	2.929934	0.921727	5.482314
H	1.239208	1.961987	3.991667
H	2.147137	3.386681	2.294753
H	1.263572	5.706619	2.323537
H	-1.082639	6.125527	1.460984
H	2.362889	-4.188396	0.551252
N	0.775724	1.227280	-1.465016
Ru	-2.028413	1.282257	-0.012719
N	-2.907077	-0.372182	-0.994083
C	-4.254411	-0.504803	-1.001269
C	-4.908731	-1.612295	-1.506030
C	-4.138740	-2.671000	-1.997578
C	-2.762631	-2.559764	-1.998265
C	-2.140102	-1.386187	-1.525756
C	-0.335970	-2.529015	1.497579
N	-0.777297	-1.228073	1.438996
C	-1.713521	-0.708724	2.301804
N	-2.433874	0.377733	1.854898
N	-1.385573	2.034140	-1.881506
C	-0.095792	1.847103	-2.329367
C	0.240151	2.188431	-3.655553
C	-0.694612	2.773916	-4.485967
C	-1.985362	3.009013	-4.001961
C	-2.285930	2.607320	-2.714454
H	-3.280997	2.734330	-2.292561
H	-2.756800	3.471921	-4.616224
H	-0.428402	3.025756	-5.513897
H	1.237592	1.948357	-4.021508
N	-0.909782	2.786102	0.967342
C	-1.368852	4.059704	0.975048
H	-2.362889	4.188396	0.551252
C	-3.339379	0.943951	2.687096
C	-3.576967	0.497015	3.972805
C	-2.813423	-0.570388	4.455753

C	-1.882124	-1.162329	3.626165
H	-1.239208	-1.961987	3.991667
H	-2.929934	-0.921727	5.482314
H	-4.326896	0.994504	4.586675
H	-3.879090	1.789822	2.265881
C	-1.129704	-3.595729	1.966852
C	-0.638997	-4.886150	1.966840
C	0.649033	-5.126430	1.478310
H	1.082639	-6.125527	1.460984
H	-1.263572	-5.706619	2.323537
H	-2.147137	-3.386681	2.294753
H	-2.136870	-3.387715	-2.329002
H	-4.611512	-3.586786	-2.356341
H	-5.997281	-1.650045	-1.488115
H	-4.797658	0.336719	-0.575906
N	3.820357	-2.415638	-0.011938
N	-3.820357	2.415638	-0.011938
C	4.837085	-3.052203	-0.014325
C	-4.837085	3.052203	-0.014325
S	-6.208024	3.910864	-0.015819
S	6.208024	-3.910864	-0.015819

Total Energy: -638.50390818 eV

³A:

Ru	0.000000	0.000000	-0.016572
Ru	2.001921	-1.266635	-0.012054
N	2.906314	0.400578	-0.973113
N	-0.780057	-1.232418	-1.477325
N	1.385294	-2.000437	-1.906671
N	2.400949	-0.392952	1.879728
N	0.778021	1.235488	1.454050
N	0.886149	-2.797947	0.946769
C	4.251586	0.537456	-0.962104
C	4.909795	1.639326	-1.475099
C	4.141295	2.687672	-1.991095
C	2.765814	2.573802	-2.005288
C	2.139626	1.405203	-1.523134
C	0.091311	-1.833082	-2.349373
C	-0.242826	-2.185783	-3.673731
C	0.699481	-2.757774	-4.504741
C	1.996982	-2.966880	-4.026578
C	2.294152	-2.555179	-2.740751
C	3.289664	-0.979768	2.713763
C	3.539013	-0.534122	3.998126
C	2.799637	0.552967	4.475294
C	1.879388	1.161327	3.645752
C	1.697516	0.706704	2.322197
C	0.348550	2.536220	1.501594
C	1.133864	3.605260	1.983605
C	0.647917	4.896767	1.962190
C	-0.626402	5.141123	1.439474
C	1.338031	-4.072475	0.927847
H	4.793432	-0.295444	-0.518780
H	5.997825	1.680833	-1.446055
H	4.615631	3.599620	-2.357476
H	2.141924	3.396911	-2.351180
H	-1.244716	-1.962398	-4.038017

H	0.433959	-3.018470	-5.530540
H	2.773767	-3.417535	-4.642951
H	3.292809	-2.663779	-2.322710
H	3.812297	-1.837608	2.296004
H	4.278895	-1.044236	4.613342
H	2.925596	0.907167	5.499778
H	1.253094	1.974007	4.011094
H	2.143660	3.396442	2.334241
H	1.268061	5.717053	2.327814
H	-1.054265	6.142035	1.404426
H	2.321065	-4.203452	0.480320
N	0.780057	1.232418	-1.477325
Ru	-2.001921	1.266635	-0.012054
N	-2.906314	-0.400578	-0.973113
C	-4.251586	-0.537456	-0.962104
C	-4.909795	-1.639326	-1.475099
C	-4.141295	-2.687672	-1.991095
C	-2.765814	-2.573802	-2.005288
C	-2.139626	-1.405203	-1.523134
C	-0.348550	-2.536220	1.501594
N	-0.778021	-1.235488	1.454050
C	-1.697516	-0.706704	2.322197
N	-2.400949	0.392952	1.879728
N	-1.385294	2.000437	-1.906671
C	-0.091311	1.833082	-2.349373
C	0.242826	2.185783	-3.673731
C	-0.699481	2.757774	-4.504741
C	-1.996982	2.966880	-4.026578
C	-2.294152	2.555179	-2.740751
H	-3.292809	2.663779	-2.322710
H	-2.773767	3.417535	-4.642951
H	-0.433959	3.018470	-5.530540
H	1.244716	1.962398	-4.038017
N	-0.886149	2.797947	0.946769
C	-1.338031	4.072475	0.927847
H	-2.321065	4.203452	0.480320
C	-3.289664	0.979768	2.713763
C	-3.539013	0.534122	3.998126
C	-2.799637	-0.552967	4.475294
C	-1.879388	-1.161327	3.645752
H	-1.253094	-1.974007	4.011094
H	-2.925596	-0.907167	5.499778
H	-4.278895	1.044236	4.613342
H	-3.812297	1.837608	2.296004
C	-1.133864	-3.605260	1.983605
C	-0.647917	-4.896767	1.962190
C	0.626402	-5.141123	1.439474
H	1.054265	-6.142035	1.404426
H	-1.268061	-5.717053	2.327814
H	-2.143660	-3.396442	2.334241
H	-2.141924	-3.396911	-2.351180
H	-4.615631	-3.599620	-2.357476
H	-5.997825	-1.680833	-1.446055
H	-4.793432	0.295444	-0.518780
N	3.790189	-2.393734	-0.011913
N	-3.790189	2.393734	-0.011913
C	4.805807	-3.033304	-0.014241
C	-4.805807	3.033304	-0.014241
S	-6.173592	3.891146	-0.019098

S 6.173592 -3.891146 -0.019098

Total Energy: -638.49036417 eV

³B:

Ru	0.000000	0.000000	0.096634
Ru	2.013086	-1.270848	-0.043893
N	2.907297	0.355694	-1.022131
N	-0.768139	-1.224479	-1.418298
N	1.389349	-2.001501	-1.887031
N	2.430843	-0.376991	1.863830
N	0.771931	1.231376	1.514232
N	0.890685	-2.785554	0.977631
C	4.255541	0.476511	-1.061352
C	4.902128	1.577936	-1.586469
C	4.124831	2.641953	-2.057915
C	2.749169	2.542793	-2.016945
C	2.130217	1.373781	-1.525258
C	0.095016	-1.805824	-2.312602
C	-0.245553	-2.104117	-3.650424
C	0.684511	-2.663538	-4.502480
C	1.979002	-2.917333	-4.034129
C	2.288092	-2.551740	-2.738998
C	3.349620	-0.958806	2.669383
C	3.617609	-0.532453	3.957391
C	2.875331	0.533449	4.473115
C	1.928985	1.142774	3.672212
C	1.729012	0.703378	2.349304
C	0.335475	2.532482	1.553712
C	1.111922	3.598963	2.051184
C	0.619949	4.888677	2.031885
C	-0.650387	5.126611	1.499084
C	1.350778	-4.057675	0.971997
H	4.802408	-0.367732	-0.645243
H	5.990931	1.608395	-1.601303
H	4.594310	3.553365	-2.431712
H	2.120591	3.375785	-2.329616
H	-1.243633	-1.852090	-4.006483
H	0.412278	-2.882092	-5.536505
H	2.744012	-3.366481	-4.666222
H	3.284553	-2.690010	-2.323830
H	3.875024	-1.801135	2.224044
H	4.376681	-1.044994	4.547431
H	3.018445	0.869804	5.501350
H	1.296923	1.939655	4.061803
H	2.117978	3.392546	2.413250
H	1.231171	5.710201	2.409172
H	-1.084924	6.124980	1.466103
H	2.330847	-4.186451	0.516365
N	0.768139	1.224479	-1.418298
Ru	-2.013086	1.270848	-0.043893
N	-2.907297	-0.355694	-1.022131
C	-4.255541	-0.476511	-1.061352
C	-4.902128	-1.577936	-1.586469
C	-4.124831	-2.641953	-2.057915
C	-2.749169	-2.542793	-2.016945

C	-2.130217	-1.373781	-1.525258
C	-0.335475	-2.532482	1.553712
N	-0.771931	-1.231376	1.514232
C	-1.729012	-0.703378	2.349304
N	-2.430843	0.376991	1.863830
N	-1.389349	2.001501	-1.887031
C	-0.095016	1.805824	-2.312602
C	0.245553	2.104117	-3.650424
C	-0.684511	2.663538	-4.502480
C	-1.979002	2.917333	-4.034129
C	-2.288092	2.551740	-2.738998
H	-3.284553	2.690010	-2.323830
H	-2.744012	3.366481	-4.666222
H	-0.412278	2.882092	-5.536505
H	1.243633	1.852090	-4.006483
N	-0.890685	2.785554	0.977631
C	-1.350778	4.057675	0.971997
H	-2.330847	4.186451	0.516365
C	-3.349620	0.958806	2.669383
C	-3.617609	0.532453	3.957391
C	-2.875331	-0.533449	4.473115
C	-1.928985	-1.142774	3.672212
H	-1.296923	-1.939655	4.061803
H	-3.018445	-0.869804	5.501350
H	-4.376681	1.044994	4.547431
H	-3.875024	1.801135	2.224044
C	-1.111922	-3.598963	2.051184
C	-0.619949	-4.888677	2.031885
C	0.650387	-5.126611	1.499084
H	1.084924	-6.124980	1.466103
H	-1.231171	-5.710201	2.409172
H	-2.117978	-3.392546	2.413250
H	-2.120591	-3.375785	-2.329616
H	-4.594310	-3.553365	-2.431712
H	-5.990931	-1.608395	-1.601303
H	-4.802408	0.367732	-0.645243
N	3.840214	-2.449090	0.052764
N	-3.840214	2.449090	0.052764
C	4.852691	-3.090195	-0.004842
C	-4.852691	3.090195	-0.004842
S	-6.215371	3.955667	-0.086773
S	6.215371	-3.955667	-0.086773

Total Energy: -638.21183239 eV

³B:

Ru	0.000000	0.000000	0.138934
Ru	2.003290	-1.215441	-0.029793
N	2.905330	0.467901	-0.896332
N	-0.757711	-1.256862	-1.376376
N	1.425118	-1.903667	-1.912219
N	2.409152	-0.344317	1.923992
N	0.771367	1.271032	1.539374
N	0.859121	-2.804442	0.877248
C	4.245048	0.647081	-0.847123
C	4.875902	1.780964	-1.323021
C	4.083254	2.811471	-1.840843
C	2.711865	2.656525	-1.879768

C	2.111799	1.463687	-1.424953
C	0.104609	-1.784017	-2.296877
C	-0.254629	-2.114575	-3.622426
C	0.687172	-2.600478	-4.506120
C	2.014598	-2.745727	-4.087784
C	2.336032	-2.366034	-2.798726
C	3.311930	-0.928299	2.741783
C	3.616564	-0.457192	4.006294
C	2.928732	0.664551	4.478032
C	1.987482	1.269349	3.668797
C	1.734430	0.771090	2.375543
C	0.361794	2.575642	1.481484
C	1.144779	3.668219	1.907795
C	0.675131	4.959893	1.775059
C	-0.579765	5.176853	1.199008
C	1.291871	-4.078107	0.752478
H	4.803651	-0.177064	-0.408606
H	5.960880	1.859439	-1.267100
H	4.535428	3.742943	-2.185713
H	2.068144	3.465048	-2.225068
H	-1.281268	-1.943662	-3.943824
H	0.396250	-2.843092	-5.529525
H	2.791705	-3.123652	-4.750494
H	3.355320	-2.430069	-2.423567
H	3.803803	-1.806740	2.329630
H	4.363041	-0.972263	4.609827
H	3.107583	1.047526	5.484098
H	1.393886	2.106964	4.032490
H	2.143065	3.477807	2.299259
H	1.294620	5.798959	2.095617
H	-0.992889	6.176679	1.072555
H	2.261131	-4.190619	0.271790
N	0.757711	1.256862	-1.376376
Ru	-2.003290	1.215441	-0.029793
N	-2.905330	-0.467901	-0.896332
C	-4.245048	-0.647081	-0.847123
C	-4.875902	-1.780964	-1.323021
C	-4.083254	-2.811471	-1.840843
C	-2.711865	-2.656525	-1.879768
C	-2.111799	-1.463687	-1.424953
C	-0.361794	-2.575642	1.481484
N	-0.771367	-1.271032	1.539374
C	-1.734430	-0.771090	2.375543
N	-2.409152	0.344317	1.923992
N	-1.425118	1.903667	-1.912219
C	-0.104609	1.784017	-2.296877
C	0.254629	2.114575	-3.622426
C	-0.687172	2.600478	-4.506120
C	-2.014598	2.745727	-4.087784
C	-2.336032	2.366034	-2.798726
H	-3.355320	2.430069	-2.423567
H	-2.791705	3.123652	-4.750494
H	-0.396250	2.843092	-5.529525
H	1.281268	1.943662	-3.943824
N	-0.859121	2.804442	0.877248
C	-1.291871	4.078107	0.752478
H	-2.261131	4.190619	0.271790
C	-3.311930	0.928299	2.741783
C	-3.616564	0.457192	4.006294

C	-2.928732	-0.664551	4.478032
C	-1.987482	-1.269349	3.668797
H	-1.393886	-2.106964	4.032490
H	-3.107583	-1.047526	5.484098
H	-4.363041	0.972263	4.609827
H	-3.803803	1.806740	2.329630
C	-1.144779	-3.668219	1.907795
C	-0.675131	-4.959893	1.775059
C	0.579765	-5.176853	1.199008
H	0.992889	-6.176679	1.072555
H	-1.294620	-5.798959	2.095617
H	-2.143065	-3.477807	2.299259
H	-2.068144	-3.465048	-2.225068
H	-4.535428	-3.742943	-2.185713
H	-5.960880	-1.859439	-1.267100
H	-4.803651	0.177064	-0.408606
N	3.729032	-2.295503	0.061191
N	-3.729032	2.295503	0.061191
C	4.724053	-2.959202	-0.024541
C	-4.724053	2.959202	-0.024541
S	-6.065342	3.850586	-0.116900
S	6.065342	-3.850586	-0.116900

Total Energy: -638.69361509 eV

⁵A:

Ru	0.000000	0.000000	-0.012105
Ru	2.024302	-1.278764	-0.012385
N	2.906656	0.383311	-0.979901
N	-0.776092	-1.228669	-1.465634
N	1.388405	-2.019282	-1.889402
N	2.422252	-0.384643	1.863191
N	0.777114	1.229155	1.440353
N	0.901413	-2.789724	0.953291
C	4.253301	0.521856	-0.971614
C	4.907518	1.631466	-1.471283
C	4.137169	2.684328	-1.975769
C	2.761856	2.566674	-1.991716
C	2.139538	1.392607	-1.520020
C	0.095921	-1.841976	-2.333073
C	-0.240272	-2.184910	-3.658794
C	0.699164	-2.756220	-4.493438
C	1.994699	-2.976982	-4.014816
C	2.293908	-2.578108	-2.726341
C	3.317056	-0.961084	2.699829
C	3.550974	-0.517544	3.987195
C	2.796553	0.558889	4.465229
C	1.876183	1.160966	3.630993
C	1.707684	0.707000	2.306539
C	0.340068	2.531124	1.492636
C	1.133949	3.598171	1.960935
C	0.649857	4.890820	1.942864
C	-0.632125	5.133685	1.439147
C	1.354168	-4.065550	0.942534
H	4.795031	-0.316970	-0.538825
H	5.995568	1.675659	-1.440508
H	4.609332	3.601412	-2.332174
H	2.136137	3.391287	-2.330847

H	-1.240949	-1.954344	-4.022042
H	0.433095	-3.007745	-5.521414
H	2.769598	-3.427438	-4.633896
H	3.290806	-2.696200	-2.305931
H	3.850993	-1.811526	2.280301
H	4.291420	-1.023198	4.605960
H	2.911229	0.909012	5.492502
H	1.239380	1.966803	3.993674
H	2.147778	3.387846	2.299212
H	1.275800	5.711656	2.296834
H	-1.059096	6.135318	1.406699
H	2.344824	-4.193838	0.510621
N	0.776092	1.228669	-1.465634
Ru	-2.024302	1.278764	-0.012385
N	-2.906656	-0.383311	-0.979901
C	-4.253301	-0.521856	-0.971614
C	-4.907518	-1.631466	-1.471283
C	-4.137169	-2.684328	-1.975769
C	-2.761856	-2.566674	-1.991716
C	-2.139538	-1.392607	-1.520020
C	-0.340068	-2.531124	1.492636
N	-0.777114	-1.229155	1.440353
C	-1.707684	-0.707000	2.306539
N	-2.422252	0.384643	1.863191
N	-1.388405	2.019282	-1.889402
C	-0.095921	1.841976	-2.333073
C	0.240272	2.184910	-3.658794
C	-0.699164	2.756220	-4.493438
C	-1.994699	2.976982	-4.014816
C	-2.293908	2.578108	-2.726341
H	-3.290806	2.696200	-2.305931
H	-2.769598	3.427438	-4.633896
H	-0.433095	3.007745	-5.521414
H	1.240949	1.954344	-4.022042
N	-0.901413	2.789724	0.953291
C	-1.354168	4.065550	0.942534
H	-2.344824	4.193838	0.510621
C	-3.317056	0.961084	2.699829
C	-3.550974	0.517544	3.987195
C	-2.796553	-0.558889	4.465229
C	-1.876183	-1.160966	3.630993
H	-1.239380	-1.966803	3.993674
H	-2.911229	-0.909012	5.492502
H	-4.291420	1.023198	4.605960
H	-3.850993	1.811526	2.280301
C	-1.133949	-3.598171	1.960935
C	-0.649857	-4.890820	1.942864
C	0.632125	-5.133685	1.439147
H	1.059096	-6.135318	1.406699
H	-1.275800	-5.711656	2.296834
H	-2.147778	-3.387846	2.299212
H	-2.136137	-3.391287	-2.330847
H	-4.609332	-3.601412	-2.332174
H	-5.995568	-1.675659	-1.440508
H	-4.795031	0.316970	-0.538825
N	3.820857	-2.413704	-0.012528
N	-3.820857	2.413704	-0.012528
C	4.834155	-3.055525	-0.013749
C	-4.834155	3.055525	-0.013749

S	-6.200384	3.921600	-0.013278
S	6.200384	-3.921600	-0.013278

Total Energy: -638.67047383 eV

Ru₃(dpa)₄(CN)₂:

¹A₁:

Ru	0.000000	0.000000	2.316861
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.316861
N	0.954055	-1.914436	2.226937
N	1.478902	-1.478902	0.000000
N	1.914436	-0.954055	-2.226937
N	-0.954055	1.914436	2.226937
N	-1.478902	1.478902	0.000000
N	-1.914436	0.954055	-2.226937
N	-1.914436	-0.954055	2.226937
N	-1.478902	-1.478902	0.000000
N	-0.954055	-1.914436	-2.226937
N	1.914436	0.954055	2.226937
N	1.478902	1.478902	0.000000
N	0.954055	1.914436	-2.226937
N	0.000000	0.000000	5.829495

N	0.000000	0.000000	-5.829495
C	0.931869	-2.743544	3.294212
H	0.488151	-2.322495	4.196179
C	1.445462	-4.028075	3.266998
H	1.413752	-4.641194	4.166783
C	1.966886	-4.507355	2.061863
H	2.333014	-5.532376	1.980952
C	1.989310	-3.680662	0.955975
H	2.342551	-4.046002	-0.007555
C	1.509888	-2.357373	1.047822
C	2.357373	-1.509888	-1.047822
C	3.680662	-1.989310	-0.955975
H	4.046002	-2.342551	0.007555
C	4.507355	-1.966886	-2.061863
H	5.532376	-2.333014	-1.980952
C	4.028075	-1.445462	-3.266998
H	4.641194	-1.413752	-4.166783
C	2.743544	-0.931869	-3.294212
H	2.322495	-0.488151	-4.196179
C	-0.931869	2.743544	3.294212
H	-0.488151	2.322495	4.196179
C	-1.445462	4.028075	3.266998
H	-1.413752	4.641194	4.166783
C	-1.966886	4.507355	2.061863
H	-2.333014	5.532376	1.980952
C	-1.989310	3.680662	0.955975
H	-2.342551	4.046002	-0.007555
C	-1.509888	2.357373	1.047822
C	-2.357373	1.509888	-1.047822
C	-3.680662	1.989310	-0.955975
H	-4.046002	2.342551	0.007555
C	-4.507355	1.966886	-2.061863
H	-5.532376	2.333014	-1.980952
C	-4.028075	1.445462	-3.266998
H	-4.641194	1.413752	-4.166783
C	-2.743544	0.931869	-3.294212
H	-2.322495	0.488151	-4.196179
C	-2.743544	-0.931869	3.294212
H	-2.322495	-0.488151	4.196179
C	-4.028075	-1.445462	3.266998
H	-4.641194	-1.413752	4.166783
C	-4.507355	-1.966886	2.061863
H	-5.532376	-2.333014	1.980952
C	-3.680662	-1.989310	0.955975
H	-4.046002	-2.342551	-0.007555
C	-2.357373	-1.509888	1.047822
C	-1.509888	-2.357373	-1.047822
C	-1.989310	-3.680662	-0.955975
H	-2.342551	-4.046002	0.007555
C	-1.966886	-4.507355	-2.061863
H	-2.333014	-5.532376	-1.980952
C	-1.445462	-4.028075	-3.266998
H	-1.413752	-4.641194	-4.166783
C	-0.931869	-2.743544	-3.294212
H	-0.488151	-2.322495	-4.196179
C	2.743544	0.931869	3.294212
H	2.322495	0.488151	4.196179
C	4.028075	1.445462	3.266998
H	4.641194	1.413752	4.166783

C	4.507355	1.966886	2.061863
H	5.532376	2.333014	1.980952
C	3.680662	1.989310	0.955975
H	4.046002	2.342551	-0.007555
C	2.357373	1.509888	1.047822
C	1.509888	2.357373	-1.047822
C	1.989310	3.680662	-0.955975
H	2.342551	4.046002	0.007555
C	1.966886	4.507355	-2.061863
H	2.333014	5.532376	-1.980952
C	1.445462	4.028075	-3.266998
H	1.413752	4.641194	-4.166783
C	0.931869	2.743544	-3.294212
H	0.488151	2.322495	-4.196179
C	0.000000	0.000000	4.649406
C	0.000000	0.000000	-4.649406

Total Energy: -628.44410320 eV

³A₂:

Ru	0.000000	0.000000	2.378768
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.378768
N	0.930143	-1.914560	2.238254
N	1.461766	-1.461766	0.000000
N	1.914560	-0.930143	-2.238254
N	-0.930143	1.914560	2.238254
N	-1.461766	1.461766	0.000000
N	-1.914560	0.930143	-2.238254
N	-1.914560	-0.930143	2.238254
N	-1.461766	-1.461766	0.000000
N	-0.930143	-1.914560	-2.238254
N	1.914560	0.930143	2.238254
N	1.461766	1.461766	0.000000
N	0.930143	1.914560	-2.238254
N	0.000000	0.000000	5.552603
N	0.000000	0.000000	-5.552603
C	0.892739	-2.773422	3.284158
H	0.445181	-2.376458	4.193538
C	1.390985	-4.062074	3.234613
H	1.338092	-4.694867	4.119859
C	1.924511	-4.519843	2.025891
H	2.283569	-5.545562	1.925791
C	1.963291	-3.667821	0.941062
H	2.322583	-4.014616	-0.027138
C	1.489404	-2.343123	1.049138
C	2.343123	-1.489404	-1.049138
C	3.667821	-1.963291	-0.941062
H	4.014616	-2.322583	0.027138
C	4.519843	-1.924511	-2.025891
H	5.545562	-2.283569	-1.925791
C	4.062074	-1.390985	-3.234613
H	4.694867	-1.338092	-4.119859
C	2.773422	-0.892739	-3.284158
H	2.376458	-0.445181	-4.193538
C	-0.892739	2.773422	3.284158
H	-0.445181	2.376458	4.193538
C	-1.390985	4.062074	3.234613

H	-1.338092	4.694867	4.119859
C	-1.924511	4.519843	2.025891
H	-2.283569	5.545562	1.925791
C	-1.963291	3.667821	0.941062
H	-2.322583	4.014616	-0.027138
C	-1.489404	2.343123	1.049138
C	-2.343123	1.489404	-1.049138
C	-3.667821	1.963291	-0.941062
H	-4.014616	2.322583	0.027138
C	-4.519843	1.924511	-2.025891
H	-5.545562	2.283569	-1.925791
C	-4.062074	1.390985	-3.234613
H	-4.694867	1.338092	-4.119859
C	-2.773422	0.892739	-3.284158
H	-2.376458	0.445181	-4.193538
C	-2.773422	-0.892739	3.284158
H	-2.376458	-0.445181	4.193538
C	-4.062074	-1.390985	3.234613
H	-4.694867	-1.338092	4.119859
C	-4.519843	-1.924511	2.025891
H	-5.545562	-2.283569	1.925791
C	-3.667821	-1.963291	0.941062
H	-4.014616	-2.322583	-0.027138
C	-2.343123	-1.489404	1.049138
C	-1.489404	-2.343123	-1.049138
C	-1.963291	-3.667821	-0.941062
H	-2.322583	-4.014616	0.027138
C	-1.924511	-4.519843	-2.025891
H	-2.283569	-5.545562	-1.925791
C	-1.390985	-4.062074	-3.234613
H	-1.338092	-4.694867	-4.119859
C	-0.892739	-2.773422	-3.284158
H	-0.445181	-2.376458	-4.193538
C	2.773422	0.892739	3.284158
H	2.376458	0.445181	4.193538
C	4.062074	1.390985	3.234613
H	4.694867	1.338092	4.119859
C	4.519843	1.924511	2.025891
H	5.545562	2.283569	1.925791
C	3.667821	1.963291	0.941062
H	4.014616	2.322583	-0.027138
C	2.343123	1.489404	1.049138
C	1.489404	2.343123	-1.049138
C	1.963291	3.667821	-0.941062
H	2.322583	4.014616	0.027138
C	1.924511	4.519843	-2.025891
H	2.283569	5.545562	-1.925791
C	1.390985	4.062074	-3.234613
H	1.338092	4.694867	-4.119859
C	0.892739	2.773422	-3.284158
H	0.445181	2.376458	-4.193538
C	0.000000	0.000000	4.367931
C	0.000000	0.000000	-4.367931

Total Energy: -630.20012602 eV

³A₂:

Ru	0.000000	0.000000	2.441114
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Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.441114
N	1.055503	-1.819214	2.283941
N	1.441778	-1.441778	0.000000
N	1.819214	-1.055503	-2.283941
N	-1.055503	1.819214	2.283941
N	-1.441778	1.441778	0.000000
N	-1.819214	1.055503	-2.283941
N	-1.819214	-1.055503	2.283941
N	-1.441778	-1.441778	0.000000
N	-1.055503	-1.819214	-2.283941
N	1.819214	1.055503	2.283941
N	1.441778	1.441778	0.000000
N	1.055503	1.819214	-2.283941
N	0.000000	0.000000	5.894354
N	0.000000	0.000000	-5.894354
C	1.135269	-2.631571	3.368367
H	0.764651	-2.190150	4.293694
C	1.630888	-3.919756	3.319463
H	1.665124	-4.516243	4.230554
C	2.044379	-4.431219	2.084363
H	2.384284	-5.463933	1.990821
C	1.995122	-3.617431	0.972096
H	2.271344	-3.997328	-0.010721
C	1.538636	-2.286470	1.082335
C	2.286470	-1.538636	-1.082335
C	3.617431	-1.995122	-0.972096
H	3.997328	-2.271344	0.010721
C	4.431219	-2.044379	-2.084363
H	5.463933	-2.384284	-1.990821
C	3.919756	-1.630888	-3.319463
H	4.516243	-1.665124	-4.230554
C	2.631571	-1.135269	-3.368367
H	2.190150	-0.764651	-4.293694
C	-1.135269	2.631571	3.368367
H	-0.764651	2.190150	4.293694
C	-1.630888	3.919756	3.319463
H	-1.665124	4.516243	4.230554
C	-2.044379	4.431219	2.084363
H	-2.384284	5.463933	1.990821
C	-1.995122	3.617431	0.972096
H	-2.271344	3.997328	-0.010721
C	-1.538636	2.286470	1.082335
C	-2.286470	1.538636	-1.082335
C	-3.617431	1.995122	-0.972096
H	-3.997328	2.271344	0.010721
C	-4.431219	2.044379	-2.084363
H	-5.463933	2.384284	-1.990821
C	-3.919756	1.630888	-3.319463
H	-4.516243	1.665124	-4.230554
C	-2.631571	1.135269	-3.368367
H	-2.190150	0.764651	-4.293694
C	-2.631571	-1.135269	3.368367
H	-2.190150	-0.764651	4.293694
C	-3.919756	-1.630888	3.319463
H	-4.516243	-1.665124	4.230554
C	-4.431219	-2.044379	2.084363
H	-5.463933	-2.384284	1.990821
C	-3.617431	-1.995122	0.972096

H	-3.997328	-2.271344	-0.010721
C	-2.286470	-1.538636	1.082335
C	-1.538636	-2.286470	-1.082335
C	-1.995122	-3.617431	-0.972096
H	-2.271344	-3.997328	0.010721
C	-2.044379	-4.431219	-2.084363
H	-2.384284	-5.463933	-1.990821
C	-1.630888	-3.919756	-3.319463
H	-1.665124	-4.516243	-4.230554
C	-1.135269	-2.631571	-3.368367
H	-0.764651	-2.190150	-4.293694
C	2.631571	1.135269	3.368367
H	2.190150	0.764651	4.293694
C	3.919756	1.630888	3.319463
H	4.516243	1.665124	4.230554
C	4.431219	2.044379	2.084363
H	5.463933	2.384284	1.990821
C	3.617431	1.995122	0.972096
H	3.997328	2.271344	-0.010721
C	2.286470	1.538636	1.082335
C	1.538636	2.286470	-1.082335
C	1.995122	3.617431	-0.972096
H	2.271344	3.997328	0.010721
C	2.044379	4.431219	-2.084363
H	2.384284	5.463933	-1.990821
C	1.630888	3.919756	-3.319463
H	1.665124	4.516243	-4.230554
C	1.135269	2.631571	-3.368367
H	0.764651	2.190150	-4.293694
C	0.000000	0.000000	4.712461
C	0.000000	0.000000	-4.712461

Total Energy: -628.25320801 eV

³E:

Ru	0.000000	0.000000	2.356238
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.356238
N	0.936994	-1.919117	2.229110
N	1.468644	-1.468644	0.000000
N	1.919117	-0.936994	-2.229110
N	-0.936994	1.919117	2.229110
N	-1.468644	1.468644	0.000000
N	-1.919117	0.936994	-2.229110
N	-1.919117	-0.936994	2.229110
N	-1.468644	-1.468644	0.000000
N	-0.936994	-1.919117	-2.229110
N	1.919117	0.936994	2.229110
N	1.468644	1.468644	0.000000
N	0.936994	1.919117	-2.229110
N	0.000000	0.000000	5.669650
N	0.000000	0.000000	-5.669650
C	0.901865	-2.767818	3.281314
H	0.455299	-2.362289	4.187544
C	1.401249	-4.057097	3.238415
H	1.353539	-4.683853	4.127998
C	1.930107	-4.522207	2.030635

H	2.288653	-5.548752	1.936219
C	1.967034	-3.677281	0.939471
H	2.323321	-4.029715	-0.027867
C	1.494369	-2.352029	1.045110
C	2.352029	-1.494369	-1.045110
C	3.677281	-1.967034	-0.939471
H	4.029715	-2.323321	0.027867
C	4.522207	-1.930107	-2.030635
H	5.548752	-2.288653	-1.936219
C	4.057097	-1.401249	-3.238415
H	4.683853	-1.353539	-4.127998
C	2.767818	-0.901865	-3.281314
H	2.362289	-0.455299	-4.187544
C	-0.901865	2.767818	3.281314
H	-0.455299	2.362289	4.187544
C	-1.401249	4.057097	3.238415
H	-1.353539	4.683853	4.127998
C	-1.930107	4.522207	2.030635
H	-2.288653	5.548752	1.936219
C	-1.967034	3.677281	0.939471
H	-2.323321	4.029715	-0.027867
C	-1.494369	2.352029	1.045110
C	-2.352029	1.494369	-1.045110
C	-3.677281	1.967034	-0.939471
H	-4.029715	2.323321	0.027867
C	-4.522207	1.930107	-2.030635
H	-5.548752	2.288653	-1.936219
C	-4.057097	1.401249	-3.238415
H	-4.683853	1.353539	-4.127998
C	-2.767818	0.901865	-3.281314
H	-2.362289	0.455299	-4.187544
C	-2.767818	-0.901865	3.281314
H	-2.362289	-0.455299	4.187544
C	-4.057097	-1.401249	3.238415
H	-4.683853	-1.353539	4.127998
C	-4.522207	-1.930107	2.030635
H	-5.548752	-2.288653	1.936219
C	-3.677281	-1.967034	0.939471
H	-4.029715	-2.323321	-0.027867
C	-2.352029	-1.494369	1.045110
C	-1.494369	-2.352029	-1.045110
C	-1.967034	-3.677281	-0.939471
H	-2.323321	-4.029715	0.027867
C	-1.930107	-4.522207	-2.030635
H	-2.288653	-5.548752	-1.936219
C	-1.401249	-4.057097	-3.238415
H	-1.353539	-4.683853	-4.127998
C	-0.901865	-2.767818	-3.281314
H	-0.455299	-2.362289	-4.187544
C	2.767818	0.901865	3.281314
H	2.362289	0.455299	4.187544
C	4.057097	1.401249	3.238415
H	4.683853	1.353539	4.127998
C	4.522207	1.930107	2.030635
H	5.548752	2.288653	1.936219
C	3.677281	1.967034	0.939471
H	4.029715	2.323321	-0.027867
C	2.352029	1.494369	1.045110
C	1.494369	2.352029	-1.045110

C	1.967034	3.677281	-0.939471
H	2.323321	4.029715	0.027867
C	1.930107	4.522207	-2.030635
H	2.288653	5.548752	-1.936219
C	1.401249	4.057097	-3.238415
H	1.353539	4.683853	-4.127998
C	0.901865	2.767818	-3.281314
H	0.455299	2.362289	-4.187544
C	0.000000	0.000000	4.487858
C	0.000000	0.000000	-4.487858

Total Energy: -629.25716626 eV

³E:

Ru	0.000000	0.000000	2.383918
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.383918
N	1.004376	-1.867962	2.256857
N	1.459388	-1.459388	0.000000
N	1.867962	-1.004376	-2.256857
N	-1.004376	1.867962	2.256857
N	-1.459388	1.459388	0.000000
N	-1.867962	1.004376	-2.256857
N	-1.867962	-1.004376	2.256857
N	-1.459388	-1.459388	0.000000
N	-1.004376	-1.867962	-2.256857
N	1.867962	1.004376	2.256857
N	1.459388	1.459388	0.000000
N	1.004376	1.867962	-2.256857
N	0.000000	0.000000	5.863211
N	0.000000	0.000000	-5.863211
C	1.038255	-2.687292	3.334558
H	0.630890	-2.257054	4.249393
C	1.548603	-3.971568	3.296858
H	1.555155	-4.574699	4.204196
C	2.012568	-4.467405	2.074431
H	2.368871	-5.495131	1.986643
C	1.991861	-3.648363	0.963560
H	2.303912	-4.020625	-0.011363
C	1.522779	-2.322067	1.065979
C	2.322067	-1.522779	-1.065979
C	3.648363	-1.991861	-0.963560
H	4.020625	-2.303912	0.011363
C	4.467405	-2.012568	-2.074431
H	5.495131	-2.368871	-1.986643
C	3.971568	-1.548603	-3.296858
H	4.574699	-1.555155	-4.204196
C	2.687292	-1.038255	-3.334558
H	2.257054	-0.630890	-4.249393
C	-1.038255	2.687292	3.334558
H	-0.630890	2.257054	4.249393
C	-1.548603	3.971568	3.296858
H	-1.555155	4.574699	4.204196
C	-2.012568	4.467405	2.074431
H	-2.368871	5.495131	1.986643
C	-1.991861	3.648363	0.963560
H	-2.303912	4.020625	-0.011363
C	-1.522779	2.322067	1.065979

C	-2.322067	1.522779	-1.065979
C	-3.648363	1.991861	-0.963560
H	-4.020625	2.303912	0.011363
C	-4.467405	2.012568	-2.074431
H	-5.495131	2.368871	-1.986643
C	-3.971568	1.548603	-3.296858
H	-4.574699	1.555155	-4.204196
C	-2.687292	1.038255	-3.334558
H	-2.257054	0.630890	-4.249393
C	-2.687292	-1.038255	3.334558
H	-2.257054	-0.630890	4.249393
C	-3.971568	-1.548603	3.296858
H	-4.574699	-1.555155	4.204196
C	-4.467405	-2.012568	2.074431
H	-5.495131	-2.368871	1.986643
C	-3.648363	-1.991861	0.963560
H	-4.020625	-2.303912	-0.011363
C	-2.322067	-1.522779	1.065979
C	-1.522779	-2.322067	-1.065979
C	-1.991861	-3.648363	-0.963560
H	-2.303912	-4.020625	0.011363
C	-2.012568	-4.467405	-2.074431
H	-2.368871	-5.495131	-1.986643
C	-1.548603	-3.971568	-3.296858
H	-1.555155	-4.574699	-4.204196
C	-1.038255	-2.687292	-3.334558
H	-0.630890	-2.257054	-4.249393
C	2.687292	1.038255	3.334558
H	2.257054	0.630890	4.249393
C	3.971568	1.548603	3.296858
H	4.574699	1.555155	4.204196
C	4.467405	2.012568	2.074431
H	5.495131	2.368871	1.986643
C	3.648363	1.991861	0.963560
H	4.020625	2.303912	-0.011363
C	2.322067	1.522779	1.065979
C	1.522779	2.322067	-1.065979
C	1.991861	3.648363	-0.963560
H	2.303912	4.020625	0.011363
C	2.012568	4.467405	-2.074431
H	2.368871	5.495131	-1.986643
C	1.548603	3.971568	-3.296858
H	1.555155	4.574699	-4.204196
C	1.038255	2.687292	-3.334558
H	0.630890	2.257054	-4.249393
C	0.000000	0.000000	4.682365
C	0.000000	0.000000	-4.682365

Total Energy: -628.42634007 eV

³E:

Ru	0.000000	0.000000	2.432736
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.432736
N	0.968811	-1.876311	2.267098
N	1.441652	-1.441652	0.000000
N	1.876311	-0.968811	-2.267098
N	-0.968811	1.876311	2.267098

N	-1.441652	1.441652	0.000000
N	-1.876311	0.968811	-2.267098
N	-1.876311	-0.968811	2.267098
N	-1.441652	-1.441652	0.000000
N	-0.968811	-1.876311	-2.267098
N	1.876311	0.968811	2.267098
N	1.441652	1.441652	0.000000
N	0.968811	1.876311	-2.267098
N	0.000000	0.000000	5.596854
N	0.000000	0.000000	-5.596854
C	0.971158	-2.731589	3.319277
H	0.555295	-2.327473	4.240776
C	1.463169	-4.020970	3.257010
H	1.438139	-4.649539	4.146483
C	1.952519	-4.487632	2.033242
H	2.303843	-5.515057	1.924473
C	1.959061	-3.637500	0.946332
H	2.286680	-3.987031	-0.032025
C	1.497160	-2.310980	1.066950
C	2.310980	-1.497160	-1.066950
C	3.637500	-1.959061	-0.946332
H	3.987031	-2.286680	0.032025
C	4.487632	-1.952519	-2.033242
H	5.515057	-2.303843	-1.924473
C	4.020970	-1.463169	-3.257010
H	4.649539	-1.438139	-4.146483
C	2.731589	-0.971158	-3.319277
H	2.327473	-0.555295	-4.240776
C	-0.971158	2.731589	3.319277
H	-0.555295	2.327473	4.240776
C	-1.463169	4.020970	3.257010
H	-1.438139	4.649539	4.146483
C	-1.952519	4.487632	2.033242
H	-2.303843	5.515057	1.924473
C	-1.959061	3.637500	0.946332
H	-2.286680	3.987031	-0.032025
C	-1.497160	2.310980	1.066950
C	-2.310980	1.497160	-1.066950
C	-3.637500	1.959061	-0.946332
H	-3.987031	2.286680	0.032025
C	-4.487632	1.952519	-2.033242
H	-5.515057	2.303843	-1.924473
C	-4.020970	1.463169	-3.257010
H	-4.649539	1.438139	-4.146483
C	-2.731589	0.971158	-3.319277
H	-2.327473	0.555295	-4.240776
C	-2.731589	-0.971158	3.319277
H	-2.327473	-0.555295	4.240776
C	-4.020970	-1.463169	3.257010
H	-4.649539	-1.438139	4.146483
C	-4.487632	-1.952519	2.033242
H	-5.515057	-2.303843	1.924473
C	-3.637500	-1.959061	0.946332
H	-3.987031	-2.286680	-0.032025
C	-2.310980	-1.497160	1.066950
C	-1.497160	-2.310980	-1.066950
C	-1.959061	-3.637500	-0.946332
H	-2.286680	-3.987031	0.032025
C	-1.952519	-4.487632	-2.033242

H	-2.303843	-5.515057	-1.924473
C	-1.463169	-4.020970	-3.257010
H	-1.438139	-4.649539	-4.146483
C	-0.971158	-2.731589	-3.319277
H	-0.555295	-2.327473	-4.240776
C	2.731589	0.971158	3.319277
H	2.327473	0.555295	4.240776
C	4.020970	1.463169	3.257010
H	4.649539	1.438139	4.146483
C	4.487632	1.952519	2.033242
H	5.515057	2.303843	1.924473
C	3.637500	1.959061	0.946332
H	3.987031	2.286680	-0.032025
C	2.310980	1.497160	1.066950
C	1.497160	2.310980	-1.066950
C	1.959061	3.637500	-0.946332
H	2.286680	3.987031	0.032025
C	1.952519	4.487632	-2.033242
H	2.303843	5.515057	-1.924473
C	1.463169	4.020970	-3.257010
H	1.438139	4.649539	-4.146483
C	0.971158	2.731589	-3.319277
H	0.555295	2.327473	-4.240776
C	0.000000	0.000000	4.409545
C	0.000000	0.000000	-4.409545

Total Energy: -630.19395301 eV

⁵B₂:

Ru	0.000000	0.000000	2.415246
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.415246
N	0.984024	-1.876049	2.260456
N	1.450967	-1.450967	0.000000
N	1.876049	-0.984024	-2.260456
N	-0.984024	1.876049	2.260456
N	-1.450967	1.450967	0.000000
N	-1.876049	0.984024	-2.260456
N	-1.876049	-0.984024	2.260456
N	-1.450967	-1.450967	0.000000
N	-0.984024	-1.876049	-2.260456
N	1.876049	0.984024	2.260456
N	1.450967	1.450967	0.000000
N	0.984024	1.876049	-2.260456
N	0.000000	0.000000	5.712378
N	0.000000	0.000000	-5.712378
C	0.998700	-2.718342	3.322022
H	0.588484	-2.303683	4.241753
C	1.494007	-4.007265	3.267903
H	1.481051	-4.626316	4.164370
C	1.970542	-4.485981	2.043616
H	2.319780	-5.514871	1.941702
C	1.968763	-3.646694	0.948143
H	2.288811	-4.004608	-0.029665
C	1.507149	-2.319223	1.064347
C	2.319223	-1.507149	-1.064347
C	3.646694	-1.968763	-0.948143

H	4.004608	-2.288811	0.029665
C	4.485981	-1.970542	-2.043616
H	5.514871	-2.319780	-1.941702
C	4.007265	-1.494007	-3.267903
H	4.626316	-1.481051	-4.164370
C	2.718342	-0.998700	-3.322022
H	2.303683	-0.588484	-4.241753
C	-0.998700	2.718342	3.322022
H	-0.588484	2.303683	4.241753
C	-1.494007	4.007265	3.267903
H	-1.481051	4.626316	4.164370
C	-1.970542	4.485981	2.043616
H	-2.319780	5.514871	1.941702
C	-1.968763	3.646694	0.948143
H	-2.288811	4.004608	-0.029665
C	-1.507149	2.319223	1.064347
C	-2.319223	1.507149	-1.064347
C	-3.646694	1.968763	-0.948143
H	-4.004608	2.288811	0.029665
C	-4.485981	1.970542	-2.043616
H	-5.514871	2.319780	-1.941702
C	-4.007265	1.494007	-3.267903
H	-4.626316	1.481051	-4.164370
C	-2.718342	0.998700	-3.322022
H	-2.303683	0.588484	-4.241753
C	-2.718342	-0.998700	3.322022
H	-2.303683	-0.588484	4.241753
C	-4.007265	-1.494007	3.267903
H	-4.626316	-1.481051	4.164370
C	-4.485981	-1.970542	2.043616
H	-5.514871	-2.319780	1.941702
C	-3.646694	-1.968763	0.948143
H	-4.004608	-2.288811	-0.029665
C	-2.319223	-1.507149	1.064347
C	-1.507149	-2.319223	-1.064347
C	-1.968763	-3.646694	-0.948143
H	-2.288811	-4.004608	0.029665
C	-1.970542	-4.485981	-2.043616
H	-2.319780	-5.514871	-1.941702
C	-1.494007	-4.007265	-3.267903
H	-1.481051	-4.626316	-4.164370
C	-0.998700	-2.718342	-3.322022
H	-0.588484	-2.303683	-4.241753
C	2.718342	0.998700	3.322022
H	2.303683	0.588484	4.241753
C	4.007265	1.494007	3.267903
H	4.626316	1.481051	4.164370
C	4.485981	1.970542	2.043616
H	5.514871	2.319780	1.941702
C	3.646694	1.968763	0.948143
H	4.004608	2.288811	-0.029665
C	2.319223	1.507149	1.064347
C	1.507149	2.319223	-1.064347
C	1.968763	3.646694	-0.948143
H	2.288811	4.004608	0.029665
C	1.970542	4.485981	-2.043616
H	2.319780	5.514871	-1.941702
C	1.494007	4.007265	-3.267903
H	1.481051	4.626316	-4.164370

C	0.998700	2.718342	-3.322022
H	0.588484	2.303683	-4.241753
C	0.000000	0.000000	4.529381
C	0.000000	0.000000	-4.529381

Total Energy: -629.68626813 eV

³A:

Ru	0.163254	2.399097	0.070217
Ru	0.000000	0.000000	-0.161648
Ru	-0.163254	-2.399097	0.070217
N	2.052925	2.102604	-0.930256
N	1.463965	-0.087281	-1.534765
N	0.831544	-2.321215	-1.872718
N	-1.703729	2.404250	0.994465
N	-1.433519	0.093696	1.360277
N	-1.073142	-2.164383	1.910568
N	1.073142	2.164383	1.910568
N	1.433519	-0.093696	1.360277
N	1.703729	-2.404250	0.994465
N	-0.831544	2.321215	-1.872718
N	-1.463965	0.087281	-1.534765
N	-2.052925	-2.102604	-0.930256
N	0.400512	5.580579	-0.053214
N	-0.400512	-5.580579	-0.053214
C	2.978902	3.090070	-0.874864
H	2.636619	4.015917	-0.415947
C	4.267649	2.965180	-1.359398
H	4.955344	3.806626	-1.282343
C	4.654369	1.740231	-1.909016
H	5.676024	1.578686	-2.256724
C	3.730525	0.717387	-1.984205
H	4.018038	-0.263614	-2.359060
C	2.412033	0.907776	-1.523594
C	1.472871	-1.197572	-2.350907
C	1.989851	-1.173836	-3.659816
H	2.420048	-0.246299	-4.035343
C	1.897295	-2.289652	-4.468331
H	2.287203	-2.260091	-5.487080
C	1.271617	-3.434707	-3.970758
H	1.169523	-4.341101	-4.566836
C	0.750119	-3.398646	-2.689947
H	0.243188	-4.262971	-2.264418
C	-2.472602	3.520516	1.044099
H	-1.997161	4.423857	0.665177
C	-3.762343	3.531263	1.538413
H	-4.321613	4.466028	1.560803
C	-4.322053	2.323530	1.969366
H	-5.354484	2.278492	2.319815
C	-3.558994	1.174359	1.918116
H	-3.978824	0.210307	2.204400
C	-2.225992	1.217305	1.461304
C	-1.515035	-0.914470	2.290464
C	-1.920466	-0.704206	3.627095
H	-2.178351	0.306608	3.941336
C	-1.948922	-1.748721	4.528024
H	-2.255175	-1.568900	5.559985
C	-1.554127	-3.024426	4.109114

H	-1.566265	-3.882156	4.780602
C	-1.110555	-3.178586	2.810926
H	-0.765964	-4.139751	2.432884
C	1.110555	3.178586	2.810926
H	0.765964	4.139751	2.432884
C	1.554127	3.024426	4.109114
H	1.566265	3.882156	4.780602
C	1.948922	1.748721	4.528024
H	2.255175	1.568900	5.559985
C	1.920466	0.704206	3.627095
H	2.178351	-0.306608	3.941336
C	1.515035	0.914470	2.290464
C	2.225992	-1.217305	1.461304
C	3.558994	-1.174359	1.918116
H	3.978824	-0.210307	2.204400
C	4.322053	-2.323530	1.969366
H	5.354484	-2.278492	2.319815
C	3.762343	-3.531263	1.538413
H	4.321613	-4.466028	1.560803
C	2.472602	-3.520516	1.044099
H	1.997161	-4.423857	0.665177
C	-0.750119	3.398646	-2.689947
H	-0.243188	4.262971	-2.264418
C	-1.271617	3.434707	-3.970758
H	-1.169523	4.341101	-4.566836
C	-1.897295	2.289652	-4.468331
H	-2.287203	2.260091	-5.487080
C	-1.989851	1.173836	-3.659816
H	-2.420048	0.246299	-4.035343
C	-1.472871	1.197572	-2.350907
C	-2.412033	-0.907776	-1.523594
C	-3.730525	-0.717387	-1.984205
H	-4.018038	0.263614	-2.359060
C	-4.654369	-1.740231	-1.909016
H	-5.676024	-1.578686	-2.256724
C	-4.267649	-2.965180	-1.359398
H	-4.955344	-3.806626	-1.282343
C	-2.978902	-3.090070	-0.874864
H	-2.636619	-4.015917	-0.415947
C	0.317858	4.398634	-0.029892
C	-0.317858	-4.398634	-0.029892

Total Energy: -630.31996565 eV

³A:

Ru	0.185237	2.407343	0.017780
Ru	0.000000	0.000000	0.017840
Ru	-0.185237	-2.407343	0.017780
N	2.048785	2.106287	-0.957003
N	1.445627	-0.110774	-1.431480
N	0.805862	-2.327266	-1.859416
N	-1.698989	2.395068	0.999734
N	-1.445266	0.109827	1.468242
N	-1.144912	-2.176575	1.898750
N	1.144912	2.176575	1.898750
N	1.445266	-0.109827	1.468242
N	1.698989	-2.395068	0.999734
N	-0.805862	2.327266	-1.859416

N	-1.445627	0.110774	-1.431480
N	-2.048785	-2.106287	-0.957003
N	0.437421	5.691823	0.017964
N	-0.437421	-5.691823	0.017964
C	2.972798	3.097039	-0.965597
H	2.630604	4.046803	-0.556993
C	4.257021	2.940043	-1.452396
H	4.945829	3.783916	-1.433910
C	4.639576	1.681789	-1.926801
H	5.659511	1.498091	-2.268895
C	3.714944	0.657161	-1.932713
H	3.995340	-0.345841	-2.252331
C	2.397766	0.879512	-1.480264
C	1.424067	-1.176387	-2.299458
C	1.901219	-1.096767	-3.624306
H	2.300131	-0.147363	-3.979702
C	1.820740	-2.188883	-4.464270
H	2.183215	-2.115124	-5.490997
C	1.245993	-3.371330	-3.988632
H	1.165459	-4.264000	-4.608035
C	0.741190	-3.386327	-2.701912
H	0.258016	-4.271189	-2.289963
C	-2.458090	3.517212	1.015407
H	-1.976157	4.402581	0.603057
C	-3.746608	3.561630	1.513959
H	-4.296091	4.502335	1.500661
C	-4.315202	2.378193	1.994562
H	-5.347783	2.355049	2.347099
C	-3.560910	1.222505	1.993133
H	-3.990666	0.275142	2.316469
C	-2.229784	1.237109	1.526868
C	-1.577067	-0.944282	2.340433
C	-2.022023	-0.790586	3.669972
H	-2.268164	0.208988	4.026322
C	-2.098388	-1.880577	4.513156
H	-2.433433	-1.750535	5.543613
C	-1.714796	-3.137567	4.036092
H	-1.763006	-4.030486	4.658372
C	-1.232540	-3.231626	2.744050
H	-0.893622	-4.180160	2.330099
C	1.232540	3.231626	2.744050
H	0.893622	4.180160	2.330099
C	1.714796	3.137567	4.036092
H	1.763006	4.030486	4.658372
C	2.098388	1.880577	4.513156
H	2.433433	1.750535	5.543613
C	2.022023	0.790586	3.669972
H	2.268164	-0.208988	4.026322
C	1.577067	0.944282	2.340433
C	2.229784	-1.237109	1.526868
C	3.560910	-1.222505	1.993133
H	3.990666	-0.275142	2.316469
C	4.315202	-2.378193	1.994562
H	5.347783	-2.355049	2.347099
C	3.746608	-3.561630	1.513959
H	4.296091	-4.502335	1.500661
C	2.458090	-3.517212	1.015407
H	1.976157	-4.402581	0.603057
C	-0.741190	3.386327	-2.701912

H	-0.258016	4.271189	-2.289963
C	-1.245993	3.371330	-3.988632
H	-1.165459	4.264000	-4.608035
C	-1.820740	2.188883	-4.464270
H	-2.183215	2.115124	-5.490997
C	-1.901219	1.096767	-3.624306
H	-2.300131	0.147363	-3.979702
C	-1.424067	1.176387	-2.299458
C	-2.397766	-0.879512	-1.480264
C	-3.714944	-0.657161	-1.932713
H	-3.995340	0.345841	-2.252331
C	-4.639576	-1.681789	-1.926801
H	-5.659511	-1.498091	-2.268895
C	-4.257021	-2.940043	-1.452396
H	-4.945829	-3.783916	-1.433910
C	-2.972798	-3.097039	-0.965597
H	-2.630604	-4.046803	-0.556993
C	0.347698	4.512033	0.017549
C	-0.347698	-4.512033	0.017549

Total Energy: -629.45477392 eV

³B:

Ru	0.189815	2.458509	0.013954
Ru	0.000000	0.000000	-0.011918
Ru	-0.189815	-2.458509	0.013954
N	2.002076	2.140271	-1.026283
N	1.427364	-0.108788	-1.431323
N	0.846588	-2.357303	-1.824558
N	-1.643599	2.425838	1.057388
N	-1.417228	0.111612	1.444638
N	-1.169966	-2.194636	1.855119
N	1.169966	2.194636	1.855119
N	1.417228	-0.111612	1.444638
N	1.643599	-2.425838	1.057388
N	-0.846588	2.357303	-1.824558
N	-1.427364	0.108788	-1.431323
N	-2.002076	-2.140271	-1.026283
N	0.440302	5.721610	-0.004194
N	-0.440302	-5.721610	-0.004194
C	2.910797	3.146044	-1.100846
H	2.559887	4.105603	-0.723327
C	4.187854	2.987022	-1.602187
H	4.863121	3.841833	-1.630159
C	4.586014	1.715534	-2.028605
H	5.603826	1.532995	-2.376689
C	3.675243	0.680607	-1.981713
H	3.963780	-0.329982	-2.267828
C	2.361286	0.903459	-1.519976
C	1.429817	-1.195186	-2.282361
C	1.888125	-1.108123	-3.613288
H	2.249404	-0.147946	-3.979521
C	1.832591	-2.206458	-4.446079
H	2.175994	-2.128067	-5.478814
C	1.308743	-3.404923	-3.950176
H	1.252117	-4.305489	-4.561139
C	0.822220	-3.429226	-2.657841
H	0.376701	-4.326927	-2.231084

C	-2.388962	3.557911	1.137446
H	-1.904301	4.450915	0.744393
C	-3.663599	3.597103	1.666064
H	-4.201921	4.543881	1.699274
C	-4.237707	2.402918	2.116023
H	-5.262945	2.378566	2.488552
C	-3.495803	1.242074	2.059455
H	-3.928497	0.288977	2.360785
C	-2.174640	1.258080	1.562680
C	-1.557784	-0.952090	2.310009
C	-1.950908	-0.785456	3.655322
H	-2.151513	0.221134	4.019979
C	-2.029874	-1.870734	4.502548
H	-2.320939	-1.730133	5.544682
C	-1.708308	-3.140205	4.009717
H	-1.767043	-4.032190	4.632748
C	-1.275635	-3.250257	2.703160
H	-0.983763	-4.208254	2.275002
C	1.275635	3.250257	2.703160
H	0.983763	4.208254	2.275002
C	1.708308	3.140205	4.009717
H	1.767043	4.032190	4.632748
C	2.029874	1.870734	4.502548
H	2.320939	1.730133	5.544682
C	1.950908	0.785456	3.655322
H	2.151513	-0.221134	4.019979
C	1.557784	0.952090	2.310009
C	2.174640	-1.258080	1.562680
C	3.495803	-1.242074	2.059455
H	3.928497	-0.288977	2.360785
C	4.237707	-2.402918	2.116023
H	5.262945	-2.378566	2.488552
C	3.663599	-3.597103	1.666064
H	4.201921	-4.543881	1.699274
C	2.388962	-3.557911	1.137446
H	1.904301	-4.450915	0.744393
C	-0.822220	3.429226	-2.657841
H	-0.376701	4.326927	-2.231084
C	-1.308743	3.404923	-3.950176
H	-1.252117	4.305489	-4.561139
C	-1.832591	2.206458	-4.446079
H	-2.175994	2.128067	-5.478814
C	-1.888125	1.108123	-3.613288
H	-2.249404	0.147946	-3.979521
C	-1.429817	1.195186	-2.282361
C	-2.361286	-0.903459	-1.519976
C	-3.675243	-0.680607	-1.981713
H	-3.963780	0.329982	-2.267828
C	-4.586014	-1.715534	-2.028605
H	-5.603826	-1.532995	-2.376689
C	-4.187854	-2.987022	-1.602187
H	-4.863121	-3.841833	-1.630159
C	-2.910797	-3.146044	-1.100846
H	-2.559887	-4.105603	-0.723327
C	0.350133	4.540390	0.002207
C	-0.350133	-4.540390	0.002207

Total Energy: -629.04730083 eV

³B:

Ru	0.182790	2.423457	0.010313
Ru	0.000000	0.000000	0.002923
Ru	-0.182790	-2.423457	0.010313
N	2.051334	2.108924	-0.934357
N	1.447714	-0.113675	-1.423702
N	0.812428	-2.340418	-1.860818
N	-1.704198	2.397984	0.965790
N	-1.438163	0.108797	1.448894
N	-1.138469	-2.187493	1.887497
N	1.138469	2.187493	1.887497
N	1.438163	-0.108797	1.448894
N	1.704198	-2.397984	0.965790
N	-0.812428	2.340418	-1.860818
N	-1.447714	0.113675	-1.423702
N	-2.051334	-2.108924	-0.934357
N	0.421650	5.576053	0.007723
N	-0.421650	-5.576053	0.007723
C	2.986757	3.090467	-0.915968
H	2.646175	4.042109	-0.511463
C	4.279883	2.924755	-1.373910
H	4.976496	3.761525	-1.332598
C	4.660208	1.666879	-1.850921
H	5.684633	1.476004	-2.174940
C	3.726035	0.651263	-1.881435
H	4.004394	-0.351956	-2.201923
C	2.402301	0.878624	-1.453909
C	1.441789	-1.186998	-2.287479
C	1.946140	-1.111307	-3.601815
H	2.357747	-0.163602	-3.946946
C	1.878752	-2.200797	-4.445990
H	2.264948	-2.127179	-5.463939
C	1.284313	-3.380077	-3.986459
H	1.207736	-4.269236	-4.611466
C	0.754667	-3.395238	-2.710569
H	0.258360	-4.279302	-2.313579
C	-2.480645	3.509489	0.955509
H	-2.008119	4.396366	0.536763
C	-3.773460	3.544742	1.441434
H	-4.336403	4.476912	1.406086
C	-4.328527	2.362526	1.940672
H	-5.361929	2.332121	2.289994
C	-3.559408	1.216725	1.959982
H	-3.980136	0.269793	2.295768
C	-2.226748	1.236427	1.499127
C	-1.574885	-0.949599	2.319397
C	-2.027151	-0.792681	3.645967
H	-2.280059	0.208038	3.994301
C	-2.102555	-1.875723	4.497450
H	-2.444517	-1.739308	5.524763
C	-1.706537	-3.133854	4.033075
H	-1.748614	-4.021412	4.663333
C	-1.219514	-3.234988	2.744267
H	-0.872184	-4.185509	2.342727
C	1.219514	3.234988	2.744267
H	0.872184	4.185509	2.342727
C	1.706537	3.133854	4.033075
H	1.748614	4.021412	4.663333

C	2.102555	1.875723	4.497450
H	2.444517	1.739308	5.524763
C	2.027151	0.792681	3.645967
H	2.280059	-0.208038	3.994301
C	1.574885	0.949599	2.319397
C	2.226748	-1.236427	1.499127
C	3.559408	-1.216725	1.959982
H	3.980136	-0.269793	2.295768
C	4.328527	-2.362526	1.940672
H	5.361929	-2.332121	2.289994
C	3.773460	-3.544742	1.441434
H	4.336403	-4.476912	1.406086
C	2.480645	-3.509489	0.955509
H	2.008119	-4.396366	0.536763
C	-0.754667	3.395238	-2.710569
H	-0.258360	4.279302	-2.313579
C	-1.284313	3.380077	-3.986459
H	-1.207736	4.269236	-4.611466
C	-1.878752	2.200797	-4.445990
H	-2.264948	2.127179	-5.463939
C	-1.946140	1.111307	-3.601815
H	-2.357747	0.163602	-3.946946
C	-1.441789	1.186998	-2.287479
C	-2.402301	-0.878624	-1.453909
C	-3.726035	-0.651263	-1.881435
H	-4.004394	0.351956	-2.201923
C	-4.660208	-1.666879	-1.850921
H	-5.684633	-1.476004	-2.174940
C	-4.279883	-2.924755	-1.373910
H	-4.976496	-3.761525	-1.332598
C	-2.986757	-3.090467	-0.915968
H	-2.646175	-4.042109	-0.511463
C	0.331693	4.392538	0.009091
C	-0.331693	-4.392538	0.009091

Total Energy: -629.45477392 eV

⁵A:

Ru	0.193290	2.406926	0.026073
Ru	0.000000	0.000000	0.027408
Ru	-0.193290	-2.406926	0.026073
N	2.053443	2.102085	-0.952610
N	1.446526	-0.115563	-1.423134
N	0.797405	-2.329809	-1.851075
N	-1.690187	2.402288	1.007827
N	-1.447198	0.115721	1.477023
N	-1.165839	-2.175583	1.900042
N	1.165839	2.175583	1.900042
N	1.447198	-0.115721	1.477023
N	1.690187	-2.402288	1.007827
N	-0.797405	2.329809	-1.851075
N	-1.446526	0.115563	-1.423134
N	-2.053443	-2.102085	-0.952610
N	0.458561	5.693054	0.027654
N	-0.458561	-5.693054	0.027654
C	2.979516	3.091403	-0.962751
H	2.639946	4.041171	-0.552015
C	4.261084	2.932982	-1.454872

H	4.951306	3.775738	-1.438785
C	4.639444	1.674506	-1.932511
H	5.657477	1.489692	-2.279531
C	3.713827	0.650904	-1.934459
H	3.992009	-0.352452	-2.254795
C	2.399048	0.874296	-1.476091
C	1.417802	-1.180262	-2.292130
C	1.891250	-1.101661	-3.618123
H	2.292319	-0.153506	-3.974245
C	1.805167	-2.193100	-4.458207
H	2.164919	-2.119862	-5.485933
C	1.227723	-3.374111	-3.981946
H	1.142813	-4.266047	-4.601847
C	0.726444	-3.388279	-2.694257
H	0.241529	-4.271553	-2.281078
C	-2.445344	3.527590	1.019937
H	-1.956956	4.411289	0.611870
C	-3.736710	3.575916	1.509417
H	-4.282732	4.518495	1.494041
C	-4.313551	2.393269	1.982320
H	-5.349131	2.373153	2.326102
C	-3.563897	1.234648	1.983858
H	-4.000080	0.288318	2.301419
C	-2.229059	1.245221	1.528980
C	-1.594471	-0.942154	2.342326
C	-2.055419	-0.791675	3.666609
H	-2.298985	0.207909	4.024571
C	-2.150754	-1.884802	4.503440
H	-2.498594	-1.757035	5.529874
C	-1.769287	-3.142292	4.025735
H	-1.831855	-4.037774	4.643297
C	-1.270858	-3.233822	2.740130
H	-0.932555	-4.182716	2.326317
C	1.270858	3.233822	2.740130
H	0.932555	4.182716	2.326317
C	1.769287	3.142292	4.025735
H	1.831855	4.037774	4.643297
C	2.150754	1.884802	4.503440
H	2.498594	1.757035	5.529874
C	2.055419	0.791675	3.666609
H	2.298985	-0.207909	4.024571
C	1.594471	0.942154	2.342326
C	2.229059	-1.245221	1.528980
C	3.563897	-1.234648	1.983858
H	4.000080	-0.288318	2.301419
C	4.313551	-2.393269	1.982320
H	5.349131	-2.373153	2.326102
C	3.736710	-3.575916	1.509417
H	4.282732	-4.518495	1.494041
C	2.445344	-3.527590	1.019937
H	1.956956	-4.411289	0.611870
C	-0.726444	3.388279	-2.694257
H	-0.241529	4.271553	-2.281078
C	-1.227723	3.374111	-3.981946
H	-1.142813	4.266047	-4.601847
C	-1.805167	2.193100	-4.458207
H	-2.164919	2.119862	-5.485933
C	-1.891250	1.101661	-3.618123
H	-2.292319	0.153506	-3.974245

C	-1.417802	1.180262	-2.292130
C	-2.399048	-0.874296	-1.476091
C	-3.713827	-0.650904	-1.934459
H	-3.992009	0.352452	-2.254795
C	-4.639444	-1.674506	-1.932511
H	-5.657477	-1.489692	-2.279531
C	-4.261084	-2.932982	-1.454872
H	-4.951306	-3.775738	-1.438785
C	-2.979516	-3.091403	-0.962751
H	-2.639946	-4.041171	-0.552015
C	0.362068	4.514123	0.025022
C	-0.362068	-4.514123	0.025022

Total Energy: -629.69783503 eV

Ru₃(dpa)₄(CCH)₂:

¹A₁:

Ru	0.000000	0.000000	2.330859
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.330859
N	0.944883	-1.921303	2.221264
N	1.478057	-1.478057	0.000000
N	1.921303	-0.944883	-2.221264
N	-0.944883	1.921303	2.221264
N	-1.478057	1.478057	0.000000
N	-1.921303	0.944883	-2.221264
N	-1.921303	-0.944883	2.221264
N	-1.478057	-1.478057	0.000000
N	-0.944883	-1.921303	-2.221264
N	1.921303	0.944883	2.221264
N	1.478057	1.478057	0.000000
N	0.944883	1.921303	-2.221264
C	0.000000	0.000000	5.848982
C	0.000000	0.000000	-5.848982
C	0.910773	-2.756651	3.282473
H	0.460880	-2.331499	4.180150
C	1.416518	-4.044677	3.250964
H	1.372218	-4.664793	4.145431
C	1.946618	-4.518503	2.047015
H	2.308126	-5.544891	1.961802
C	1.982064	-3.684499	0.947090
H	2.339749	-4.044769	-0.016721
C	1.505350	-2.359723	1.043714
C	2.359723	-1.505350	-1.043714
C	3.684499	-1.982064	-0.947090
H	4.044769	-2.339749	0.016721
C	4.518503	-1.946618	-2.047015
H	5.544891	-2.308126	-1.961802
C	4.044677	-1.416518	-3.250964
H	4.664793	-1.372218	-4.145431

C	2.756651	-0.910773	-3.282473
H	2.331499	-0.460880	-4.180150
C	-0.910773	2.756651	3.282473
H	-0.460880	2.331499	4.180150
C	-1.416518	4.044677	3.250964
H	-1.372218	4.664793	4.145431
C	-1.946618	4.518503	2.047015
H	-2.308126	5.544891	1.961802
C	-1.982064	3.684499	0.947090
H	-2.339749	4.044769	-0.016721
C	-1.505350	2.359723	1.043714
C	-2.359723	1.505350	-1.043714
C	-3.684499	1.982064	-0.947090
H	-4.044769	2.339749	0.016721
C	-4.518503	1.946618	-2.047015
H	-5.544891	2.308126	-1.961802
C	-4.044677	1.416518	-3.250964
H	-4.664793	1.372218	-4.145431
C	-2.756651	0.910773	-3.282473
H	-2.331499	0.460880	-4.180150
C	-2.756651	-0.910773	3.282473
H	-2.331499	-0.460880	4.180150
C	-4.044677	-1.416518	3.250964
H	-4.664793	-1.372218	4.145431
C	-4.518503	-1.946618	2.047015
H	-5.544891	-2.308126	1.961802
C	-3.684499	-1.982064	0.947090
H	-4.044769	-2.339749	-0.016721
C	-2.359723	-1.505350	1.043714
C	-1.505350	-2.359723	-1.043714
C	-1.982064	-3.684499	-0.947090
H	-2.339749	-4.044769	0.016721
C	-1.946618	-4.518503	-2.047015
H	-2.308126	-5.544891	-1.961802
C	-1.416518	-4.044677	-3.250964
H	-1.372218	-4.664793	-4.145431
C	-0.910773	-2.756651	-3.282473
H	-0.460880	-2.331499	-4.180150
C	2.756651	0.910773	3.282473
H	2.331499	0.460880	4.180150
C	4.044677	1.416518	3.250964
H	4.664793	1.372218	4.145431
C	4.518503	1.946618	2.047015
H	5.544891	2.308126	1.961802
C	3.684499	1.982064	0.947090
H	4.044769	2.339749	-0.016721
C	2.359723	1.505350	1.043714
C	1.505350	2.359723	-1.043714
C	1.982064	3.684499	-0.947090
H	2.339749	4.044769	0.016721
C	1.946618	4.518503	-2.047015
H	2.308126	5.544891	-1.961802
C	1.416518	4.044677	-3.250964
H	1.372218	4.664793	-4.145431
C	0.910773	2.756651	-3.282473
H	0.460880	2.331499	-4.180150
C	0.000000	0.000000	4.609242
C	0.000000	0.000000	-4.609242
H	0.000000	0.000000	6.924182

H	0.000000	0.000000	-6.924182
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Total Energy: -633.78045391 eV

³A₂:

Ru	0.000000	0.000000	2.380397
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.380397
N	0.921714	-1.917923	2.234353
N	1.462786	-1.462786	0.000000
N	1.917923	-0.921714	-2.234353
N	-0.921714	1.917923	2.234353
N	-1.462786	1.462786	0.000000
N	-1.917923	0.921714	-2.234353
N	-1.917923	-0.921714	2.234353
N	-1.462786	-1.462786	0.000000
N	-0.921714	-1.917923	-2.234353
N	1.917923	0.921714	2.234353
N	1.462786	1.462786	0.000000
N	0.921714	1.917923	-2.234353
C	0.000000	0.000000	5.601347
C	0.000000	0.000000	-5.601347
C	0.867707	-2.781014	3.275063
H	0.409643	-2.378857	4.177314
C	1.361031	-4.071887	3.226030
H	1.293007	-4.710030	4.106470
C	1.909854	-4.525695	2.022249
H	2.267118	-5.552092	1.921931
C	1.963797	-3.669264	0.941507
H	2.331174	-4.014208	-0.024296
C	1.489332	-2.343900	1.048416
C	2.343900	-1.489332	-1.048416
C	3.669264	-1.963797	-0.941507
H	4.014208	-2.331174	0.024296
C	4.525695	-1.909854	-2.022249
H	5.552092	-2.267118	-1.921931
C	4.071887	-1.361031	-3.226030
H	4.710030	-1.293007	-4.106470
C	2.781014	-0.867707	-3.275063
H	2.378857	-0.409643	-4.177314
C	-0.867707	2.781014	3.275063
H	-0.409643	2.378857	4.177314
C	-1.361031	4.071887	3.226030
H	-1.293007	4.710030	4.106470
C	-1.909854	4.525695	2.022249
H	-2.267118	5.552092	1.921931
C	-1.963797	3.669264	0.941507
H	-2.331174	4.014208	-0.024296
C	-1.489332	2.343900	1.048416
C	-2.343900	1.489332	-1.048416
C	-3.669264	1.963797	-0.941507
H	-4.014208	2.331174	0.024296
C	-4.525695	1.909854	-2.022249
H	-5.552092	2.267118	-1.921931
C	-4.071887	1.361031	-3.226030
H	-4.710030	1.293007	-4.106470
C	-2.781014	0.867707	-3.275063
H	-2.378857	0.409643	-4.177314

C	-2.781014	-0.867707	3.275063
H	-2.378857	-0.409643	4.177314
C	-4.071887	-1.361031	3.226030
H	-4.710030	-1.293007	4.106470
C	-4.525695	-1.909854	2.022249
H	-5.552092	-2.267118	1.921931
C	-3.669264	-1.963797	0.941507
H	-4.014208	-2.331174	-0.024296
C	-2.343900	-1.489332	1.048416
C	-1.489332	-2.343900	-1.048416
C	-1.963797	-3.669264	-0.941507
H	-2.331174	-4.014208	0.024296
C	-1.909854	-4.525695	-2.022249
H	-2.267118	-5.552092	-1.921931
C	-1.361031	-4.071887	-3.226030
H	-1.293007	-4.710030	-4.106470
C	-0.867707	-2.781014	-3.275063
H	-0.409643	-2.378857	-4.177314
C	2.781014	0.867707	3.275063
H	2.378857	0.409643	4.177314
C	4.071887	1.361031	3.226030
H	4.710030	1.293007	4.106470
C	4.525695	1.909854	2.022249
H	5.552092	2.267118	1.921931
C	3.669264	1.963797	0.941507
H	4.014208	2.331174	-0.024296
C	2.343900	1.489332	1.048416
C	1.489332	2.343900	-1.048416
C	1.963797	3.669264	-0.941507
H	2.331174	4.014208	0.024296
C	1.909854	4.525695	-2.022249
H	2.267118	5.552092	-1.921931
C	1.361031	4.071887	-3.226030
H	1.293007	4.710030	-4.106470
C	0.867707	2.781014	-3.275063
H	0.409643	2.378857	-4.177314
C	0.000000	0.000000	4.364819
C	0.000000	0.000000	-4.364819
H	0.000000	0.000000	-6.674293
H	0.000000	0.000000	6.674293

Total Energy: -635.66428077 eV

³A₂:

Ru	0.000000	0.000000	2.450433
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.450433
N	1.055641	-1.819911	2.283018
N	1.441203	-1.441203	0.000000
N	1.819911	-1.055641	-2.283018
N	-1.055641	1.819911	2.283018
N	-1.441203	1.441203	0.000000
N	-1.819911	1.055641	-2.283018
N	-1.819911	-1.055641	2.283018
N	-1.441203	-1.441203	0.000000
N	-1.055641	-1.819911	-2.283018
N	1.819911	1.055641	2.283018
N	1.441203	1.441203	0.000000

N	1.055641	1.819911	-2.283018
C	0.000000	0.000000	5.933088
C	0.000000	0.000000	-5.933088
C	1.129859	-2.634069	3.366193
H	0.755961	-2.185211	4.287704
C	1.620703	-3.924509	3.315762
H	1.650090	-4.523824	4.224947
C	2.035822	-4.435132	2.080554
H	2.372197	-5.468861	1.985363
C	1.991458	-3.618903	0.969679
H	2.267041	-3.997614	-0.013634
C	1.538329	-2.286414	1.081631
C	2.286414	-1.538329	-1.081631
C	3.618903	-1.991458	-0.969679
H	3.997614	-2.267041	0.013634
C	4.435132	-2.035822	-2.080554
H	5.468861	-2.372197	-1.985363
C	3.924509	-1.620703	-3.315762
H	4.523824	-1.650090	-4.224947
C	2.634069	-1.129859	-3.366193
H	2.185211	-0.755961	-4.287704
C	-1.129859	2.634069	3.366193
H	-0.755961	2.185211	4.287704
C	-1.620703	3.924509	3.315762
H	-1.650090	4.523824	4.224947
C	-2.035822	4.435132	2.080554
H	-2.372197	5.468861	1.985363
C	-1.991458	3.618903	0.969679
H	-2.267041	3.997614	-0.013634
C	-1.538329	2.286414	1.081631
C	-2.286414	1.538329	-1.081631
C	-3.618903	1.991458	-0.969679
H	-3.997614	2.267041	0.013634
C	-4.435132	2.035822	-2.080554
H	-5.468861	2.372197	-1.985363
C	-3.924509	1.620703	-3.315762
H	-4.523824	1.650090	-4.224947
C	-2.634069	1.129859	-3.366193
H	-2.185211	0.755961	-4.287704
C	-2.634069	-1.129859	3.366193
H	-2.185211	-0.755961	4.287704
C	-3.924509	-1.620703	3.315762
H	-4.523824	-1.650090	4.224947
C	-4.435132	-2.035822	2.080554
H	-5.468861	-2.372197	1.985363
C	-3.618903	-1.991458	0.969679
H	-3.997614	-2.267041	-0.013634
C	-2.286414	-1.538329	1.081631
C	-1.538329	-2.286414	-1.081631
C	-1.991458	-3.618903	-0.969679
H	-2.267041	-3.997614	0.013634
C	-2.035822	-4.435132	-2.080554
H	-2.372197	-5.468861	-1.985363
C	-1.620703	-3.924509	-3.315762
H	-1.650090	-4.523824	-4.224947
C	-1.129859	-2.634069	-3.366193
H	-0.755961	-2.185211	-4.287704
C	2.634069	1.129859	3.366193
H	2.185211	0.755961	4.287704

C	3.924509	1.620703	3.315762
H	4.523824	1.650090	4.224947
C	4.435132	2.035822	2.080554
H	5.468861	2.372197	1.985363
C	3.618903	1.991458	0.969679
H	3.997614	2.267041	-0.013634
C	2.286414	1.538329	1.081631
C	1.538329	2.286414	-1.081631
C	1.991458	3.618903	-0.969679
H	2.267041	3.997614	0.013634
C	2.035822	4.435132	-2.080554
H	2.372197	5.468861	-1.985363
C	1.620703	3.924509	-3.315762
H	1.650090	4.523824	-4.224947
C	1.129859	2.634069	-3.366193
H	0.755961	2.185211	-4.287704
C	0.000000	0.000000	4.692164
C	0.000000	0.000000	-4.692164
H	0.000000	0.000000	-7.008384
H	0.000000	0.000000	7.008384

Total Energy: -633.46639456 eV

³E:

Ru	0.000000	0.000000	2.362595
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.362595
N	0.918345	-1.929316	2.220692
N	1.468695	-1.468695	0.000000
N	1.929316	-0.918345	-2.220692
N	-0.918345	1.929316	2.220692
N	-1.468695	1.468695	0.000000
N	-1.929316	0.918345	-2.220692
N	-1.929316	-0.918345	2.220692
N	-1.468695	-1.468695	0.000000
N	-0.918345	-1.929316	-2.220692
N	1.929316	0.918345	2.220692
N	1.468695	1.468695	0.000000
N	0.918345	1.929316	-2.220692
C	0.000000	0.000000	5.705611
C	0.000000	0.000000	-5.705611
C	0.862519	-2.787105	3.264176
H	0.406167	-2.378325	4.164822
C	1.353183	-4.080014	3.216842
H	1.286554	-4.716139	4.098775
C	1.899602	-4.537066	2.013367
H	2.254120	-5.564726	1.915070
C	1.957622	-3.683050	0.930472
H	2.326679	-4.028927	-0.034371
C	1.486916	-2.356878	1.039536
C	2.356878	-1.486916	-1.039536
C	3.683050	-1.957622	-0.930472
H	4.028927	-2.326679	0.034371
C	4.537066	-1.899602	-2.013367
H	5.564726	-2.254120	-1.915070
C	4.080014	-1.353183	-3.216842
H	4.716139	-1.286554	-4.098775
C	2.787105	-0.862519	-3.264176

H	2.378325	-0.406167	-4.164822
C	-0.862519	2.787105	3.264176
H	-0.406167	2.378325	4.164822
C	-1.353183	4.080014	3.216842
H	-1.286554	4.716139	4.098775
C	-1.899602	4.537066	2.013367
H	-2.254120	5.564726	1.915070
C	-1.957622	3.683050	0.930472
H	-2.326679	4.028927	-0.034371
C	-1.486916	2.356878	1.039536
C	-2.356878	1.486916	-1.039536
C	-3.683050	1.957622	-0.930472
H	-4.028927	2.326679	0.034371
C	-4.537066	1.899602	-2.013367
H	-5.564726	2.254120	-1.915070
C	-4.080014	1.353183	-3.216842
H	-4.716139	1.286554	-4.098775
C	-2.787105	0.862519	-3.264176
H	-2.378325	0.406167	-4.164822
C	-2.787105	-0.862519	3.264176
H	-2.378325	-0.406167	4.164822
C	-4.080014	-1.353183	3.216842
H	-4.716139	-1.286554	4.098775
C	-4.537066	-1.899602	2.013367
H	-5.564726	-2.254120	1.915070
C	-3.683050	-1.957622	0.930472
H	-4.028927	-2.326679	-0.034371
C	-2.356878	-1.486916	1.039536
C	-1.486916	-2.356878	-1.039536
C	-1.957622	-3.683050	-0.930472
H	-2.326679	-4.028927	0.034371
C	-1.899602	-4.537066	-2.013367
H	-2.254120	-5.564726	-1.915070
C	-1.353183	-4.080014	-3.216842
H	-1.286554	-4.716139	-4.098775
C	-0.862519	-2.787105	-3.264176
H	-0.406167	-2.378325	-4.164822
C	2.787105	0.862519	3.264176
H	2.378325	0.406167	4.164822
C	4.080014	1.353183	3.216842
H	4.716139	1.286554	4.098775
C	4.537066	1.899602	2.013367
H	5.564726	2.254120	1.915070
C	3.683050	1.957622	0.930472
H	4.028927	2.326679	-0.034371
C	2.356878	1.486916	1.039536
C	1.486916	2.356878	-1.039536
C	1.957622	3.683050	-0.930472
H	2.326679	4.028927	0.034371
C	1.899602	4.537066	-2.013367
H	2.254120	5.564726	-1.915070
C	1.353183	4.080014	-3.216842
H	1.286554	4.716139	-4.098775
C	0.862519	2.787105	-3.264176
H	0.406167	2.378325	-4.164822
C	0.000000	0.000000	4.467354
C	0.000000	0.000000	-4.467354
H	0.000000	0.000000	-6.779850
H	0.000000	0.000000	6.779850

Total Energy: -634.66910614 eV

³E:

Ru	0.000000	0.000000	2.395808
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.395808
N	0.993386	-1.875728	2.251776
N	1.458762	-1.458762	0.000000
N	1.875728	-0.993386	-2.251776
N	-0.993386	1.875728	2.251776
N	-1.458762	1.458762	0.000000
N	-1.875728	0.993386	-2.251776
N	-1.875728	-0.993386	2.251776
N	-1.458762	-1.458762	0.000000
N	-0.993386	-1.875728	-2.251776
N	1.875728	0.993386	2.251776
N	1.458762	1.458762	0.000000
N	0.993386	1.875728	-2.251776
C	0.000000	0.000000	5.890634
C	0.000000	0.000000	-5.890634
C	1.011631	-2.703702	3.322943
H	0.599244	-2.269101	4.234332
C	1.511528	-3.992259	3.279607
H	1.504238	-4.603445	4.181659
C	1.984680	-4.482199	2.057814
H	2.334732	-5.511702	1.965399
C	1.979929	-3.654372	0.953446
H	2.298237	-4.020332	-0.021967
C	1.516639	-2.325614	1.061918
C	2.325614	-1.516639	-1.061918
C	3.654372	-1.979929	-0.953446
H	4.020332	-2.298237	0.021967
C	4.482199	-1.984680	-2.057814
H	5.511702	-2.334732	-1.965399
C	3.992259	-1.511528	-3.279607
H	4.603445	-1.504238	-4.181659
C	2.703702	-1.011631	-3.322943
H	2.269101	-0.599244	-4.234332
C	-1.011631	2.703702	3.322943
H	-0.599244	2.269101	4.234332
C	-1.511528	3.992259	3.279607
H	-1.504238	4.603445	4.181659
C	-1.984680	4.482199	2.057814
H	-2.334732	5.511702	1.965399
C	-1.979929	3.654372	0.953446
H	-2.298237	4.020332	-0.021967
C	-1.516639	2.325614	1.061918
C	-2.325614	1.516639	-1.061918
C	-3.654372	1.979929	-0.953446
H	-4.020332	2.298237	0.021967
C	-4.482199	1.984680	-2.057814
H	-5.511702	2.334732	-1.965399
C	-3.992259	1.511528	-3.279607
H	-4.603445	1.504238	-4.181659
C	-2.703702	1.011631	-3.322943
H	-2.269101	0.599244	-4.234332
C	-2.703702	-1.011631	3.322943

H	-2.269101	-0.599244	4.234332
C	-3.992259	-1.511528	3.279607
H	-4.603445	-1.504238	4.181659
C	-4.482199	-1.984680	2.057814
H	-5.511702	-2.334732	1.965399
C	-3.654372	-1.979929	0.953446
H	-4.020332	-2.298237	-0.021967
C	-2.325614	-1.516639	1.061918
C	-1.516639	-2.325614	-1.061918
C	-1.979929	-3.654372	-0.953446
H	-2.298237	-4.020332	0.021967
C	-1.984680	-4.482199	-2.057814
H	-2.334732	-5.511702	-1.965399
C	-1.511528	-3.992259	-3.279607
H	-1.504238	-4.603445	-4.181659
C	-1.011631	-2.703702	-3.322943
H	-0.599244	-2.269101	-4.234332
C	2.703702	1.011631	3.322943
H	2.269101	0.599244	4.234332
C	3.992259	1.511528	3.279607
H	4.603445	1.504238	4.181659
C	4.482199	1.984680	2.057814
H	5.511702	2.334732	1.965399
C	3.654372	1.979929	0.953446
H	4.020332	2.298237	-0.021967
C	2.325614	1.516639	1.061918
C	1.516639	2.325614	-1.061918
C	1.979929	3.654372	-0.953446
H	2.298237	4.020332	0.021967
C	1.984680	4.482199	-2.057814
H	2.334732	5.511702	-1.965399
C	1.511528	3.992259	-3.279607
H	1.504238	4.603445	-4.181659
C	1.011631	2.703702	-3.322943
H	0.599244	2.269101	-4.234332
C	0.000000	0.000000	4.650396
C	0.000000	0.000000	-4.650396
H	0.000000	0.000000	-6.965891
H	0.000000	0.000000	6.965891

Total Energy: -633.69038205 eV

³E:

Ru	0.000000	0.000000	2.434509
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.434509
N	0.967820	-1.876604	2.265802
N	1.442300	-1.442300	0.000000
N	1.876604	-0.967820	-2.265802
N	-0.967820	1.876604	2.265802
N	-1.442300	1.442300	0.000000
N	-1.876604	0.967820	-2.265802

N	-1.876604	-0.967820	2.265802
N	-1.442300	-1.442300	0.000000
N	-0.967820	-1.876604	-2.265802
N	1.876604	0.967820	2.265802
N	1.442300	1.442300	0.000000
N	0.967820	1.876604	-2.265802
C	0.000000	0.000000	5.650259
C	0.000000	0.000000	-5.650259
C	0.966941	-2.732151	3.317335
H	0.547242	-2.321023	4.234828
C	1.460519	-4.021531	3.256829
H	1.433954	-4.650987	4.145813
C	1.953614	-4.488209	2.034078
H	2.306097	-5.515363	1.925871
C	1.961494	-3.637882	0.947191
H	2.290786	-3.987631	-0.030442
C	1.498431	-2.310995	1.066554
C	2.310995	-1.498431	-1.066554
C	3.637882	-1.961494	-0.947191
H	3.987631	-2.290786	0.030442
C	4.488209	-1.953614	-2.034078
H	5.515363	-2.306097	-1.925871
C	4.021531	-1.460519	-3.256829
H	4.650987	-1.433954	-4.145813
C	2.732151	-0.966941	-3.317335
H	2.321023	-0.547242	-4.234828
C	-0.966941	2.732151	3.317335
H	-0.547242	2.321023	4.234828
C	-1.460519	4.021531	3.256829
H	-1.433954	4.650987	4.145813
C	-1.953614	4.488209	2.034078
H	-2.306097	5.515363	1.925871
C	-1.961494	3.637882	0.947191
H	-2.290786	3.987631	-0.030442
C	-1.498431	2.310995	1.066554
C	-2.310995	1.498431	-1.066554
C	-3.637882	1.961494	-0.947191
H	-3.987631	2.290786	0.030442
C	-4.488209	1.953614	-2.034078
H	-5.515363	2.306097	-1.925871
C	-4.021531	1.460519	-3.256829
H	-4.650987	1.433954	-4.145813
C	-2.732151	0.966941	-3.317335
H	-2.321023	0.547242	-4.234828
C	-2.732151	-0.966941	3.317335
H	-2.321023	-0.547242	4.234828
C	-4.021531	-1.460519	3.256829
H	-4.650987	-1.433954	4.145813
C	-4.488209	-1.953614	2.034078
H	-5.515363	-2.306097	1.925871
C	-3.637882	-1.961494	0.947191
H	-3.987631	-2.290786	-0.030442
C	-2.310995	-1.498431	1.066554
C	-1.498431	-2.310995	-1.066554
C	-1.961494	-3.637882	-0.947191
H	-2.290786	-3.987631	0.030442
C	-1.953614	-4.488209	-2.034078
H	-2.306097	-5.515363	-1.925871
C	-1.460519	-4.021531	-3.256829

H	-1.433954	-4.650987	-4.145813
C	-0.966941	-2.732151	-3.317335
H	-0.547242	-2.321023	-4.234828
C	2.732151	0.966941	3.317335
H	2.321023	0.547242	4.234828
C	4.021531	1.460519	3.256829
H	4.650987	1.433954	4.145813
C	4.488209	1.953614	2.034078
H	5.515363	2.306097	1.925871
C	3.637882	1.961494	0.947191
H	3.987631	2.290786	-0.030442
C	2.310995	1.498431	1.066554
C	1.498431	2.310995	-1.066554
C	1.961494	3.637882	-0.947191
H	2.290786	3.987631	0.030442
C	1.953614	4.488209	-2.034078
H	2.306097	5.515363	-1.925871
C	1.460519	4.021531	-3.256829
H	1.433954	4.650987	-4.145813
C	0.966941	2.732151	-3.317335
H	0.547242	2.321023	-4.234828
C	0.000000	0.000000	4.411168
C	0.000000	0.000000	-4.411168
H	0.000000	0.000000	-6.723164
H	0.000000	0.000000	6.723164

Total Energy: -635.54712754 eV

⁵B₂:

Ru	0.000000	0.000000	2.420886
Ru	0.000000	0.000000	0.000000
Ru	0.000000	0.000000	-2.420886
N	0.979418	-1.879032	2.257376
N	1.451064	-1.451064	0.000000
N	1.879032	-0.979418	-2.257376
N	-0.979418	1.879032	2.257376
N	-1.451064	1.451064	0.000000
N	-1.879032	0.979418	-2.257376
N	-1.879032	-0.979418	2.257376
N	-1.451064	-1.451064	0.000000
N	-0.979418	-1.879032	-2.257376
N	1.879032	0.979418	2.257376
N	1.451064	1.451064	0.000000
N	0.979418	1.879032	-2.257376
C	0.000000	0.000000	5.756815
C	0.000000	0.000000	-5.756815
C	0.983491	-2.725085	3.315470
H	0.567987	-2.304216	4.230815
C	1.472373	-4.016942	3.259440
H	1.449008	-4.640710	4.152510
C	1.955967	-4.493027	2.036419
H	2.301295	-5.523060	1.932470
C	1.964646	-3.649279	0.944295
H	2.288207	-4.004483	-0.033311
C	1.505564	-2.320434	1.062539
C	2.320434	-1.505564	-1.062539
C	3.649279	-1.964646	-0.944295
H	4.004483	-2.288207	0.033311

C	4.493027	-1.955967	-2.036419
H	5.523060	-2.301295	-1.932470
C	4.016942	-1.472373	-3.259440
H	4.640710	-1.449008	-4.152510
C	2.725085	-0.983491	-3.315470
H	2.304216	-0.567987	-4.230815
C	-0.983491	2.725085	3.315470
H	-0.567987	2.304216	4.230815
C	-1.472373	4.016942	3.259440
H	-1.449008	4.640710	4.152510
C	-1.955967	4.493027	2.036419
H	-2.301295	5.523060	1.932470
C	-1.964646	3.649279	0.944295
H	-2.288207	4.004483	-0.033311
C	-1.505564	2.320434	1.062539
C	-2.320434	1.505564	-1.062539
C	-3.649279	1.964646	-0.944295
H	-4.004483	2.288207	0.033311
C	-4.493027	1.955967	-2.036419
H	-5.523060	2.301295	-1.932470
C	-4.016942	1.472373	-3.259440
H	-4.640710	1.449008	-4.152510
C	-2.725085	0.983491	-3.315470
H	-2.304216	0.567987	-4.230815
C	-2.725085	-0.983491	3.315470
H	-2.304216	-0.567987	4.230815
C	-4.016942	-1.472373	3.259440
H	-4.640710	-1.449008	4.152510
C	-4.493027	-1.955967	2.036419
H	-5.523060	-2.301295	1.932470
C	-3.649279	-1.964646	0.944295
H	-4.004483	-2.288207	-0.033311
C	-2.320434	-1.505564	1.062539
C	-1.505564	-2.320434	-1.062539
C	-1.964646	-3.649279	-0.944295
H	-2.288207	-4.004483	0.033311
C	-1.955967	-4.493027	-2.036419
H	-2.301295	-5.523060	-1.932470
C	-1.472373	-4.016942	-3.259440
H	-1.449008	-4.640710	-4.152510
C	-0.983491	-2.725085	-3.315470
H	-0.567987	-2.304216	-4.230815
C	2.725085	0.983491	3.315470
H	2.304216	0.567987	4.230815
C	4.016942	1.472373	3.259440
H	4.640710	1.449008	4.152510
C	4.493027	1.955967	2.036419
H	5.523060	2.301295	1.932470
C	3.649279	1.964646	0.944295
H	4.004483	2.288207	-0.033311
C	2.320434	1.505564	1.062539
C	1.505564	2.320434	-1.062539
C	1.964646	3.649279	-0.944295
H	2.288207	4.004483	0.033311
C	1.955967	4.493027	-2.036419
H	2.301295	5.523060	-1.932470
C	1.472373	4.016942	-3.259440
H	1.449008	4.640710	-4.152510
C	0.983491	2.725085	-3.315470

H	0.567987	2.304216	-4.230815
C	0.000000	0.000000	4.517982
C	0.000000	0.000000	-4.517982
H	0.000000	0.000000	6.831019
H	0.000000	0.000000	-6.831019

Total Energy: -635.01021424 eV

¹A:

Ru	0.160489	2.392914	0.065389
Ru	0.000000	0.000000	-0.175940
Ru	-0.160489	-2.392914	0.065389
N	2.066747	2.087475	-0.911576
N	1.466791	-0.089969	-1.539827
N	0.815657	-2.312098	-1.888576
N	-1.714421	2.392944	0.976555
N	-1.430216	0.091060	1.365666
N	-1.038789	-2.158874	1.918048
N	1.038789	2.158874	1.918048
N	1.430216	-0.091060	1.365666
N	1.714421	-2.392944	0.976555
N	-0.815657	2.312098	-1.888576
N	-1.466791	0.089969	-1.539827
N	-2.066747	-2.087475	-0.911576
C	0.439553	5.626120	-0.045803
C	-0.439553	-5.626120	-0.045803
C	2.998135	3.066901	-0.836593
H	2.651213	3.987071	-0.368104
C	4.290214	2.939018	-1.314097
H	4.984383	3.773620	-1.220772
C	4.672369	1.718899	-1.877682
H	5.694921	1.555240	-2.221915
C	3.742464	0.702276	-1.969609
H	4.025650	-0.276764	-2.352951
C	2.423053	0.895762	-1.513223
C	1.469644	-1.194100	-2.362705
C	1.992203	-1.172427	-3.669335
H	2.435930	-0.249250	-4.039893
C	1.885411	-2.283938	-4.482637
H	2.278348	-2.256154	-5.500351
C	1.239856	-3.420987	-3.991389
H	1.122920	-4.321526	-4.593955
C	0.716874	-3.383074	-2.710519
H	0.195298	-4.238011	-2.281331
C	-2.497201	3.499991	0.990933
H	-2.024406	4.393698	0.585393
C	-3.787336	3.510166	1.483751
H	-4.360049	4.437124	1.475543
C	-4.330781	2.309364	1.955552
H	-5.362331	2.262728	2.309077
C	-3.554884	1.168114	1.936873
H	-3.963981	0.207724	2.250014
C	-2.224654	1.210354	1.467397
C	-1.494998	-0.913057	2.297915
C	-1.889793	-0.705760	3.639205
H	-2.161237	0.301366	3.953488
C	-1.884745	-1.746354	4.545058
H	-2.180466	-1.566989	5.580143

C	-1.467129	-3.015978	4.128211
H	-1.450638	-3.869182	4.805538
C	-1.039418	-3.167994	2.824032
H	-0.680772	-4.121556	2.438584
C	1.039418	3.167994	2.824032
H	0.680772	4.121556	2.438584
C	1.467129	3.015978	4.128211
H	1.450638	3.869182	4.805538
C	1.884745	1.746354	4.545058
H	2.180466	1.566989	5.580143
C	1.889793	0.705760	3.639205
H	2.161237	-0.301366	3.953488
C	1.494998	0.913057	2.297915
C	2.224654	-1.210354	1.467397
C	3.554884	-1.168114	1.936873
H	3.963981	-0.207724	2.250014
C	4.330781	-2.309364	1.955552
H	5.362331	-2.262728	2.309077
C	3.787336	-3.510166	1.483751
H	4.360049	-4.437124	1.475543
C	2.497201	-3.499991	0.990933
H	2.024406	-4.393698	0.585393
C	-0.716874	3.383074	-2.710519
H	-0.195298	4.238011	-2.281331
C	-1.239856	3.420987	-3.991389
H	-1.122920	4.321526	-4.593955
C	-1.885411	2.283938	-4.482637
H	-2.278348	2.256154	-5.500351
C	-1.992203	1.172427	-3.669335
H	-2.435930	0.249250	-4.039893
C	-1.469644	1.194100	-2.362705
C	-2.423053	-0.895762	-1.513223
C	-3.742464	-0.702276	-1.969609
H	-4.025650	0.276764	-2.352951
C	-4.672369	-1.718899	-1.877682
H	-5.694921	-1.555240	-2.221915
C	-4.290214	-2.939018	-1.314097
H	-4.984383	-3.773620	-1.220772
C	-2.998135	-3.066901	-0.836593
H	-2.651213	-3.987071	-0.368104
C	0.320839	4.393733	-0.033634
C	-0.320839	-4.393733	-0.033634
H	0.538548	6.694454	-0.051222
H	-0.538548	-6.694454	-0.051222

Total Energy: -635.55066191 eV

³A:

Ru	0.160404	2.403720	0.066086
Ru	0.000000	0.000000	-0.161696
Ru	-0.160404	-2.403720	0.066086
N	2.056839	2.098936	-0.920616
N	1.462509	-0.085787	-1.537758
N	0.825110	-2.318858	-1.875247
N	-1.710484	2.398972	0.982160
N	-1.431230	0.092690	1.361682
N	-1.062139	-2.164252	1.909775
N	1.062139	2.164252	1.909775

N	1.431230	-0.092690	1.361682
N	1.710484	-2.398972	0.982160
N	-0.825110	2.318858	-1.875247
N	-1.462509	0.085787	-1.537758
N	-2.056839	-2.098936	-0.920616
C	0.421078	5.634313	-0.034981
C	-0.421078	-5.634313	-0.034981
C	2.989145	3.077795	-0.842663
H	2.640240	3.999001	-0.377862
C	4.283346	2.947562	-1.311893
H	4.978021	3.781405	-1.216051
C	4.666923	1.725860	-1.871646
H	5.691314	1.560095	-2.209230
C	3.736425	0.710557	-1.967440
H	4.021130	-0.269094	-2.347572
C	2.414405	0.905190	-1.517848
C	1.475109	-1.198018	-2.350518
C	2.001337	-1.179633	-3.656375
H	2.442175	-0.256100	-4.029280
C	1.903188	-2.294078	-4.466045
H	2.299836	-2.267253	-5.482352
C	1.261714	-3.433119	-3.973231
H	1.151015	-4.336399	-4.572728
C	0.734573	-3.393420	-2.694684
H	0.216482	-4.249689	-2.263832
C	-2.490484	3.508120	1.008026
H	-2.012165	4.406303	0.619148
C	-3.785493	3.514230	1.488545
H	-4.355423	4.442989	1.488905
C	-4.337499	2.308360	1.935204
H	-5.372827	2.258530	2.276454
C	-3.563228	1.166059	1.908440
H	-3.977109	0.202252	2.204142
C	-2.227737	1.212903	1.457545
C	-1.510446	-0.916186	2.290243
C	-1.917493	-0.707828	3.626715
H	-2.182624	0.301497	3.939522
C	-1.935806	-1.751409	4.529377
H	-2.242504	-1.572465	5.561190
C	-1.528682	-3.024120	4.111719
H	-1.530194	-3.880209	4.785608
C	-1.086846	-3.176569	2.812296
H	-0.733650	-4.132780	2.427833
C	1.086846	3.176569	2.812296
H	0.733650	4.132780	2.427833
C	1.528682	3.024120	4.111719
H	1.530194	3.880209	4.785608
C	1.935806	1.751409	4.529377
H	2.242504	1.572465	5.561190
C	1.917493	0.707828	3.626715
H	2.182624	-0.301497	3.939522
C	1.510446	0.916186	2.290243
C	2.227737	-1.212903	1.457545
C	3.563228	-1.166059	1.908440
H	3.977109	-0.202252	2.204142
C	4.337499	-2.308360	1.935204
H	5.372827	-2.258530	2.276454
C	3.785493	-3.514230	1.488545
H	4.355423	-4.442989	1.488905

C	2.490484	-3.508120	1.008026
H	2.012165	-4.406303	0.619148
C	-0.734573	3.393420	-2.694684
H	-0.216482	4.249689	-2.263832
C	-1.261714	3.433119	-3.973231
H	-1.151015	4.336399	-4.572728
C	-1.903188	2.294078	-4.466045
H	-2.299836	2.267253	-5.482352
C	-2.001337	1.179633	-3.656375
H	-2.442175	0.256100	-4.029280
C	-1.475109	1.198018	-2.350518
C	-2.414405	-0.905190	-1.517848
C	-3.736425	-0.710557	-1.967440
H	-4.021130	0.269094	-2.347572
C	-4.666923	-1.725860	-1.871646
H	-5.691314	-1.560095	-2.209230
C	-4.283346	-2.947562	-1.311893
H	-4.978021	-3.781405	-1.216051
C	-2.989145	-3.077795	-0.842663
H	-2.640240	-3.999001	-0.377862
C	0.321026	4.400259	-0.023059
C	-0.321026	-4.400259	-0.023059
H	0.510218	6.703497	-0.040161
H	-0.510218	-6.703497	-0.040161

Total Energy: -635.66451633 eV

³A:

Ru	0.185481	2.413092	0.021336
Ru	0.000000	0.000000	0.022739
Ru	-0.185481	-2.413092	0.021336
N	2.052736	2.100896	-0.942636
N	1.444370	-0.111112	-1.429511
N	0.790471	-2.321000	-1.863601
N	-1.705451	2.390949	0.989264
N	-1.443916	0.111489	1.473888
N	-1.130580	-2.171187	1.908973
N	1.130580	2.171187	1.908973
N	1.443916	-0.111489	1.473888
N	1.705451	-2.390949	0.989264
N	-0.790471	2.321000	-1.863601
N	-1.444370	0.111112	-1.429511
N	-2.052736	-2.100896	-0.942636
C	0.438584	5.741460	0.021545
C	-0.438584	-5.741460	0.021545
C	2.982130	3.086090	-0.933851
H	2.635793	4.028829	-0.510559
C	4.266458	2.929574	-1.421673
H	4.961802	3.767710	-1.387325
C	4.641273	1.677416	-1.918878
H	5.659774	1.493906	-2.265297
C	3.711612	0.657463	-1.939553
H	3.987087	-0.342147	-2.273373
C	2.396493	0.878148	-1.478762
C	1.413643	-1.171930	-2.301883
C	1.882020	-1.088622	-3.630051

H	2.287141	-0.140783	-3.982272
C	1.781704	-2.173455	-4.477400
H	2.135485	-2.095757	-5.506928
C	1.196248	-3.352643	-4.005714
H	1.097643	-4.237974	-4.633172
C	0.704519	-3.372184	-2.713410
H	0.215246	-4.251331	-2.294926
C	-2.472239	3.507392	0.982532
H	-1.986696	4.385267	0.557021
C	-3.763033	3.550640	1.476381
H	-4.321737	4.485391	1.443718
C	-4.323516	2.371930	1.978197
H	-5.356383	2.347646	2.329991
C	-3.562193	1.221168	1.996261
H	-3.987025	0.276265	2.332773
C	-2.231341	1.235977	1.527784
C	-1.571122	-0.940768	2.347917
C	-2.017701	-0.787028	3.677325
H	-2.273749	0.211205	4.030145
C	-2.079442	-1.874345	4.525238
H	-2.413693	-1.743679	5.555906
C	-1.679921	-3.128440	4.053297
H	-1.713243	-4.017877	4.681642
C	-1.201384	-3.222885	2.759394
H	-0.851493	-4.166193	2.340454
C	1.201384	3.222885	2.759394
H	0.851493	4.166193	2.340454
C	1.679921	3.128440	4.053297
H	1.713243	4.017877	4.681642
C	2.079442	1.874345	4.525238
H	2.413693	1.743679	5.555906
C	2.017701	0.787028	3.677325
H	2.273749	-0.211205	4.030145
C	1.571122	0.940768	2.347917
C	2.231341	-1.235977	1.527784
C	3.562193	-1.221168	1.996261
H	3.987025	-0.276265	2.332773
C	4.323516	-2.371930	1.978197
H	5.356383	-2.347646	2.329991
C	3.763033	-3.550640	1.476381
H	4.321737	-4.485391	1.443718
C	2.472239	-3.507392	0.982532
H	1.986696	-4.385267	0.557021
C	-0.704519	3.372184	-2.713410
H	-0.215246	4.251331	-2.294926
C	-1.196248	3.352643	-4.005714
H	-1.097643	4.237974	-4.633172
C	-1.781704	2.173455	-4.477400
H	-2.135485	2.095757	-5.506928
C	-1.882020	1.088622	-3.630051
H	-2.287141	0.140783	-3.982272
C	-1.413643	1.171930	-2.301883
C	-2.396493	-0.878148	-1.478762
C	-3.711612	-0.657463	-1.939553
H	-3.987087	0.342147	-2.273373
C	-4.641273	-1.677416	-1.918878
H	-5.659774	-1.493906	-2.265297
C	-4.266458	-2.929574	-1.421673
H	-4.961802	-3.767710	-1.387325

C	-2.982130	-3.086090	-0.933851
H	-2.635793	-4.028829	-0.510559
C	0.345396	4.505906	0.021127
C	-0.345396	-4.505906	0.021127
H	0.519725	6.812559	0.023656
H	-0.519725	-6.812559	0.023656

Total Energy: -634.75945935 eV

³B:

Ru	0.185354	2.418491	0.020955
Ru	0.000000	0.000000	-0.010580
Ru	-0.185354	-2.418491	0.020955
N	2.042546	2.110221	-0.984034
N	1.438352	-0.108724	-1.452483
N	0.784546	-2.322129	-1.868174
N	-1.689554	2.401693	1.023302
N	-1.425716	0.111751	1.466733
N	-1.104848	-2.170668	1.905327
N	1.104848	2.170668	1.905327
N	1.425716	-0.111751	1.466733
N	1.689554	-2.401693	1.023302
N	-0.784546	2.322129	-1.868174
N	-1.438352	0.108724	-1.452483
N	-2.042546	-2.110221	-0.984034
C	0.438422	5.734712	-0.001995
C	-0.438422	-5.734712	-0.001995
C	2.961341	3.104630	-1.015538
H	2.619608	4.049030	-0.593191
C	4.232902	2.955852	-1.537265
H	4.917525	3.803471	-1.536529
C	4.610862	1.699677	-2.022322
H	5.622138	1.521696	-2.391600
C	3.692135	0.670093	-2.003097
H	3.969114	-0.332211	-2.327936
C	2.384911	0.885462	-1.518146
C	1.399366	-1.174555	-2.320216
C	1.851435	-1.094430	-3.653588
H	2.247606	-0.145823	-4.014095
C	1.747568	-2.183472	-4.495464
H	2.089840	-2.108980	-5.529285
C	1.173137	-3.362543	-4.010573
H	1.071031	-4.251838	-4.631593
C	0.696603	-3.378020	-2.712542
H	0.217777	-4.258164	-2.285197
C	-2.450329	3.521719	1.057371
H	-1.977571	4.402459	0.624122
C	-3.721909	3.565622	1.597036
H	-4.274252	4.504702	1.597949
C	-4.272636	2.382025	2.099889
H	-5.292613	2.358515	2.487141
C	-3.518547	1.227153	2.072531
H	-3.936650	0.279335	2.409096
C	-2.203120	1.241029	1.560818
C	-1.524309	-0.935562	2.350571
C	-1.917373	-0.770930	3.695935
H	-2.150666	0.231618	4.052637
C	-1.957882	-1.852505	4.552111

H	-2.253202	-1.712878	5.593438
C	-1.588188	-3.113428	4.072516
H	-1.609964	-3.999940	4.705334
C	-1.156390	-3.218481	2.763616
H	-0.831110	-4.166893	2.337163
C	1.156390	3.218481	2.763616
H	0.831110	4.166893	2.337163
C	1.588188	3.113428	4.072516
H	1.609964	3.999940	4.705334
C	1.957882	1.852505	4.552111
H	2.253202	1.712878	5.593438
C	1.917373	0.770930	3.695935
H	2.150666	-0.231618	4.052637
C	1.524309	0.935562	2.350571
C	2.203120	-1.241029	1.560818
C	3.518547	-1.227153	2.072531
H	3.936650	-0.279335	2.409096
C	4.272636	-2.382025	2.099889
H	5.292613	-2.358515	2.487141
C	3.721909	-3.565622	1.597036
H	4.274252	-4.504702	1.597949
C	2.450329	-3.521719	1.057371
H	1.977571	-4.402459	0.624122
C	-0.696603	3.378020	-2.712542
H	-0.217777	4.258164	-2.285197
C	-1.173137	3.362543	-4.010573
H	-1.071031	4.251838	-4.631593
C	-1.747568	2.183472	-4.495464
H	-2.089840	2.108980	-5.529285
C	-1.851435	1.094430	-3.653588
H	-2.247606	0.145823	-4.014095
C	-1.399366	1.174555	-2.320216
C	-2.384911	-0.885462	-1.518146
C	-3.692135	-0.670093	-2.003097
H	-3.969114	0.332211	-2.327936
C	-4.610862	-1.699677	-2.022322
H	-5.622138	-1.521696	-2.391600
C	-4.232902	-2.955852	-1.537265
H	-4.917525	-3.803471	-1.536529
C	-2.961341	-3.104630	-1.015538
H	-2.619608	-4.049030	-0.593191
C	0.344758	4.497738	0.006201
C	-0.344758	-4.497738	0.006201
H	0.520432	6.805622	-0.005920
H	-0.520432	-6.805622	-0.005920

Total Energy: -634.40287474 eV

³B:

Ru	0.174219	2.373469	0.018386
Ru	0.000000	0.000000	0.010241
Ru	-0.174219	-2.373469	0.018386
N	2.083781	2.081235	-0.890640
N	1.459209	-0.107222	-1.447283
N	0.752547	-2.293884	-1.903082
N	-1.751150	2.366191	0.933359
N	-1.455586	0.105706	1.475779
N	-1.066684	-2.157493	1.940561

N	1.066684	2.157493	1.940561
N	1.455586	-0.105706	1.475779
N	1.751150	-2.366191	0.933359
N	-0.752547	2.293884	-1.903082
N	-1.459209	0.107222	-1.447283
N	-2.083781	-2.081235	-0.890640
C	0.413166	5.585532	0.017053
C	-0.413166	-5.585532	0.017053
C	3.025426	3.050314	-0.822737
H	2.690961	3.979374	-0.363667
C	4.313335	2.902243	-1.304275
H	5.018203	3.729157	-1.225084
C	4.675649	1.669736	-1.857200
H	5.693766	1.491089	-2.207343
C	3.737252	0.660038	-1.925498
H	4.008320	-0.327615	-2.296890
C	2.420609	0.868069	-1.461055
C	1.410923	-1.155284	-2.327566
C	1.899235	-1.085509	-3.649928
H	2.344983	-0.152011	-3.991334
C	1.761829	-2.157440	-4.508025
H	2.130480	-2.085386	-5.532719
C	1.116107	-3.313620	-4.058009
H	0.979263	-4.184516	-4.698052
C	0.618039	-3.325681	-2.768058
H	0.090409	-4.190058	-2.368045
C	-2.538617	3.465264	0.878254
H	-2.073932	4.336193	0.418684
C	-3.829101	3.508295	1.373237
H	-4.403618	4.431346	1.303998
C	-4.365918	2.340871	1.926092
H	-5.395817	2.314627	2.286150
C	-3.588141	1.202187	1.980663
H	-3.998877	0.263963	2.351752
C	-2.260005	1.213947	1.502407
C	-1.548203	-0.932821	2.363436
C	-2.005208	-0.785537	3.690879
H	-2.305146	0.205021	4.030826
C	-2.018374	-1.862173	4.553974
H	-2.361200	-1.731946	5.581930
C	-1.555548	-3.103131	4.104195
H	-1.542863	-3.982205	4.747508
C	-1.077024	-3.194090	2.809988
H	-0.685958	-4.128243	2.410115
C	1.077024	3.194090	2.809988
H	0.685958	4.128243	2.410115
C	1.555548	3.103131	4.104195
H	1.542863	3.982205	4.747508
C	2.018374	1.862173	4.553974
H	2.361200	1.731946	5.581930
C	2.005208	0.785537	3.690879
H	2.305146	-0.205021	4.030826
C	1.548203	0.932821	2.363436
C	2.260005	-1.213947	1.502407
C	3.588141	-1.202187	1.980663
H	3.998877	-0.263963	2.351752
C	4.365918	-2.340871	1.926092
H	5.395817	-2.314627	2.286150
C	3.829101	-3.508295	1.373237

H	4.403618	-4.431346	1.303998
C	2.538617	-3.465264	0.878254
H	2.073932	-4.336193	0.418684
C	-0.618039	3.325681	-2.768058
H	-0.090409	4.190058	-2.368045
C	-1.116107	3.313620	-4.058009
H	-0.979263	4.184516	-4.698052
C	-1.761829	2.157440	-4.508025
H	-2.130480	2.085386	-5.532719
C	-1.899235	1.085509	-3.649928
H	-2.344983	0.152011	-3.991334
C	-1.410923	1.155284	-2.327566
C	-2.420609	-0.868069	-1.461055
C	-3.737252	-0.660038	-1.925498
H	-4.008320	0.327615	-2.296890
C	-4.675649	-1.669736	-1.857200
H	-5.693766	-1.491089	-2.207343
C	-4.313335	-2.902243	-1.304275
H	-5.018203	-3.729157	-1.225084
C	-3.025426	-3.050314	-0.822737
H	-2.690961	-3.979374	-0.363667
C	0.320211	4.352469	0.017191
C	-0.320211	-4.352469	0.017191
H	0.492915	6.655753	0.016489
H	-0.492915	-6.655753	0.016489

Total Energy: -635.66085333 eV

⁵A:

Ru	0.192624	2.413106	0.025812
Ru	0.000000	0.000000	0.027863
Ru	-0.192624	-2.413106	0.025812
N	2.054164	2.100299	-0.950505
N	1.445467	-0.114744	-1.423955
N	0.792385	-2.325626	-1.855809
N	-1.693723	2.399479	1.005049
N	-1.446438	0.115716	1.478713
N	-1.157382	-2.172949	1.904037
N	1.157382	2.172949	1.904037
N	1.446438	-0.115716	1.478713
N	1.693723	-2.399479	1.005049
N	-0.792385	2.325626	-1.855809
N	-1.445467	0.114744	-1.423955
N	-2.054164	-2.100299	-0.950505
C	0.455825	5.740526	0.019774
C	-0.455825	-5.740526	0.019774
C	2.982353	3.087009	-0.954199
H	2.636390	4.033293	-0.538897
C	4.265309	2.927438	-1.443675
H	4.958504	3.767721	-1.421120
C	4.641727	1.670191	-1.927285
H	5.659960	1.484229	-2.273071
C	3.713325	0.649058	-1.935499
H	3.988996	-0.353986	-2.258882
C	2.398125	0.873858	-1.477004
C	1.413795	-1.176522	-2.295074
C	1.880755	-1.092824	-3.623750
H	2.282781	-0.143963	-3.976875

C	1.782869	-2.178641	-4.469892
H	2.135436	-2.100941	-5.499773
C	1.201019	-3.359103	-3.996400
H	1.104810	-4.245658	-4.622353
C	0.709586	-3.378391	-2.704419
H	0.221661	-4.258128	-2.285517
C	-2.452129	3.522039	1.010377
H	-1.959386	4.400830	0.595043
C	-3.744162	3.569418	1.499710
H	-4.294377	4.509534	1.477234
C	-4.316783	2.388024	1.982074
H	-5.351915	2.366526	2.327076
C	-3.563278	1.231807	1.990030
H	-3.995803	0.285669	2.312996
C	-2.229032	1.243549	1.531627
C	-1.587892	-0.940610	2.345992
C	-2.038516	-0.788057	3.674202
H	-2.283796	0.211742	4.030364
C	-2.117496	-1.878311	4.516619
H	-2.454832	-1.748384	5.546357
C	-1.731732	-3.135295	4.039746
H	-1.780455	-4.028162	4.662268
C	-1.246816	-3.228467	2.748596
H	-0.904680	-4.173295	2.326957
C	1.246816	3.228467	2.748596
H	0.904680	4.173295	2.326957
C	1.731732	3.135295	4.039746
H	1.780455	4.028162	4.662268
C	2.117496	1.878311	4.516619
H	2.454832	1.748384	5.546357
C	2.038516	0.788057	3.674202
H	2.283796	-0.211742	4.030364
C	1.587892	0.940610	2.345992
C	2.229032	-1.243549	1.531627
C	3.563278	-1.231807	1.990030
H	3.995803	-0.285669	2.312996
C	4.316783	-2.388024	1.982074
H	5.351915	-2.366526	2.327076
C	3.744162	-3.569418	1.499710
H	4.294377	-4.509534	1.477234
C	2.452129	-3.522039	1.010377
H	1.959386	-4.400830	0.595043
C	-0.709586	3.378391	-2.704419
H	-0.221661	4.258128	-2.285517
C	-1.201019	3.359103	-3.996400
H	-1.104810	4.245658	-4.622353
C	-1.782869	2.178641	-4.469892
H	-2.135436	2.100941	-5.499773
C	-1.880755	1.092824	-3.623750
H	-2.282781	0.143963	-3.976875
C	-1.413795	1.176522	-2.295074
C	-2.398125	-0.873858	-1.477004
C	-3.713325	-0.649058	-1.935499
H	-3.988996	0.353986	-2.258882
C	-4.641727	-1.670191	-1.927285
H	-5.659960	-1.484229	-2.273071
C	-4.265309	-2.927438	-1.443675
H	-4.958504	-3.767721	-1.421120
C	-2.982353	-3.087009	-0.954199

H	-2.636390	-4.033293	-0.538897
C	0.358338	4.505663	0.022206
C	-0.358338	-4.505663	0.022206
H	-0.538901	-6.811564	0.018603
H	0.538901	6.811564	0.018603

Total Energy: -635.02167387 eV

Table S2 Cartesian Coordinates of the central scattering regions:

Linear Ru₃(L₄)(NCS)₂

Au	0.00000000e+00,	0.00000000e+00,	7.06330299e+00
Au	-1.44179070e+00,	2.49725485e+00,	7.06330299e+00
Au	-2.88358140e+00,	4.99450970e+00,	7.06330299e+00
Au	-4.32537222e+00,	7.49176455e+00,	7.06330299e+00
Au	2.88358140e+00,	0.00000000e+00,	7.06330299e+00
Au	1.44179070e+00,	2.49725485e+00,	7.06330299e+00
Au	1.33226763e-15,	4.99450970e+00,	7.06330299e+00
Au	-1.44179070e+00,	7.49176455e+00,	7.06330299e+00
Au	5.76716280e+00,	0.00000000e+00,	7.06330299e+00
Au	4.32537222e+00,	2.49725485e+00,	7.06330299e+00
Au	2.88358140e+00,	4.99450970e+00,	7.06330299e+00
Au	1.44179070e+00,	7.49176455e+00,	7.06330299e+00
Au	8.65074444e+00,	0.00000000e+00,	7.06330299e+00
Au	7.20895386e+00,	2.49725485e+00,	7.06330299e+00
Au	5.76716280e+00,	4.99450970e+00,	7.06330299e+00
Au	4.32537222e+00,	7.49176455e+00,	7.06330299e+00
Au	-4.32537222e+00,	9.15660095e+00,	9.41773796e+00
Au	2.22044605e-16,	1.66483653e+00,	9.41773796e+00
Au	-1.44179070e+00,	4.16209126e+00,	9.41773796e+00
Au	-2.88358140e+00,	6.65934610e+00,	9.41773796e+00
Au	-1.44179070e+00,	9.15660095e+00,	9.41773796e+00
Au	2.88358140e+00,	1.66483653e+00,	9.41773796e+00
Au	1.44179070e+00,	4.16209126e+00,	9.41773796e+00
Au	-4.44089210e-16,	6.65934610e+00,	9.41773796e+00
Au	1.44179070e+00,	9.15660095e+00,	9.41773796e+00
Au	5.76716280e+00,	1.66483653e+00,	9.41773796e+00
Au	4.32537222e+00,	4.16209126e+00,	9.41773796e+00
Au	2.88358140e+00,	6.65934610e+00,	9.41773796e+00
Au	4.32537222e+00,	9.15660095e+00,	9.41773796e+00
Au	8.65074444e+00,	1.66483653e+00,	9.41773796e+00
Au	7.20895386e+00,	4.16209126e+00,	9.41773796e+00
Au	5.76716280e+00,	6.65934610e+00,	9.41773796e+00
Au	-2.88358140e+00,	8.32418251e+00,	1.17721720e+01
Au	1.44179070e+00,	8.32418263e-01,	1.17721720e+01
Au	4.44089210e-16,	3.32967305e+00,	1.17721720e+01
Au	-1.44179070e+00,	5.82692766e+00,	1.17721720e+01
Au	1.77635684e-15,	8.32418251e+00,	1.17721720e+01
Au	4.32537222e+00,	8.32418263e-01,	1.17721720e+01
Au	2.88358140e+00,	3.32967305e+00,	1.17721720e+01
Au	1.44179070e+00,	5.82692766e+00,	1.17721720e+01
Au	2.88358140e+00,	8.32418251e+00,	1.17721720e+01
Au	7.20895386e+00,	8.32418263e-01,	1.17721720e+01
Au	5.76716280e+00,	3.32967305e+00,	1.17721720e+01
Au	4.32537222e+00,	5.82692766e+00,	1.17721720e+01
Au	5.76716280e+00,	8.32418251e+00,	1.17721720e+01
Au	1.00925350e+01,	8.32418263e-01,	1.17721720e+01
Au	8.65074444e+00,	3.32967305e+00,	1.17721720e+01

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Au -1.44179070e+00, 4.16209126e+00, 3.03221737e+01
Au -2.88358140e+00, 6.65934610e+00, 3.03221737e+01
Au -1.44179070e+00, 9.15660095e+00, 3.03221737e+01
Au 2.88358140e+00, 1.66483653e+00, 3.03221737e+01
Au 1.44179070e+00, 4.16209126e+00, 3.03221737e+01
Au -4.44089210e-16, 6.65934610e+00, 3.03221737e+01
Au 1.44179070e+00, 9.15660095e+00, 3.03221737e+01
Au 5.76716280e+00, 1.66483653e+00, 3.03221737e+01
Au 4.32537222e+00, 4.16209126e+00, 3.03221737e+01
Au 2.88358140e+00, 6.65934610e+00, 3.03221737e+01
Au 4.32537222e+00, 9.15660095e+00, 3.03221737e+01

Au	8.65074444e+00,	1.66483653e+00,	3.03221737e+01
Au	7.20895386e+00,	4.16209126e+00,	3.03221737e+01
Au	5.76716280e+00,	6.65934610e+00,	3.03221737e+01
Au	-2.88358140e+00,	8.32418251e+00,	3.26766079e+01
Au	1.44179070e+00,	8.32418263e-01,	3.26766079e+01
Au	4.44089210e-16,	3.32967305e+00,	3.26766079e+01
Au	-1.44179070e+00,	5.82692766e+00,	3.26766079e+01
Au	1.77635684e-15,	8.32418251e+00,	3.26766079e+01
Au	4.32537222e+00,	8.32418263e-01,	3.26766079e+01
Au	2.88358140e+00,	3.32967305e+00,	3.26766079e+01
Au	1.44179070e+00,	5.82692766e+00,	3.26766079e+01
Au	2.88358140e+00,	8.32418251e+00,	3.26766079e+01
Au	7.20895386e+00,	8.32418263e-01,	3.26766079e+01
Au	5.76716280e+00,	3.32967305e+00,	3.26766079e+01
Au	4.32537222e+00,	5.82692766e+00,	3.26766079e+01
Au	5.76716280e+00,	8.32418251e+00,	3.26766079e+01
Au	1.00925350e+01,	8.32418263e-01,	3.26766079e+01
Au	8.65074444e+00,	3.32967305e+00,	3.26766079e+01
Au	7.20895386e+00,	5.82692766e+00,	3.26766079e+01

Bent Ru₃(L₄)(NCS)₂

Au	0.00000000e+00,	0.00000000e+00,	7.06330299e+00
Au	-1.44179070e+00,	2.49725485e+00,	7.06330299e+00
Au	-2.88358140e+00,	4.99450970e+00,	7.06330299e+00
Au	-4.32537222e+00,	7.49176455e+00,	7.06330299e+00
Au	2.88358140e+00,	0.00000000e+00,	7.06330299e+00
Au	1.44179070e+00,	2.49725485e+00,	7.06330299e+00
Au	1.33226763e-15,	4.99450970e+00,	7.06330299e+00
Au	-1.44179070e+00,	7.49176455e+00,	7.06330299e+00
Au	5.76716280e+00,	0.00000000e+00,	7.06330299e+00
Au	4.32537222e+00,	2.49725485e+00,	7.06330299e+00
Au	2.88358140e+00,	4.99450970e+00,	7.06330299e+00
Au	1.44179070e+00,	7.49176455e+00,	7.06330299e+00
Au	8.65074444e+00,	0.00000000e+00,	7.06330299e+00
Au	7.20895386e+00,	2.49725485e+00,	7.06330299e+00
Au	5.76716280e+00,	4.99450970e+00,	7.06330299e+00
Au	4.32537222e+00,	7.49176455e+00,	7.06330299e+00
Au	-4.32537222e+00,	9.15660095e+00,	9.41773796e+00
Au	2.22044605e-16,	1.66483653e+00,	9.41773796e+00
Au	-1.44179070e+00,	4.16209126e+00,	9.41773796e+00
Au	-2.88358140e+00,	6.65934610e+00,	9.41773796e+00
Au	-1.44179070e+00,	9.15660095e+00,	9.41773796e+00
Au	2.88358140e+00,	1.66483653e+00,	9.41773796e+00
Au	1.44179070e+00,	4.16209126e+00,	9.41773796e+00
Au	-4.44089210e-16,	6.65934610e+00,	9.41773796e+00
Au	1.44179070e+00,	9.15660095e+00,	9.41773796e+00
Au	5.76716280e+00,	1.66483653e+00,	9.41773796e+00
Au	4.32537222e+00,	4.16209126e+00,	9.41773796e+00
Au	2.88358140e+00,	6.65934610e+00,	9.41773796e+00
Au	4.32537222e+00,	9.15660095e+00,	9.41773796e+00
Au	8.65074444e+00,	1.66483653e+00,	9.41773796e+00
Au	7.20895386e+00,	4.16209126e+00,	9.41773796e+00
Au	5.76716280e+00,	6.65934610e+00,	9.41773796e+00
Au	-2.88358140e+00,	8.32418251e+00,	1.17721720e+01
Au	1.44179070e+00,	8.32418263e-01,	1.17721720e+01
Au	4.44089210e-16,	3.32967305e+00,	1.17721720e+01
Au	-1.44179070e+00,	5.82692766e+00,	1.17721720e+01
Au	1.77635684e-15,	8.32418251e+00,	1.17721720e+01

Au	4.32537222e+00,	8.32418263e-01,	1.17721720e+01
Au	2.88358140e+00,	3.32967305e+00,	1.17721720e+01
Au	1.44179070e+00,	5.82692766e+00,	1.17721720e+01
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Au	5.76716280e+00,	3.32967305e+00,	1.17721720e+01
Au	4.32537222e+00,	5.82692766e+00,	1.17721720e+01
Au	5.76716280e+00,	8.32418251e+00,	1.17721720e+01
Au	1.00925350e+01,	8.32418263e-01,	1.17721720e+01
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H	5.37180532,	5.9678465 ,	17.86266174
H	6.27076185,	6.9963467 ,	19.84503701
C	5.26580537,	6.57473122,	19.82497754
C	4.38323534,	7.37584614,	21.96537974
H	4.73600972,	8.40577864,	21.91162863
H	3.66765363,	7.55149268,	23.89080253
H	0.21582544,	4.23982482,	17.95628562
H	-0.50589525,	3.24444269,	20.02421679
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C	1.38544965,	2.63314985,	21.91495278
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H	1.88598717,	2.41690015,	23.90985336
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Au	-1.44179070e+00,	9.15660095e+00,	3.01221720e+01
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Au	7.20895386e+00,	4.16209126e+00,	3.01221720e+01
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Au	-2.88358140e+00,	8.32418251e+00,	3.24766062e+01
Au	1.44179070e+00,	8.32418263e-01,	3.24766062e+01
Au	4.44089210e-16,	3.32967305e+00,	3.24766062e+01
Au	-1.44179070e+00,	5.82692766e+00,	3.24766062e+01
Au	1.77635684e-15,	8.32418251e+00,	3.24766062e+01
Au	4.32537222e+00,	8.32418263e-01,	3.24766062e+01
Au	2.88358140e+00,	3.32967305e+00,	3.24766062e+01
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Au	7.20895386e+00,	8.32418263e-01,	3.24766062e+01
Au	5.76716280e+00,	3.32967305e+00,	3.24766062e+01
Au	4.32537222e+00,	5.82692766e+00,	3.24766062e+01
Au	5.76716280e+00,	8.32418251e+00,	3.24766062e+01
Au	1.00925350e+01,	8.32418263e-01,	3.24766062e+01
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