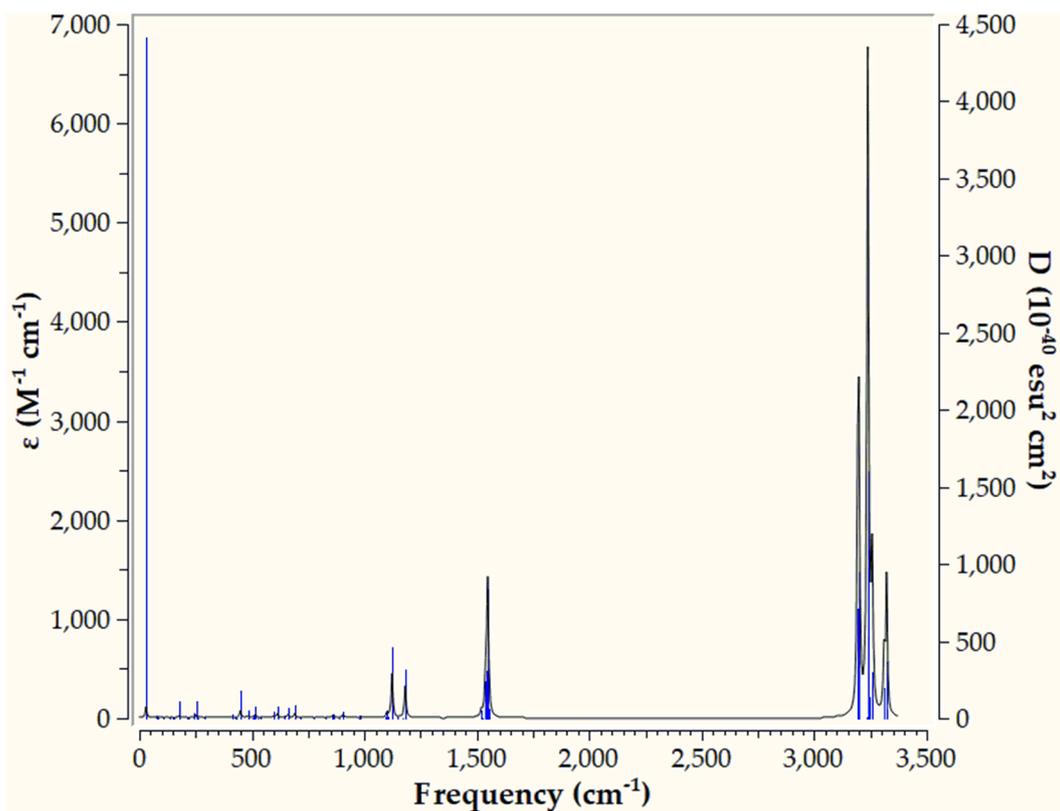
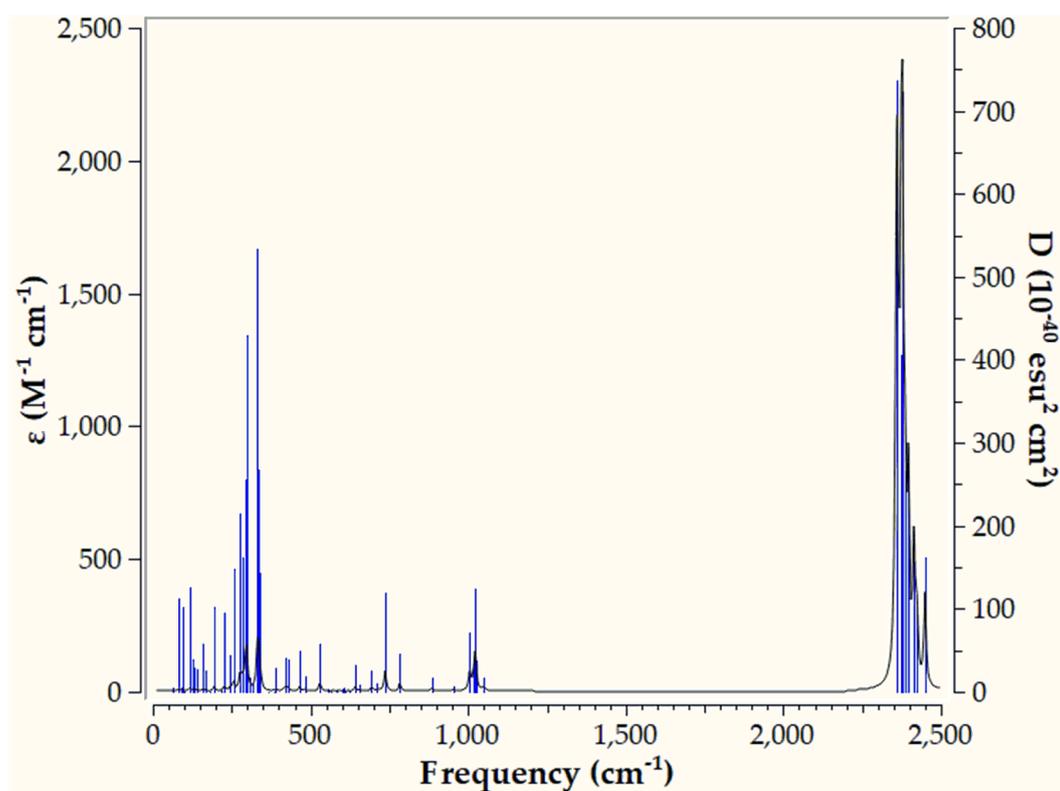


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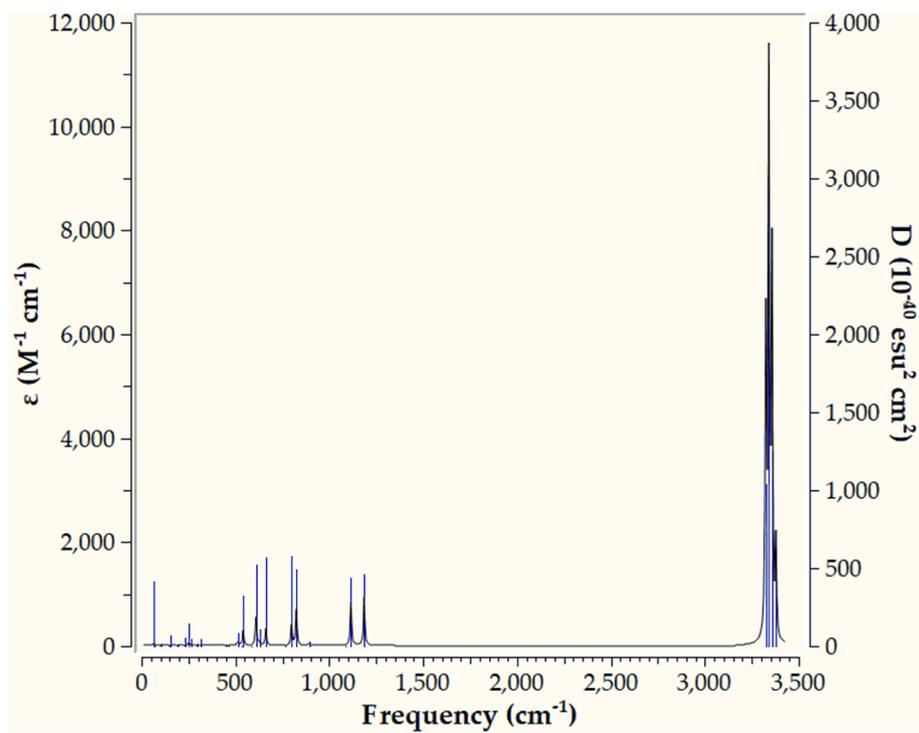


(a)

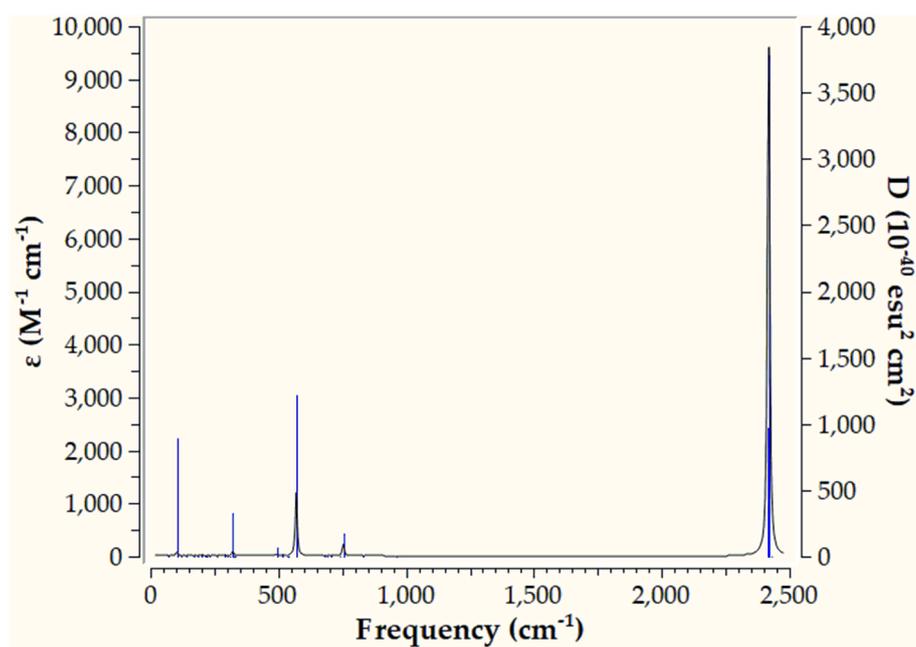


(b)

Figure S1: Simulated IR spectra of **2''_Ru** (a) and **3''_Ru** (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

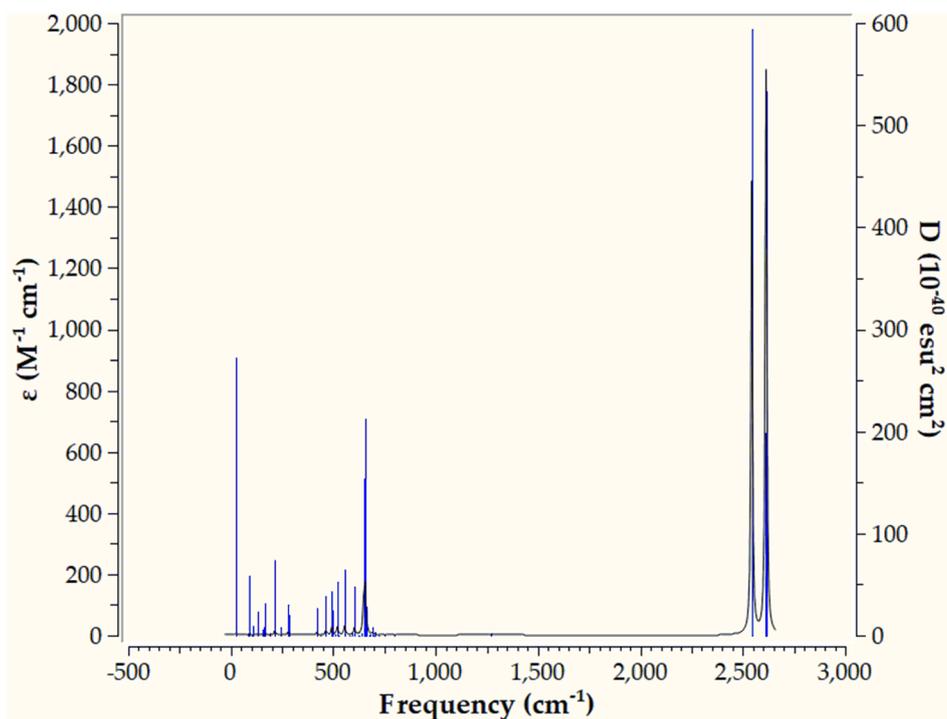


(a)

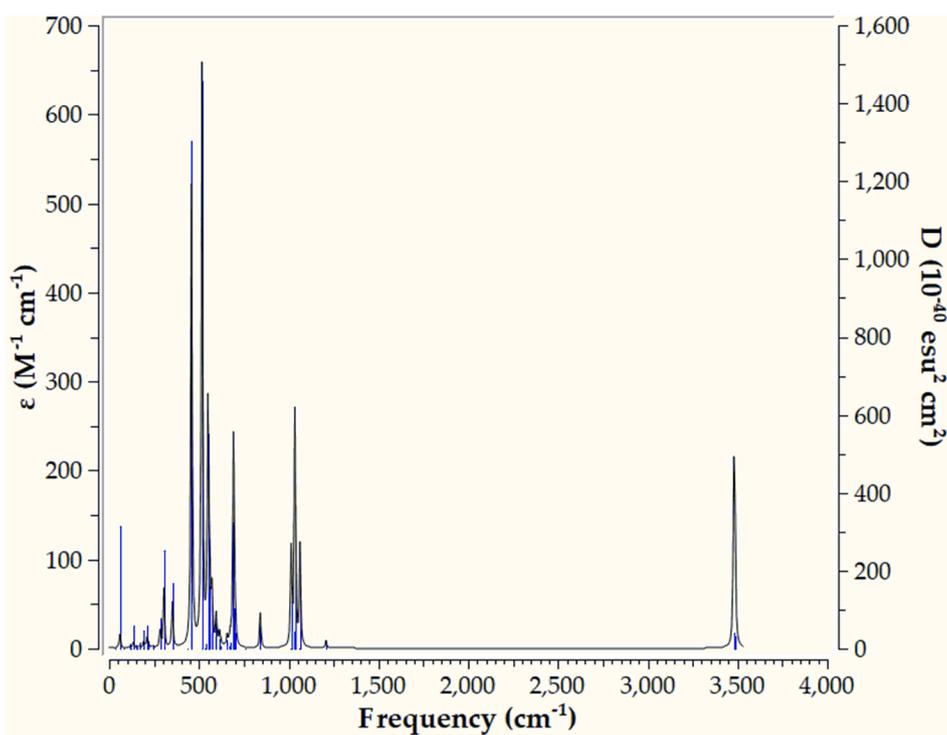


(b)

Figure S2: Simulated IR spectra of 4''_Ru (a) and 5''_Ru (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

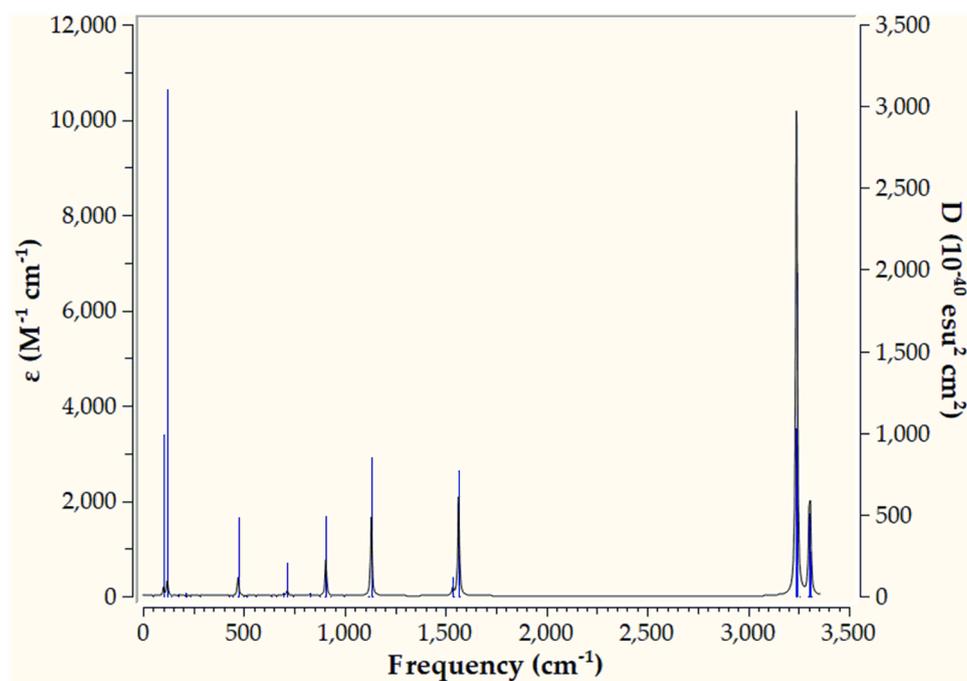


(a)

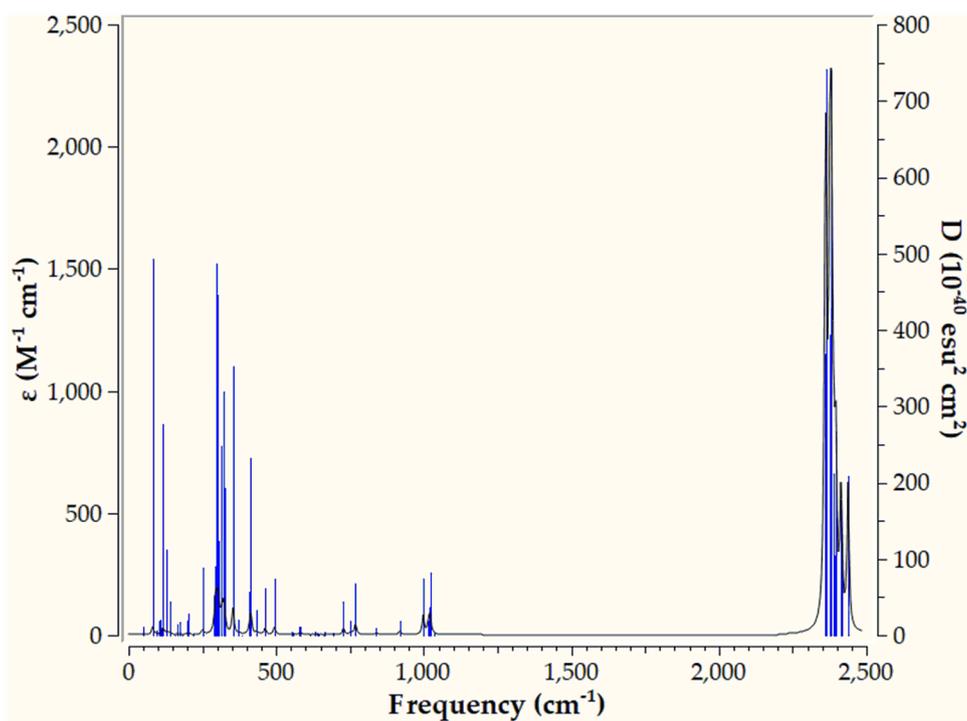


(b)

Figure S3: Simulated IR spectra of $6''_{\text{Ru}}$ (a) and $7''_{\text{Ru}}$ (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

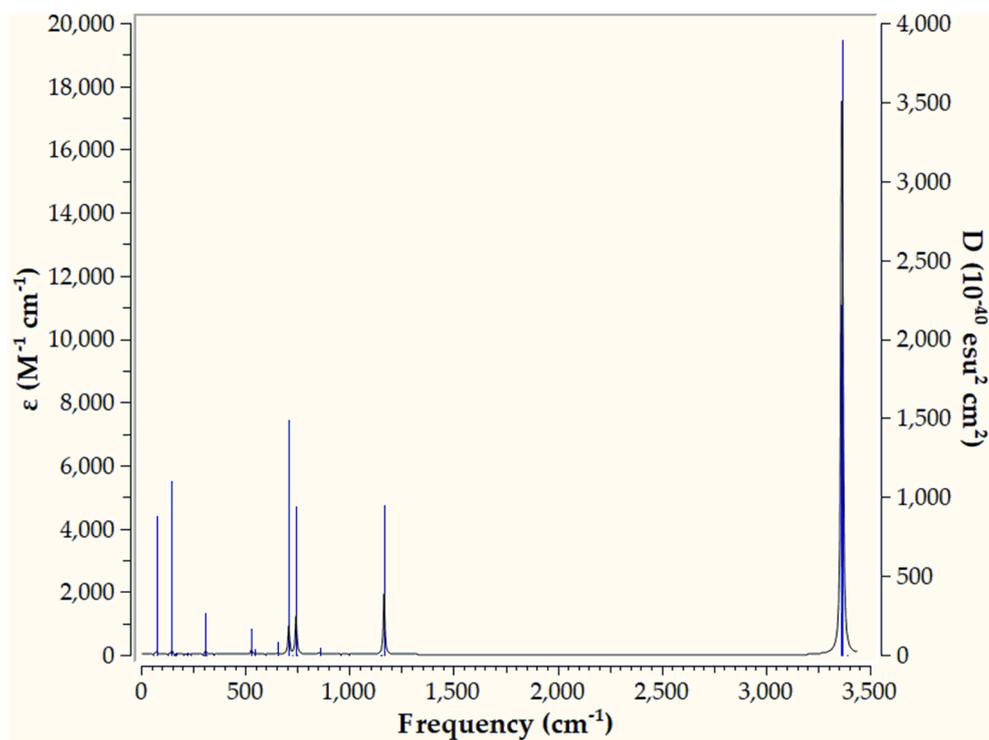


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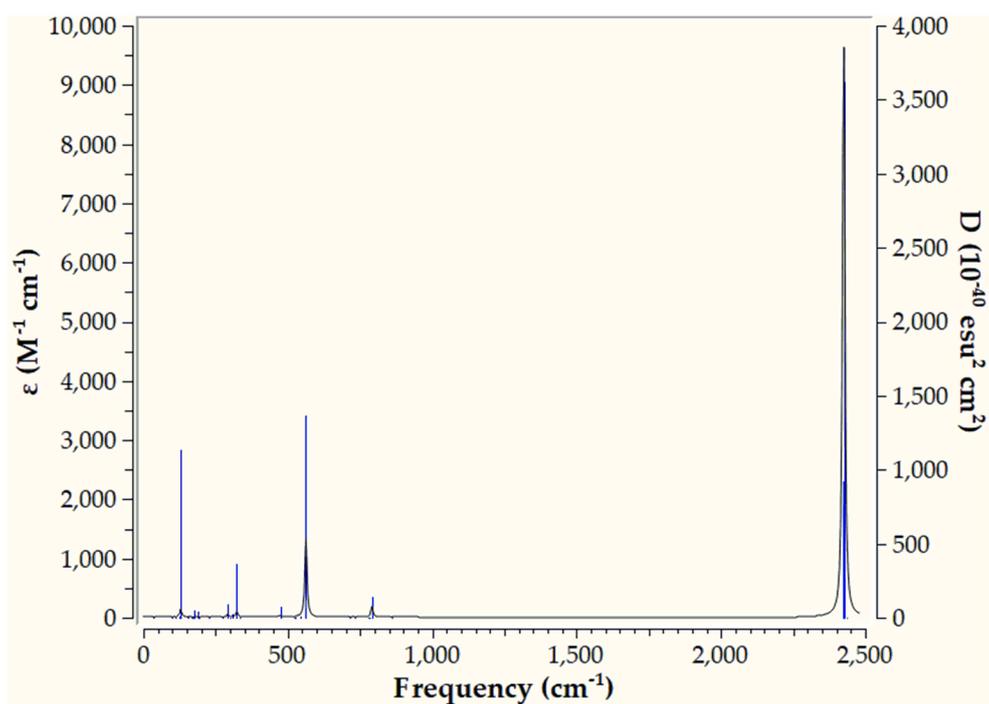


(b)

Figure S4: Simulated IR spectra of 2''_Os (a) and 3''_Os (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.



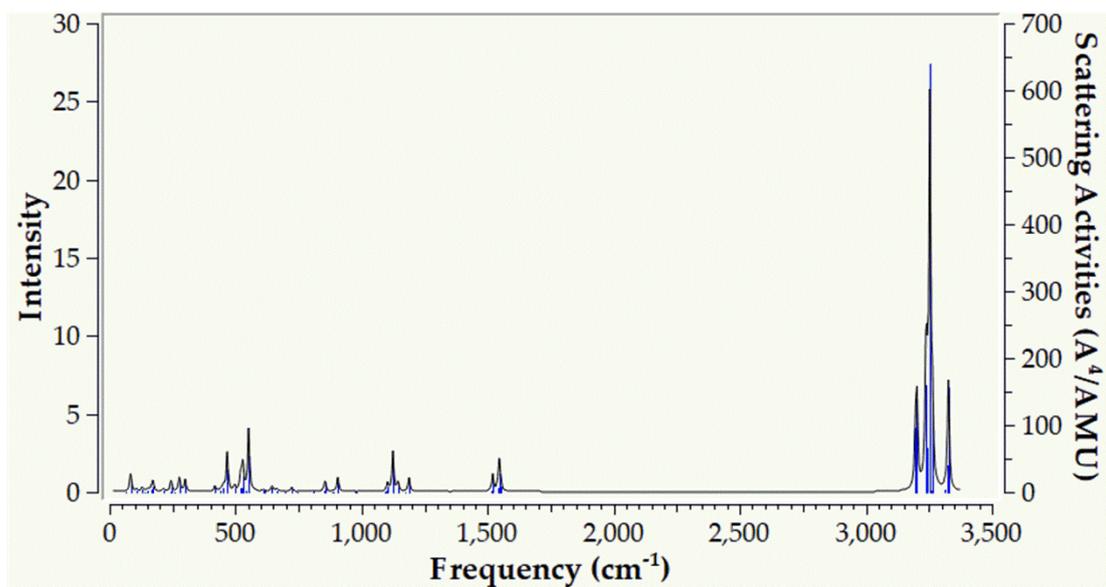
(a)



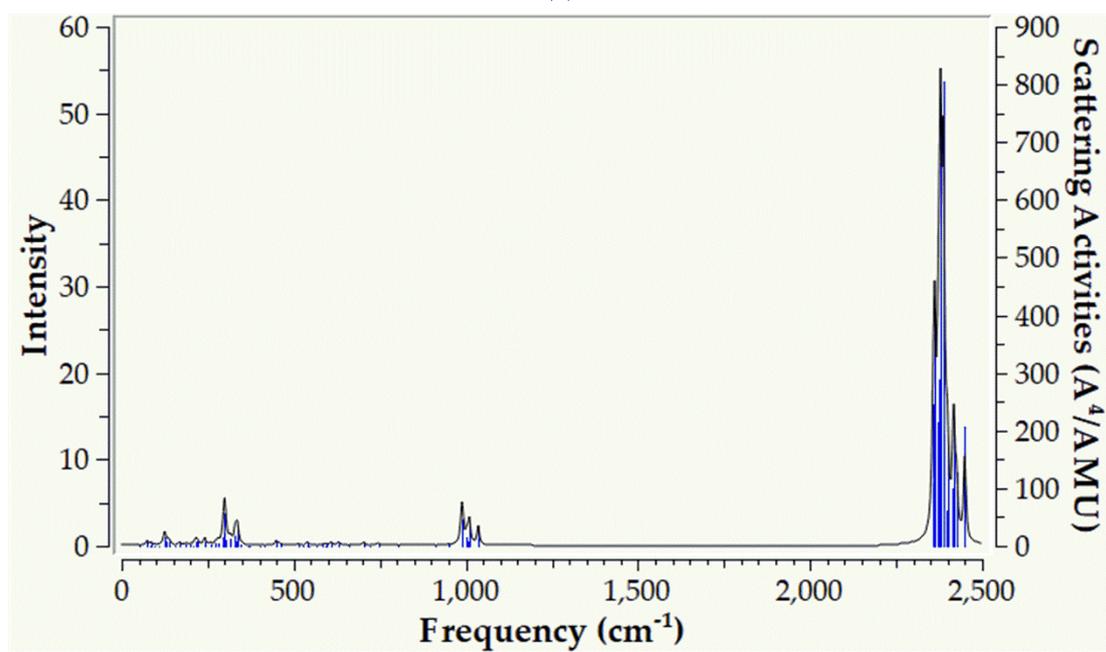
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Figure S5: Simulated IR spectra of 4''_Os (a) and 5''_Os (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

Figure S6: NTO pairs for the most significant electronic transitions of the simulated absorption spectra of **4** (hole, h^+ at the left, electron, e^- at the right).

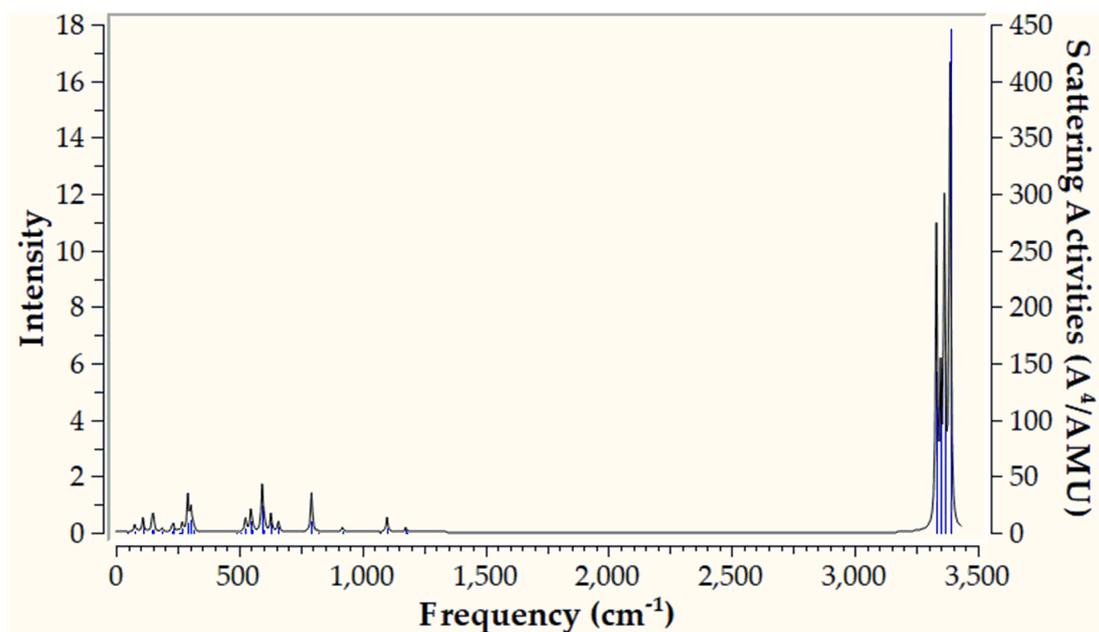


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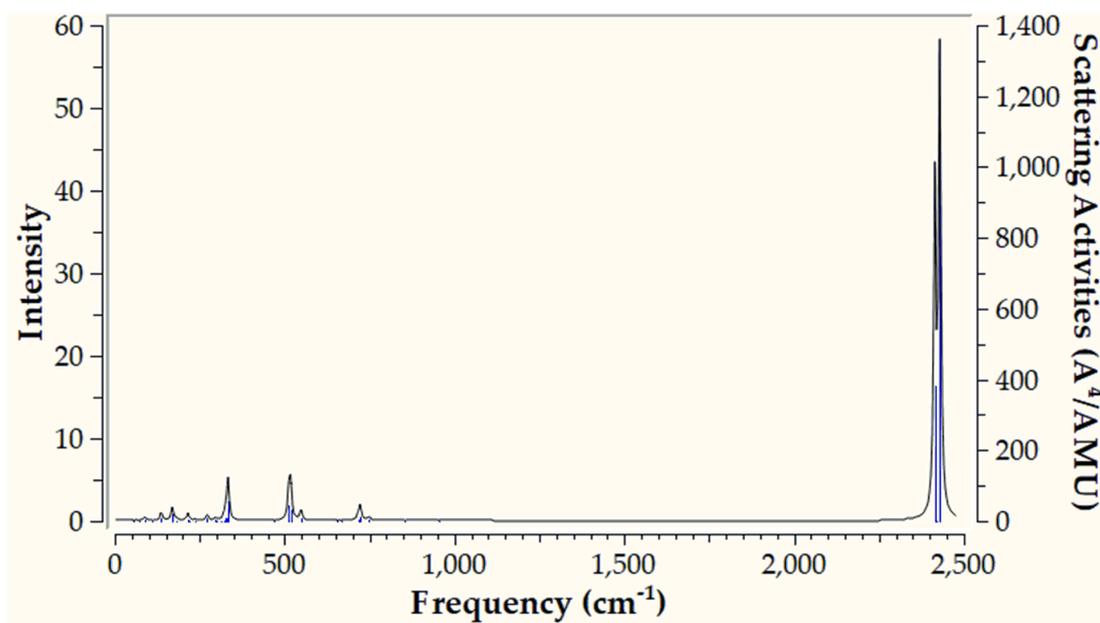


(b)

Figure S7: Simulated IR spectra of 6''_Os (a) and 7''_Os (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

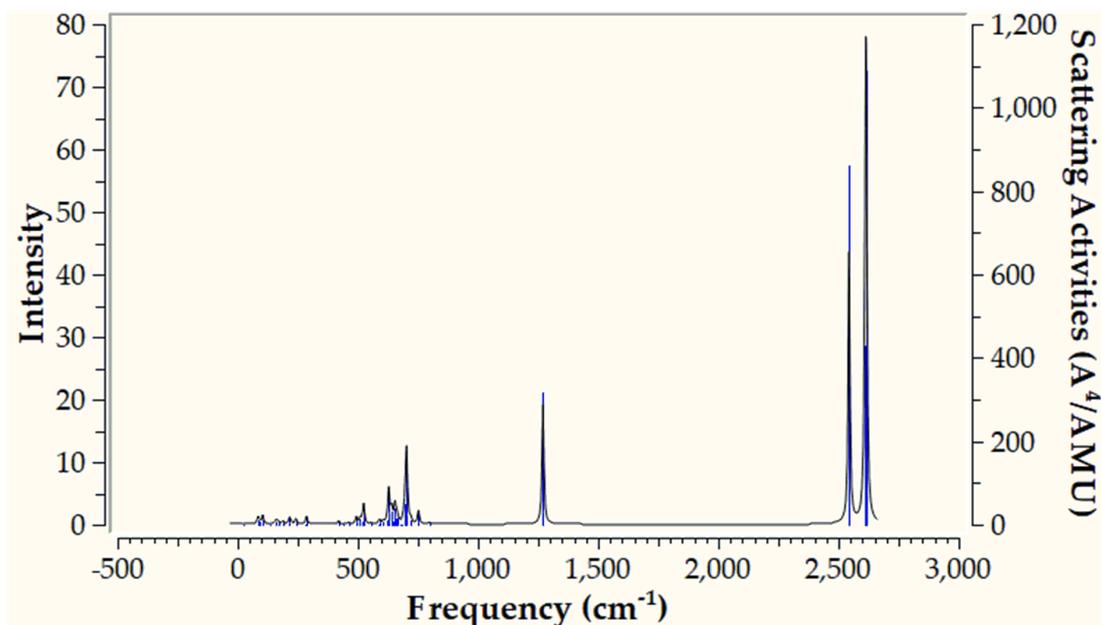


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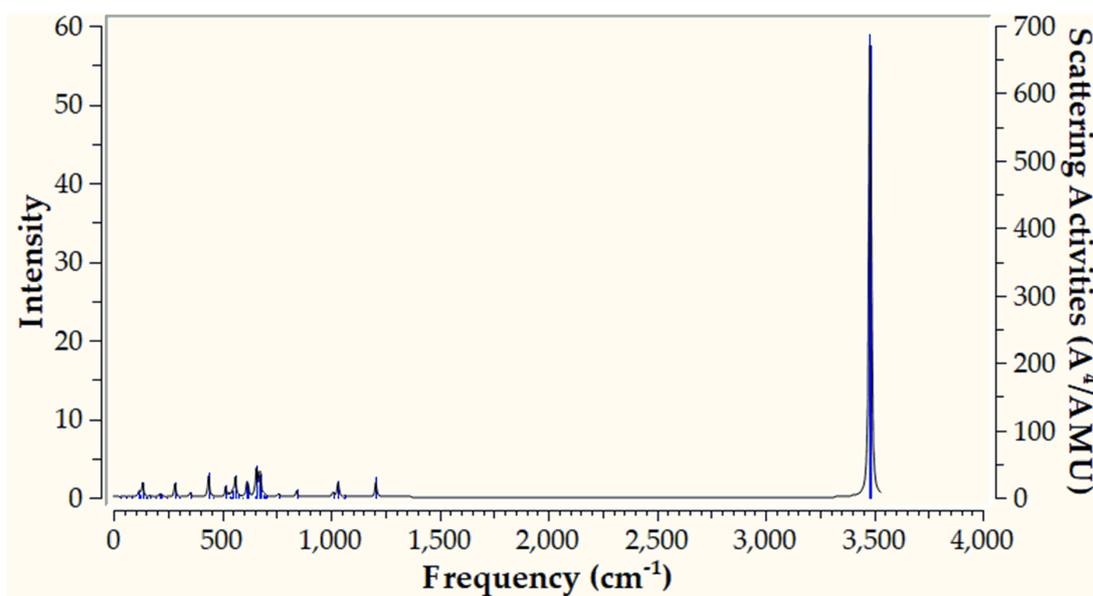


(b)

Figure S8: Simulated Raman spectra of 4''_Ru (a) and 5''_Ru (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

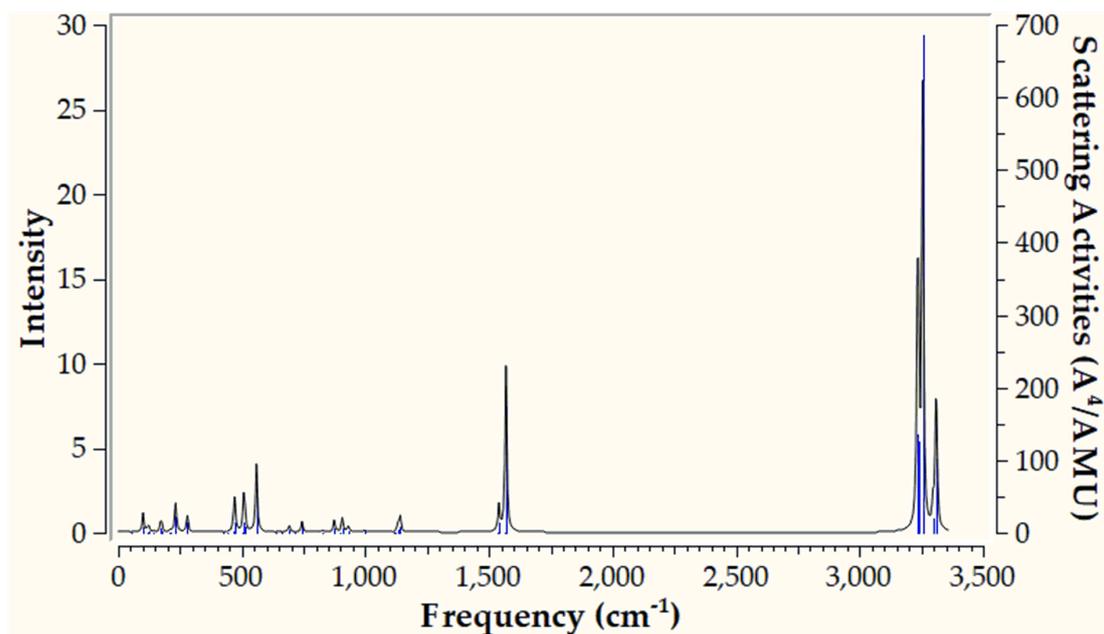


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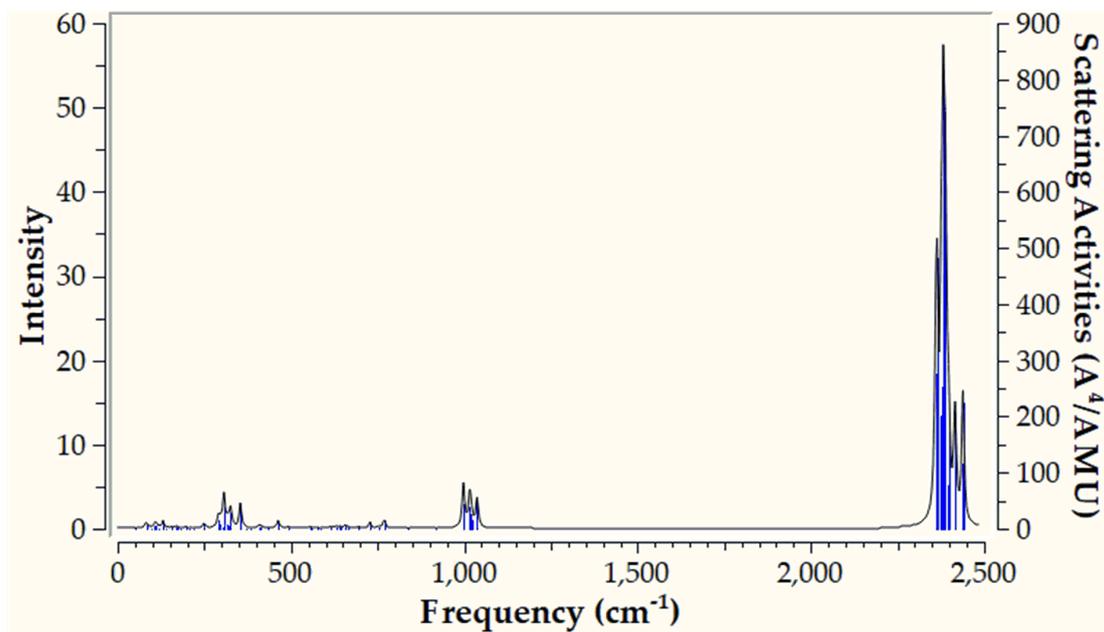


(b)

Figure S9: Simulated Raman spectra of $6''\text{-Ru}$ (a) and $7''\text{-Ru}$ (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

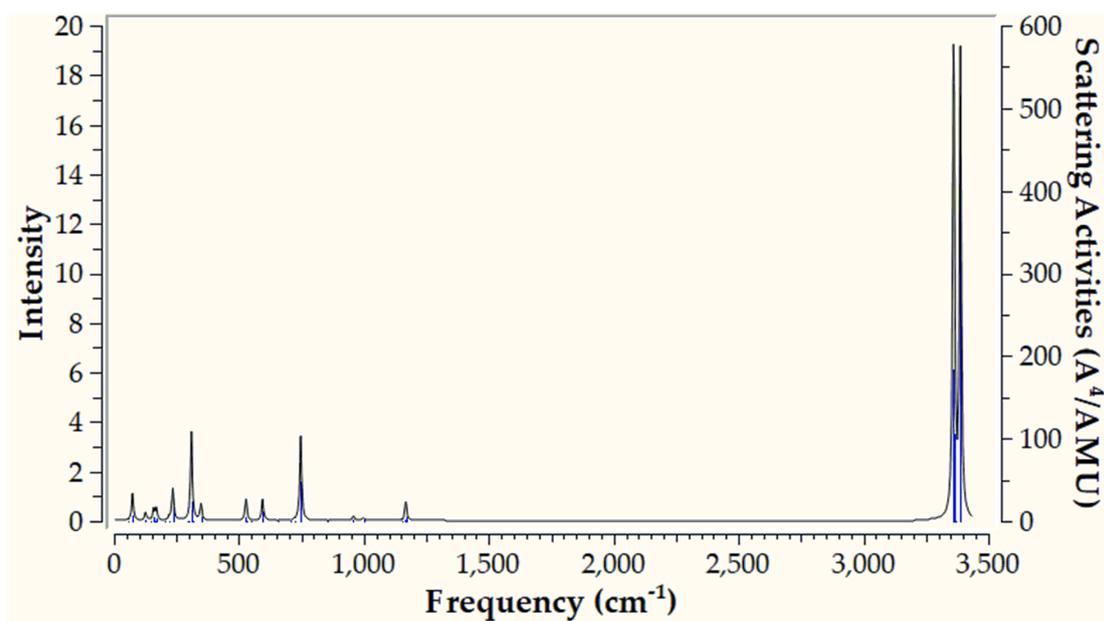


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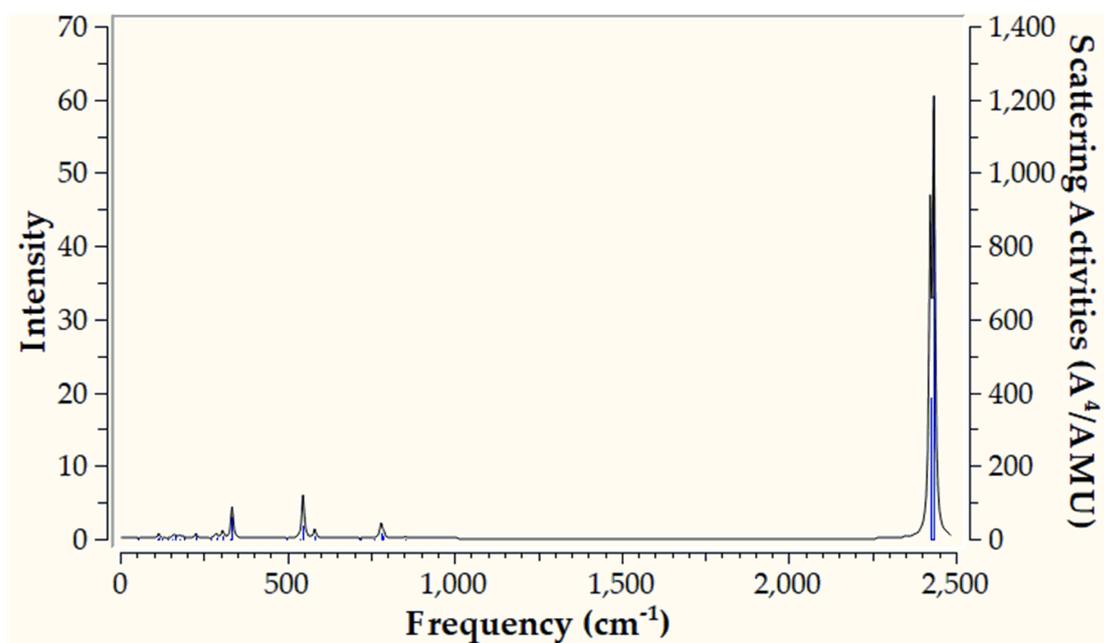


(b)

Figure S10: Simulated Raman spectra of 2''_Os (a) and 3''_Os (a) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

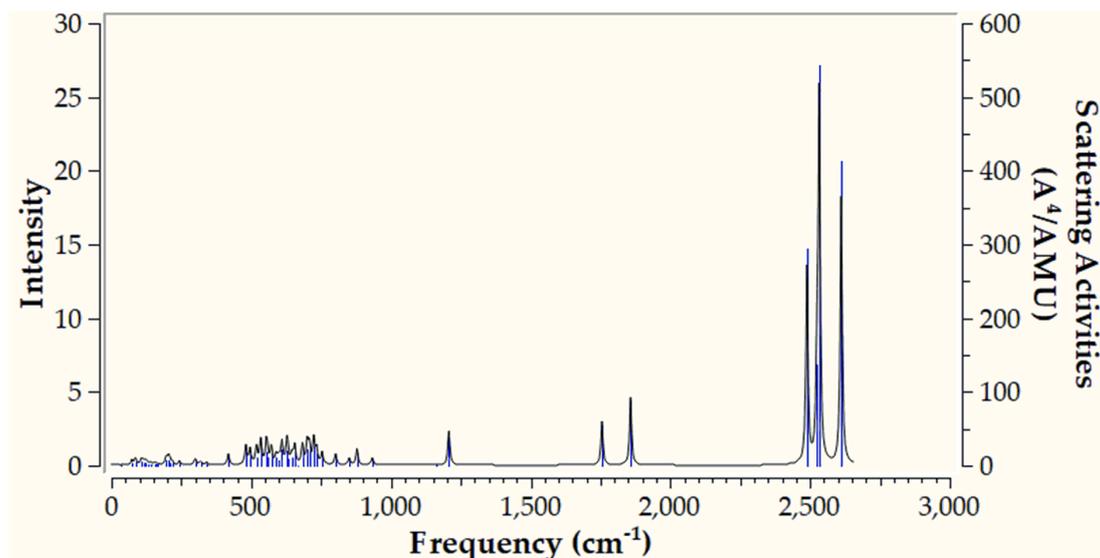


(a)

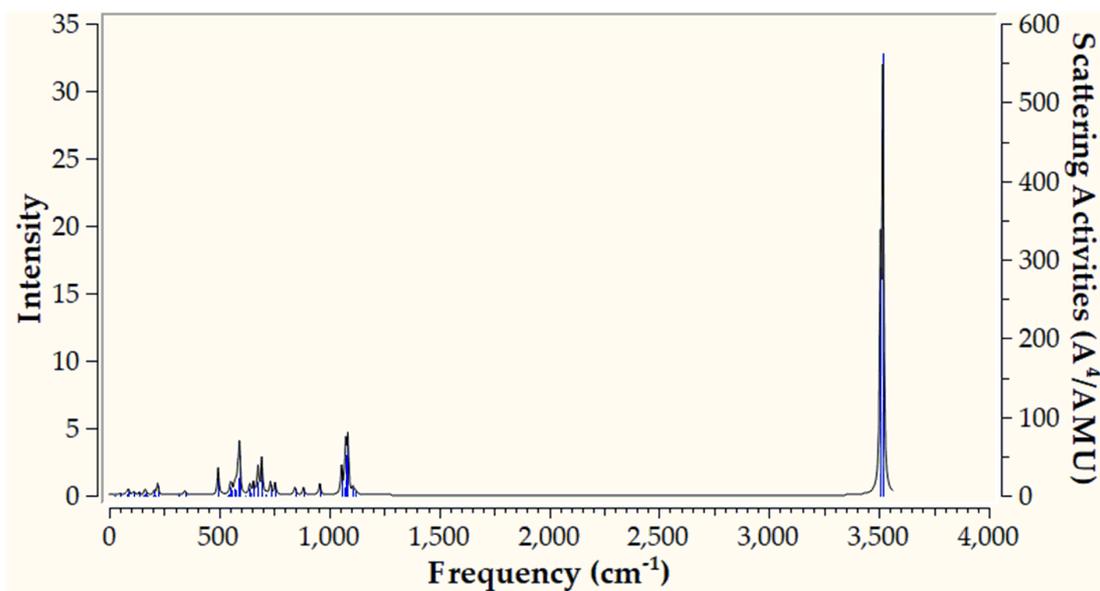


(b)

Figure S11: Simulated Raman spectra of 4''_Os (a) and 5''_Os (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.



(a)



(b)

Figure S12: Simulated Raman spectra of 6''_Os (a) and 7''_Os (b) calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase.

Table S1: Cartesian Coordinates and Energetic Data of the optimized geometries of all species calculated at the PBE0/LANL2DZ(M)U6-31G(d,p)(E) level of theory in the gas phase..

1_Ru			
Ru	-1.238788000	0.691362000	-0.566209000
Ru	0.002979000	-1.450228000	-0.556506000
Ru	1.236970000	0.696096000	-0.568372000
H	-0.005142000	2.701196000	-1.708965000
H	-0.004253000	1.294506000	-2.860023000
H	-1.151440000	-0.699381000	-2.848934000
H	-2.361013000	-1.395531000	-1.684424000
H	1.149453000	-0.695059000	-2.850921000
H	2.365078000	-1.385975000	-1.689756000
C	1.405043000	-0.835513000	-1.793441000
C	-1.403606000	-0.840873000	-1.790759000
C	-0.003794000	1.593725000	-1.804662000
Sum of electronic and zero-point Energies=			-402.267931
Sum of electronic and thermal Energies=			-402.260075
Sum of electronic and thermal Enthalpies=			-402.259131
Sum of electronic and thermal Free Energies=			-402.302219

2_Ru			
Ru	0.879694000	-1.261335000	0.231516000
Ru	0.879683000	1.261322000	0.231529000
Ru	-1.304117000	0.000004000	0.301073000
N	-0.685224000	-1.382593000	-0.950035000
N	1.707915000	0.000004000	-1.026305000
N	-0.685220000	1.382590000	-0.950039000
H	-1.201337000	-2.278741000	-0.906084000
H	-0.594053000	-1.169396000	-1.950712000
H	1.429507000	0.000007000	-2.015014000
H	2.742976000	0.000008000	-1.032263000
H	-0.594041000	1.169387000	-1.950714000
H	-1.201330000	2.278740000	-0.906094000
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Sum of electronic and thermal Energies=			-451.044821
Sum of electronic and thermal Enthalpies=			-451.043877
Sum of electronic and thermal Free Energies=			-451.086168

3_Ru			
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Ru	2.001577000	-1.155652000	0.068998000
Ru	-2.001578000	-1.155652000	0.068997000
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H	-1.718837000	0.991942000	-2.059887000
H	1.718836000	0.991941000	-2.059888000
H	2.887863000	1.667169000	-0.312701000
H	0.000001000	-1.983802000	-2.059872000
H	0.000000000	-3.334551000	-0.313291000
P	1.687831000	0.974355000	-0.640537000
P	-1.687831000	0.974356000	-0.640537000

P	0.000000000	-1.948744000	-0.640508000
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Sum of electronic and thermal Energies=			-1310.569917
Sum of electronic and thermal Enthalpies=			-1310.568973
Sum of electronic and thermal Free Energies=			-1310.622278

4_Ru

Ru	0.000000000	1.636857000	-0.157041000
Ru	1.417560000	-0.818429000	-0.157041000
Ru	-1.417560000	-0.818429000	-0.157041000
H	-2.022788000	1.167857000	1.453347000
H	2.022788000	1.167857000	1.453347000
H	0.000000000	-2.335715000	1.453347000
O	0.000000000	-1.714559000	0.682060000
O	-1.484852000	0.857280000	0.682060000
O	1.484852000	0.857280000	0.682060000
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Sum of electronic and thermal Energies=			-510.476718
Sum of electronic and thermal Enthalpies=			-510.475773
Sum of electronic and thermal Free Energies=			-510.519523

5_Ru

Ru	0.000000000	1.762081000	-0.294315000
Ru	1.526007000	-0.881041000	-0.294315000
Ru	-1.526007000	-0.881041000	-0.294315000
H	-2.174265000	1.255312000	1.957911000
H	2.174265000	1.255312000	1.957911000
H	0.000000000	-2.510625000	1.957911000
S	1.721966000	0.994177000	0.686997000
S	0.000000000	-1.988355000	0.686997000
S	-1.721966000	0.994177000	0.686997000
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Sum of electronic and thermal Energies=			-1479.262970
Sum of electronic and thermal Enthalpies=			-1479.262026
Sum of electronic and thermal Free Energies=			-1479.311488

6_Ru

Ru	-1.420589000	-0.379781000	-0.178955000
Ru	0.381334000	1.419574000	-0.179179000
Ru	1.039143000	-1.040023000	-0.179037000
H	-0.540317000	-2.007163000	2.154534000
H	-1.469371000	1.474476000	2.152911000
H	2.011906000	0.537189000	2.153081000
B	-1.005780000	1.006213000	1.144743000
B	1.374793000	0.367671000	1.144829000
B	-0.368477000	-1.372754000	1.145436000
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Sum of electronic and thermal Energies=			-357.699092
Sum of electronic and thermal Enthalpies=			-357.698148
Sum of electronic and thermal Free Energies=			-357.741305

7_Ru

Ru	0.000000000	1.571258000	-0.132865000
Ru	-1.360749000	-0.785629000	-0.132865000
Ru	1.360749000	-0.785629000	-0.132865000
H	-2.014490000	1.163066000	1.507297000
H	0.000000000	-2.326133000	1.507297000
H	2.014490000	1.163066000	1.507297000
N	1.570594000	0.906783000	0.619820000
N	-1.570594000	0.906783000	0.619820000
N	0.000000000	-1.813566000	0.619820000
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Sum of electronic and thermal Energies=			-447.283559
Sum of electronic and thermal Enthalpies=			-447.282615
Sum of electronic and thermal Free Energies=			-447.325071

1_Os

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Os	-1.004663000	1.078966000	0.000000000
Os	0.350072000	-0.658166000	-1.271823000
C	0.350072000	1.343717000	-1.462381000
C	0.350072000	1.343717000	1.462381000
C	1.907845000	-0.654596000	0.000000000
H	2.515307000	-1.582878000	0.000000000
H	2.553470000	0.233180000	0.000000000
H	1.275245000	1.872731000	-1.199526000
H	-0.061863000	1.723507000	-2.419910000
H	-0.061863000	1.723507000	2.419910000
H	1.275245000	1.872731000	1.199526000
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Sum of electronic and thermal Energies=			-390.568656
Sum of electronic and thermal Enthalpies=			-390.567712
Sum of electronic and thermal Free Energies=			-390.613627

2_Os

Os	0.357813000	-0.675073000	1.299305000
Os	-1.054098000	1.077467000	0.000000000
Os	0.357813000	-0.675073000	-1.299305000
N	0.357813000	1.329573000	-1.404599000
N	0.357813000	1.329573000	1.404599000
N	1.884077000	-0.564767000	0.000000000
H	2.535750000	-1.367801000	0.000000000
H	2.488154000	0.267001000	0.000000000
H	1.214699000	1.847448000	-1.171932000
H	0.036284000	1.734408000	-2.300086000
H	0.036284000	1.734408000	2.300086000
H	1.214699000	1.847448000	1.171932000
Sum of electronic and zero-point Energies=			-439.327823
Sum of electronic and thermal Energies=			-439.320200
Sum of electronic and thermal Enthalpies=			-439.319256
Sum of electronic and thermal Free Energies=			-439.363980

3_Os

Os	0.286238000	-0.765051000	1.326970000
Os	-1.216082000	0.974419000	0.000000000
Os	0.286238000	-0.765051000	-1.326970000
P	0.286238000	1.491888000	-1.631533000
P	0.286238000	1.491888000	1.631533000
P	2.133458000	-0.647524000	0.000000000
H	2.988342000	-1.778269000	0.000000000
H	2.966217000	0.491496000	0.000000000
H	1.430544000	2.269964000	-1.355844000
H	-0.245268000	1.967517000	-2.856559000
H	-0.245268000	1.967517000	2.856559000
H	1.430544000	2.269964000	1.355844000
Sum of electronic and zero-point Energies=			-1298.977919
Sum of electronic and thermal Energies=			-1298.967895
Sum of electronic and thermal Enthalpies=			-1298.966951
Sum of electronic and thermal Free Energies=			-1299.016401

4_Os

Os	0.000000000	1.647684000	-0.100791000
Os	1.426936000	-0.823842000	-0.100791000
Os	-1.426936000	-0.823842000	-0.100791000
H	-2.063421000	1.191317000	1.536128000
H	2.063421000	1.191317000	1.536128000
H	0.000000000	-2.382634000	1.536128000
O	0.000000000	-1.759100000	0.765503000
O	-1.523425000	0.879550000	0.765503000
O	1.523425000	0.879550000	0.765503000
Sum of electronic and zero-point Energies=			-498.719070
Sum of electronic and thermal Energies=			-498.710500
Sum of electronic and thermal Enthalpies=			-498.709555
Sum of electronic and thermal Free Energies=			-498.757380

5_Os

Os	0.000000000	1.743936000	-0.193087000
Os	1.510293000	-0.871968000	-0.193087000
Os	-1.510293000	-0.871968000	-0.193087000
H	-2.339430000	1.350671000	2.007445000
H	2.339430000	1.350671000	2.007445000
H	0.000000000	-2.701341000	2.007445000
S	1.781186000	1.028368000	0.791698000
S	0.000000000	-2.056737000	0.791698000
S	-1.781186000	1.028368000	0.791698000
Sum of electronic and zero-point Energies=			-1467.524024
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Sum of electronic and thermal Enthalpies=			-1467.512645
Sum of electronic and thermal Free Energies=			-1467.566472

6_Os

Os	0.000000000	1.458347000	-0.107829000
Os	1.262965000	-0.729173000	-0.107829000

Os	-1.262965000	-0.729173000	-0.107829000
B	-1.345343000	0.776734000	1.199780000
H	-1.922831000	1.110147000	2.196137000
B	0.000000000	-1.553468000	1.199780000
H	0.000000000	-2.220294000	2.196137000
B	1.345343000	0.776734000	1.199780000
H	1.922831000	1.110147000	2.196137000
Sum of electronic and zero-point Energies=			-349.172553
Sum of electronic and thermal Energies=			-349.164712
Sum of electronic and thermal Enthalpies=			-349.163768
Sum of electronic and thermal Free Energies=			-349.207570

7_Os

H	0.789752000	3.087537000	0.416259000
H	-3.069444000	-0.860307000	0.414346000
H	2.281370000	-2.226038000	0.415353000
N	1.578561000	-1.540274000	0.164325000
N	0.546464000	2.136629000	0.163780000
N	-2.123961000	-0.595929000	0.162643000
Os	1.311744000	0.368265000	-0.020717000
Os	-0.336864000	-1.320040000	-0.020463000
Os	-0.975000000	0.951721000	-0.020415000
Sum of electronic and zero-point Energies=			-437.840238
Sum of electronic and thermal Energies=			-437.831856
Sum of electronic and thermal Enthalpies=			-437.830912
Sum of electronic and thermal Free Energies=			-437.877531

1'_Ru

Ru	-1.397397000	0.695944000	-0.830672000
Ru	0.000000000	-1.407791000	-1.176640000
Ru	1.397397000	0.695944000	-0.830672000
N	0.000000000	0.156968000	0.516859000
N	0.000000000	0.112768000	1.680440000
H	0.000000000	2.724871000	-1.749340000
H	0.000000000	1.380178000	-2.966439000
H	-1.718520000	-0.632906000	-3.077301000
H	-2.463057000	-1.518467000	-1.629456000
H	1.718520000	-0.632906000	-3.077301000
H	2.463057000	-1.518467000	-1.629456000
C	1.655922000	-0.839261000	-1.999822000
C	-1.655922000	-0.839261000	-1.999822000
C	0.000000000	1.622387000	-1.892020000
Sum of electronic and zero-point Energies=			-511.643411
Sum of electronic and thermal Energies=			-511.632497
Sum of electronic and thermal Enthalpies=			-511.631553
Sum of electronic and thermal Free Energies=			-511.682228

2'_Ru

Ru	1.007995000	-1.298073000	0.136082000
Ru	1.007995000	1.298073000	0.136082000
Ru	-1.899533000	0.000000000	-0.125948000
N	-0.730507000	-1.455216000	-0.869275000
N	1.837539000	0.000000000	-1.066903000
N	-0.730508000	1.455215000	-0.869276000
N	-0.140895000	0.000000000	1.193834000
N	-1.093568000	0.000001000	1.873107000
H	-1.142798000	-2.385383000	-0.687180000
H	-0.633617000	-1.424368000	-1.892852000
H	1.561106000	0.000000000	-2.057966000
H	2.873198000	0.000000000	-1.045873000
H	-0.633618000	1.424367000	-1.892852000
H	-1.142798000	2.385382000	-0.687181000
Sum of electronic and zero-point Energies=			-560.419690
Sum of electronic and thermal Energies=			-560.409867
Sum of electronic and thermal Enthalpies=			-560.408923
Sum of electronic and thermal Free Energies=			-560.456501

3'_Ru

Ru	0.000000000	1.652326000	0.226234000
Ru	1.430956000	-0.826163000	0.226234000
Ru	-1.430956000	-0.826163000	0.226234000
N	0.000000000	0.000000000	2.743308000
N	0.000000000	0.000000000	1.600139000
H	-2.857274000	1.649648000	-0.975747000
H	-1.418258000	0.818832000	-2.499564000
H	1.418258000	0.818832000	-2.499564000
H	2.857274000	1.649648000	-0.975747000
H	0.000000000	-1.637664000	-2.499564000
H	0.000000000	-3.299296000	-0.975747000
P	1.632500000	0.942524000	-1.107579000
P	-1.632500000	0.942524000	-1.107579000
P	0.000000000	-1.885048000	-1.107579000
Sum of electronic and zero-point Energies=			-1420.048382
Sum of electronic and thermal Energies=			-1420.035033
Sum of electronic and thermal Enthalpies=			-1420.034088
Sum of electronic and thermal Free Energies=			-1420.089861

4'_Ru

Ru	-0.352124000	1.605467000	0.070459000
Ru	-1.572420000	-0.891074000	0.432003000
Ru	1.193528000	-0.746047000	-0.298628000
H	1.194668000	1.254725000	-2.013025000
H	-2.738897000	1.058826000	-0.880083000
H	-0.626369000	-2.300986000	-1.543773000
O	-0.421892000	-1.623838000	-0.856674000
O	0.910306000	0.931612000	-1.124078000
O	-2.005139000	0.790661000	-0.273897000
N	2.853588000	-0.082398000	0.694055000

N	3.784858000	0.167075000	1.235283000
Sum of electronic and zero-point Energies=			-619.937302
Sum of electronic and thermal Energies=			-619.926499
Sum of electronic and thermal Enthalpies=			-619.925555
Sum of electronic and thermal Free Energies=			-619.976398

5'_Ru

Ru	-0.015537000	1.493862000	-0.275596000
Ru	1.057515000	-0.819466000	0.123119000
Ru	-1.358859000	-0.649778000	-0.767269000
H	-2.088253000	0.780483000	1.756436000
H	0.061308000	0.584565000	2.552622000
H	-1.186142000	-1.469420000	2.114357000
S	1.005045000	0.869218000	1.610026000
S	-0.764147000	-1.982014000	0.923103000
S	-2.096678000	1.092168000	0.426726000
N	2.849844000	-0.154504000	-0.732968000
N	3.842777000	0.061823000	-1.168788000
Sum of electronic and zero-point Energies=			-1588.769556
Sum of electronic and thermal Energies=			-1588.757664
Sum of electronic and thermal Enthalpies=			-1588.756720
Sum of electronic and thermal Free Energies=			-1588.809676

6'_Ru

Ru	0.000000000	1.571351000	-0.014990000
Ru	-1.360830000	-0.785676000	-0.014990000
Ru	1.360830000	-0.785676000	-0.014990000
B	-1.291117000	0.745427000	-1.223081000
B	0.000000000	-1.490853000	-1.223081000
B	1.291117000	0.745427000	-1.223081000
H	-1.841367000	1.063114000	-2.248861000
H	0.000000000	-2.126228000	-2.248861000
H	1.841367000	1.063114000	-2.248861000
N	0.000000000	0.000000000	1.351078000
N	0.000000000	0.000000000	2.516284000
Sum of electronic and zero-point Energies=			-467.081877
Sum of electronic and thermal Energies=			-467.071441
Sum of electronic and thermal Enthalpies=			-467.070497
Sum of electronic and thermal Free Energies=			-467.117871

7'_Ru

N	-1.072522000	-0.498625000	0.000000000
N	-2.094638000	0.120182000	0.000000000
H	1.155379000	1.529952000	1.909772000
H	2.384008000	-1.259810000	0.000000000
H	1.155379000	1.529952000	-1.909772000
N	0.306744000	1.033263000	-1.611287000
N	0.306744000	1.033263000	1.611287000
N	1.359415000	-1.244567000	0.000000000
Ru	0.306744000	-0.869256000	-1.505170000
Ru	0.306744000	-0.869256000	1.505170000

Ru	-0.530192000	1.627041000	0.000000000
Sum of electronic and zero-point Energies=			-556.629690
Sum of electronic and thermal Energies=			-556.620519
Sum of electronic and thermal Enthalpies=			-556.619575
Sum of electronic and thermal Free Energies=			-556.665653

1'_Os

Os	0.937167000	-1.036200000	0.021351000
Os	-1.452595000	-0.377234000	-0.178308000
Os	0.249970000	1.367608000	0.036139000
H	2.031511000	0.493410000	1.916596000
H	0.325554000	0.081978000	2.389355000
H	-2.396986000	1.906564000	1.133603000
H	-2.291494000	1.605957000	-0.689330000
H	-1.044293000	-2.782452000	-0.266501000
H	-0.916814000	-2.508759000	1.536257000
C	-1.785849000	1.501546000	0.324547000
C	-0.710000000	-2.088014000	0.548462000
C	1.020065000	0.242784000	1.559217000
N	2.751288000	0.065899000	-0.973713000
N	2.009010000	0.898126000	-0.659310000
Sum of electronic and zero-point Energies=			-499.030288
Sum of electronic and thermal Energies=			-499.019593
Sum of electronic and thermal Enthalpies=			-499.018649
Sum of electronic and thermal Free Energies=			-499.069295

2'_Os

Os	-1.116046000	0.779447000	-0.195361000
Os	0.115680000	-1.494740000	0.067946000
Os	1.429867000	0.713115000	0.374976000
N	1.790152000	-0.853954000	-0.831510000
N	-0.941560000	-0.764537000	-1.468322000
N	0.497895000	1.653536000	-1.128640000
H	0.549270000	2.683275000	-1.090292000
H	0.752331000	1.416754000	-2.094282000
H	1.789416000	-0.714554000	-1.849574000
H	2.652230000	-1.388565000	-0.634122000
H	-1.811219000	-1.267056000	-1.702651000
H	-0.472699000	-0.602694000	-2.367564000
N	-2.782538000	0.111127000	0.799832000
N	-3.721294000	-0.140688000	1.332053000
Sum of electronic and zero-point Energies=			-548.785202
Sum of electronic and thermal Energies=			-548.774923
Sum of electronic and thermal Enthalpies=			-548.773979
Sum of electronic and thermal Free Energies=			-548.824591

3'_Os

Os	0.000005000	2.112346000	0.292289000
Os	1.584185000	-0.889524000	0.517527000
Os	-1.584126000	-0.889510000	0.517582000
N	-0.000121000	-0.684829000	1.808351000

N	-0.00002000	0.319256000	1.022829000
H	-2.950546000	1.658700000	-0.697831000
H	-1.557634000	0.803159000	-2.216023000
H	1.557652000	0.803201000	-2.216045000
H	2.950562000	1.658731000	-0.697848000
H	-0.00004000	-1.712372000	-2.152956000
H	0.00008000	-3.347195000	-0.632501000
P	1.674508000	1.052343000	-0.829112000
P	-1.674489000	1.052318000	-0.829093000
P	0.00003000	-1.936624000	-0.758944000
Sum of electronic and zero-point Energies=			-1407.352488
Sum of electronic and thermal Energies=			-1407.340911
Sum of electronic and thermal Enthalpies=			-1407.339967
Sum of electronic and thermal Free Energies=			-1407.392764

4'_Os

Os	-1.242631000	-0.673718000	-0.148070000
Os	1.317411000	-0.842357000	0.248511000
Os	0.300961000	1.429745000	-0.113754000
N	-3.404048000	0.575006000	1.685209000
N	-2.603977000	0.171937000	1.032374000
H	-1.265731000	1.139213000	-2.320384000
H	0.582087000	-2.291442000	-1.860615000
H	2.917897000	1.329194000	0.544671000
O	-0.957771000	0.899313000	-1.412177000
O	0.349150000	-1.710028000	-1.098343000
O	2.016816000	0.955151000	0.713655000
Sum of electronic and zero-point Energies=			-608.230198
Sum of electronic and thermal Energies=			-608.219445
Sum of electronic and thermal Enthalpies=			-608.218501
Sum of electronic and thermal Free Energies=			-608.269921

5'_Os

N	-0.749228000	-0.237720000	0.000000000
N	-0.871443000	-1.512516000	0.000000000
Os	-1.106434000	1.664877000	0.000000000
Os	0.316879000	-0.933501000	1.577796000
Os	0.316879000	-0.933501000	-1.577796000
H	1.564457000	1.830730000	-1.419964000
H	1.564457000	1.830730000	1.419964000
H	2.788520000	-0.212896000	0.000000000
S	0.316879000	1.399122000	-1.767925000
S	0.316879000	1.399122000	1.767925000
S	1.950655000	-1.287960000	0.000000000
Sum of electronic and zero-point Energies=			-1575.983904
Sum of electronic and thermal Energies=			-1575.972897
Sum of electronic and thermal Enthalpies=			-1575.971953
Sum of electronic and thermal Free Energies=			-1576.024194

6'_Os

Os	2.465937000	-0.000070000	0.449066000
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Os	-1.527057000	-2.352960000	-0.032625000
Os	-1.526909000	2.353041000	-0.032628000
N	4.214781000	-0.000081000	-2.089851000
N	3.489652000	-0.000075000	-1.245664000
H	1.413706000	2.511028000	-1.296542000
H	1.486314000	2.994496000	0.722850000
H	1.486151000	-2.994597000	0.722786000
H	1.413538000	-2.511078000	-1.296594000
H	-3.493288000	0.000102000	0.898250000
H	-3.385230000	0.000097000	-1.184151000
S	1.006778000	-1.975805000	-0.089181000
S	1.006900000	1.975748000	-0.089147000
S	-2.523802000	0.000070000	-0.095911000
Sum of electronic and zero-point Energies=			-1576.089588
Sum of electronic and thermal Energies=			-1576.074626
Sum of electronic and thermal Enthalpies=			-1576.073682
Sum of electronic and thermal Free Energies=			-1576.138804

7'_Os

Os	-1.472270000	-0.686466000	-0.101450000
Os	1.472489000	-0.686210000	-0.101273000
Os	-0.000245000	1.492602000	0.199229000
B	-1.375354000	1.019282000	-1.127826000
B	1.375852000	1.019854000	-1.126906000
B	0.000374000	-1.175316000	-1.406017000
H	-2.005974000	1.424437000	-2.064659000
H	2.007864000	1.423360000	-2.063523000
H	0.000342000	-1.545344000	-2.552155000
N	0.000252000	-0.868214000	1.248793000
N	-0.000907000	-1.236914000	2.358301000
Sum of electronic and zero-point Energies=			-458.511551
Sum of electronic and thermal Energies=			-458.501413
Sum of electronic and thermal Enthalpies=			-458.500469
Sum of electronic and thermal Free Energies=			-458.550264

8'_Os

N	0.007565000	0.000000000	1.024686000
N	-1.010678000	0.000000000	1.784009000
Os	-1.720391000	0.000000000	-0.066626000
Os	0.900960000	1.504132000	0.031681000
Os	0.900960000	-1.504132000	0.031681000
H	-1.033586000	2.002105000	-1.623471000
H	2.281548000	0.000000000	-1.582040000
H	-1.033586000	-2.002105000	-1.623471000
N	-0.853226000	-1.601217000	-0.699736000
N	-0.853226000	1.601217000	-0.699736000
N	1.793770000	0.000000000	-0.683926000
Sum of electronic and zero-point Energies=			-547.112720
Sum of electronic and thermal Energies=			-547.103910
Sum of electronic and thermal Enthalpies=			-547.102966
Sum of electronic and thermal Free Energies=			-547.150067

1''_Ru			
Ru	1.578286000	0.911224000	1.252425000
Ru	0.000000000	-1.822448000	1.252425000
Ru	-1.578286000	0.911224000	1.252425000
Ru	-1.578286000	0.911224000	-1.252425000
Ru	0.000000000	-1.822448000	-1.252425000
Ru	1.578286000	0.911224000	-1.252425000
N	0.000000000	0.000000000	-0.681730000
N	0.000000000	0.000000000	0.681730000
H	0.000000000	2.912686000	1.047611000
H	0.000000000	2.399663000	2.820956000
H	2.078169000	-1.199831000	2.820956000
H	2.522460000	-1.456343000	1.047611000
H	-2.078169000	-1.199831000	2.820956000
H	-2.522460000	-1.456343000	1.047611000
H	0.000000000	2.912686000	-1.047611000
H	0.000000000	2.399663000	-2.820956000
H	-2.078169000	-1.199831000	-2.820956000
H	-2.522460000	-1.456343000	-1.047611000
H	2.078169000	-1.199831000	-2.820956000
H	2.522460000	-1.456343000	-1.047611000
C	1.794606000	-1.036116000	1.766222000
C	1.794606000	-1.036116000	-1.766222000
C	-1.794606000	-1.036116000	-1.766222000
C	0.000000000	2.072232000	-1.766222000
C	0.000000000	2.072232000	1.766222000
C	-1.794606000	-1.036116000	1.766222000
Sum of electronic and zero-point Energies=			-913.948986
Sum of electronic and thermal Energies=			-913.929834
Sum of electronic and thermal Enthalpies=			-913.928890
Sum of electronic and thermal Free Energies=			-913.993185

2''_Ru			
Ru	1.192322000	0.000240000	1.783919000
Ru	1.400544000	1.629703000	-0.917976000
Ru	1.400730000	-1.629746000	-0.917679000
N	1.813375000	-1.842244000	1.053254000
N	1.813023000	1.842663000	1.052959000
N	2.175922000	-0.000049000	-1.832715000
Ru	-1.401426000	-1.627895000	-0.916674000
Ru	-1.401623000	1.627541000	-0.917012000
Ru	-1.182704000	0.000146000	1.790456000
N	-1.830785000	-1.825201000	1.051522000
N	-2.179408000	-0.000326000	-1.829539000
N	-1.830976000	1.825226000	1.051152000
N	-0.675610000	-0.000049000	-0.057291000
N	0.682584000	0.000020000	-0.058231000
H	1.376281000	-2.717168000	1.410060000
H	2.831961000	-2.023862000	1.203032000
H	2.831571000	2.024453000	1.202799000
H	1.375767000	2.717609000	1.409499000

H	3.223062000	0.000007000	-1.793439000
H	1.980563000	-0.000150000	-2.861654000
H	-1.409443000	-2.702703000	1.421489000
H	-2.852813000	-1.990753000	1.196782000
H	-3.226363000	-0.000409000	-1.785614000
H	-1.989816000	-0.000405000	-2.859560000
H	-2.853017000	1.990721000	1.196392000
H	-1.409724000	2.702836000	1.420957000
Sum of electronic and zero-point Energies=			-1010.558779
Sum of electronic and thermal Energies=			-1010.540495
Sum of electronic and thermal Enthalpies=			-1010.539551
Sum of electronic and thermal Free Energies=			-1010.606228

3''_Ru

Ru	2.429895000	-0.450887000	-0.000098000
Ru	-0.478401000	-1.381298000	-1.669929000
Ru	-0.478160000	-1.380736000	1.670460000
Ru	-1.454438000	0.801174000	1.322869000
Ru	-1.454628000	0.800732000	-1.322930000
Ru	1.505617000	1.982546000	-0.000439000
N	-0.068165000	0.743139000	-0.000120000
N	0.384302000	-0.592317000	0.000071000
H	2.443954000	-0.920817000	3.082432000
H	2.307301000	-2.925486000	1.980859000
H	2.307016000	-2.926156000	-1.980203000
H	2.443515000	-0.921856000	-3.082469000
H	-0.500942000	-4.098295000	0.000724000
H	-2.587516000	-3.193823000	0.000719000
H	1.280828000	2.251398000	3.064562000
H	-0.112523000	3.714112000	2.040057000
H	-4.252584000	1.478553000	0.000060000
H	-4.276577000	-0.800241000	0.000444000
H	-0.112801000	3.713426000	-2.041296000
H	1.280391000	2.250352000	-3.065502000
P	1.832506000	-1.578335000	-1.971655000
P	0.291759000	2.343886000	-2.044306000
P	-3.411376000	0.324355000	0.000189000
P	0.292047000	2.344575000	2.043478000
P	1.832789000	-1.577669000	1.971926000
P	-1.204923000	-2.858431000	0.000565000
Sum of electronic and zero-point Energies=			-2729.888699
Sum of electronic and thermal Energies=			-2729.864724
Sum of electronic and thermal Enthalpies=			-2729.863779
Sum of electronic and thermal Free Energies=			-2729.940827

4''_Ru

Ru	1.549041000	0.894339000	-1.395720000
Ru	-1.549041000	0.894339000	-1.395720000
Ru	0.000000000	-1.788679000	-1.395720000
Ru	0.000000000	-1.817311000	1.352407000
Ru	-1.573838000	0.908656000	1.352407000

Ru	1.573838000	0.908656000	1.352407000
N	0.000000000	0.000000000	0.606894000
N	0.000000000	0.000000000	-0.748454000
H	2.432643000	-1.404487000	-2.431232000
H	0.000000000	2.808974000	-2.431232000
H	-2.432643000	-1.404487000	-2.431232000
H	2.213659000	-1.278057000	2.710509000
H	-2.213659000	-1.278057000	2.710509000
H	0.000000000	2.556113000	2.710509000
O	1.854237000	-1.070544000	-1.682932000
O	0.000000000	2.141089000	-1.682932000
O	0.000000000	1.926493000	1.927529000
O	1.668392000	-0.963247000	1.927529000
O	-1.854237000	-1.070544000	-1.682932000
O	-1.668392000	-0.963247000	1.927529000
Sum of electronic and zero-point Energies=			-1129.539605
Sum of electronic and thermal Energies=			-1129.521469
Sum of electronic and thermal Enthalpies=			-1129.520525
Sum of electronic and thermal Free Energies=			-1129.585811

5''_Ru

Ru	0.000000000	1.922689000	1.254660000
Ru	0.000000000	1.922689000	-1.254660000
Ru	1.665098000	-0.961345000	1.254660000
Ru	1.665098000	-0.961345000	-1.254660000
Ru	-1.665098000	-0.961345000	-1.254660000
Ru	-1.665098000	-0.961345000	1.254660000
N	0.000000000	0.000000000	0.704986000
N	0.000000000	0.000000000	-0.704986000
H	-2.453423000	1.416485000	3.108590000
H	0.000000000	-2.832969000	3.108590000
H	0.000000000	-2.832969000	-3.108590000
H	2.453423000	1.416485000	-3.108590000
H	-2.453423000	1.416485000	-3.108590000
H	2.453423000	1.416485000	3.108590000
S	-2.137989000	1.234368000	1.771068000
S	-2.137989000	1.234368000	-1.771068000
S	2.137989000	1.234368000	1.771068000
S	2.137989000	1.234368000	-1.771068000
S	0.000000000	-2.468737000	1.771068000
S	0.000000000	-2.468737000	-1.771068000
Sum of electronic and zero-point Energies=			-3067.242550
Sum of electronic and thermal Energies=			-3067.221250
Sum of electronic and thermal Enthalpies=			-3067.220306
Sum of electronic and thermal Free Energies=			-3067.290726

6''_Ru

Ru	1.452448000	-0.738337000	2.018649000
Ru	-1.453097000	-0.737379000	2.017160000
Ru	0.000704000	1.372216000	1.342288000
B	-0.001070000	-1.026495000	3.329373000

B	-1.431242000	1.092167000	2.696675000
B	1.431406000	1.091311000	2.697951000
H	-0.001479000	-1.201013000	4.527131000
H	-1.959230000	1.716888000	3.578002000
H	1.959381000	1.715376000	3.579745000
N	0.000484000	-0.494597000	-0.649642000
N	0.000484000	-0.494597000	0.649642000
Ru	0.000704000	1.372216000	-1.342288000
Ru	-1.453097000	-0.737379000	-2.017160000
Ru	1.452448000	-0.738337000	-2.018649000
B	-1.431242000	1.092167000	-2.696675000
B	-0.001070000	-1.026495000	-3.329373000
B	1.431406000	1.091311000	-2.697951000
H	-1.959230000	1.716888000	-3.578002000
H	-0.001479000	-1.201013000	-4.527131000
H	1.959381000	1.715376000	-3.579745000
Sum of electronic and zero-point Energies=			-824.832872
Sum of electronic and thermal Energies=			-824.813818
Sum of electronic and thermal Enthalpies=			-824.812874
Sum of electronic and thermal Free Energies=			-824.882875

7''_Ru

Ru	0.813603000	1.478595000	1.404631000
Ru	0.844660000	-1.461397000	1.404680000
Ru	-1.730371000	-0.018002000	1.960156000
H	2.807187000	0.029802000	2.388307000
H	-0.664319000	-2.044242000	3.363572000
H	-0.707213000	2.029750000	3.363935000
N	-0.269198000	-0.003035000	-0.665371000
N	-0.269198000	-0.003035000	0.665371000
Ru	-1.730371000	-0.018002000	-1.960156000
Ru	0.844660000	-1.461397000	-1.404680000
Ru	0.813603000	1.478595000	-1.404631000
H	-0.664319000	-2.044242000	-3.363572000
H	2.807187000	0.029802000	-2.388307000
H	-0.707213000	2.029750000	-3.363935000
N	2.022542000	0.021406000	1.732605000
N	-0.735581000	-1.628009000	2.431087000
N	-0.769614000	1.612505000	2.431305000
N	-0.769614000	1.612505000	-2.431305000
N	-0.735581000	-1.628009000	-2.431087000
N	2.022542000	0.021406000	-1.732605000
Sum of electronic and zero-point Energies=			-1004.013298
Sum of electronic and thermal Energies=			-1003.995720
Sum of electronic and thermal Enthalpies=			-1003.994775
Sum of electronic and thermal Free Energies=			-1004.060690

1''_Os

Os	0.000000000	1.901992000	1.256764000
Os	1.647174000	-0.950996000	1.256764000
Os	-1.647174000	-0.950996000	1.256764000

Os	-1.647174000	-0.950996000	-1.256764000
Os	1.647174000	-0.950996000	-1.256764000
Os	0.000000000	1.901992000	-1.256764000
N	0.000000000	0.000000000	-0.715605000
N	0.000000000	0.000000000	0.715605000
H	-2.646701000	1.528074000	1.509569000
H	-1.684484000	0.972537000	2.989237000
H	1.684484000	0.972537000	2.989237000
H	2.646701000	1.528074000	1.509569000
H	0.000000000	-1.945075000	2.989237000
H	0.000000000	-3.056148000	1.509569000
H	-2.646701000	1.528074000	-1.509569000
H	-1.684484000	0.972537000	-2.989237000
H	0.000000000	-1.945075000	-2.989237000
H	0.000000000	-3.056148000	-1.509569000
H	1.684484000	0.972537000	-2.989237000
H	2.646701000	1.528074000	-1.509569000
C	1.730030000	0.998833000	1.863368000
C	1.730030000	0.998833000	-1.863368000
C	0.000000000	-1.997666000	-1.863368000
C	-1.730030000	0.998833000	-1.863368000
C	-1.730030000	0.998833000	1.863368000
C	0.000000000	-1.997666000	1.863368000
Sum of electronic and zero-point Energies=			-885.176273
Sum of electronic and thermal Energies=			-885.157889
Sum of electronic and thermal Enthalpies=			-885.156945
Sum of electronic and thermal Free Energies=			-885.222470

2''_Os			
Os	0.000000000	-1.868247000	1.285863000
Os	-1.617949000	0.934123000	1.285863000
Os	1.617949000	0.934123000	1.285863000
Os	1.617950000	0.934124000	-1.285950000
Os	-1.617950000	0.934124000	-1.285950000
Os	0.000000000	-1.868248000	-1.285950000
N	0.000000000	0.000000000	-0.709286000
N	0.000000000	0.000000000	0.709153000
N	0.000000000	2.083860000	1.870114000
N	1.804675000	-1.041930000	1.870114000
N	-1.805059000	-1.042151000	-1.869425000
N	0.000000000	2.084302000	-1.869425000
N	1.805059000	-1.042151000	-1.869425000
N	-1.804675000	-1.041930000	1.870114000
H	0.000000000	2.290135000	2.893985000
H	0.000000000	3.034436000	1.442618000
H	2.627898000	-1.517218000	1.442618000
H	1.983315000	-1.145068000	2.893985000
H	-1.984017000	-1.145473000	-2.893199000
H	-2.628048000	-1.517304000	-1.441347000
H	0.000000000	2.290946000	-2.893199000
H	0.000000000	3.034608000	-1.441347000

H	2.628048000	-1.517304000	-1.441347000
H	1.984017000	-1.145473000	-2.893199000
H	-1.983315000	-1.145068000	2.893985000
H	-2.627898000	-1.517218000	1.442618000
Sum of electronic and zero-point Energies=			-985.295806
Sum of electronic and thermal Energies=			-985.277364
Sum of electronic and thermal Enthalpies=			-985.276420
Sum of electronic and thermal Free Energies=			-985.343688

3''_Os

Os	2.368109000	-0.780547000	-0.000020000
Os	-0.644026000	-1.337855000	-1.661081000
Os	-0.643751000	-1.337237000	1.661599000
Os	-1.350733000	0.932302000	1.332756000
Os	-1.351050000	0.931751000	-1.332905000
Os	1.754244000	1.750924000	-0.000467000
N	0.031169000	0.701519000	-0.000172000
N	0.327273000	-0.727849000	0.000073000
H	2.394767000	-1.207592000	3.127537000
H	1.977536000	-3.181518000	2.061299000
H	1.977259000	-3.182767000	-2.060203000
H	2.394429000	-1.209135000	-3.127136000
H	-1.424997000	-3.965372000	0.000610000
H	-3.227850000	-2.598200000	0.000438000
H	1.411123000	2.132576000	3.121690000
H	0.234421000	3.694679000	1.978490000
H	-3.961667000	2.178294000	-0.000310000
H	-4.431612000	-0.071461000	0.001003000
H	0.233377000	3.693892000	-1.978276000
H	1.409856000	2.132643000	-3.123307000
P	1.664337000	-1.788737000	-2.046288000
P	0.540572000	2.300419000	-2.007947000
P	-3.374898000	0.876962000	0.000143000
P	0.540955000	2.301032000	2.007167000
P	1.664649000	-1.787487000	2.046864000
P	-1.808148000	-2.591619000	0.000582000
Sum of electronic and zero-point Energies=			-2704.642152
Sum of electronic and thermal Energies=			-2704.617933
Sum of electronic and thermal Enthalpies=			-2704.616989
Sum of electronic and thermal Free Energies=			-2704.696642

4''_Os

Os	0.000000000	-1.833029000	1.301040000
Os	-1.587450000	0.916515000	1.301040000
Os	1.587450000	0.916515000	1.301040000
Os	1.587632000	0.916620000	-1.301197000
Os	-1.587632000	0.916620000	-1.301197000
Os	0.000000000	-1.833240000	-1.301197000
N	0.000000000	0.000000000	-0.709429000
N	0.000000000	0.000000000	0.708449000
H	2.396683000	-1.383726000	2.472212000

H	-2.396683000	-1.383726000	2.472212000
H	0.000000000	2.767451000	2.472212000
H	2.396976000	-1.383895000	-2.471223000
H	0.000000000	2.767790000	-2.471223000
H	-2.396976000	-1.383895000	-2.471223000
O	1.821626000	-1.051716000	1.721719000
O	-1.821626000	-1.051716000	1.721719000
O	-1.822610000	-1.052284000	-1.720064000
O	1.822610000	-1.052284000	-1.720064000
O	0.000000000	2.103433000	1.721719000
O	0.000000000	2.104568000	-1.720064000
Sum of electronic and zero-point Energies=			-1104.255459
Sum of electronic and thermal Energies=			-1104.236888
Sum of electronic and thermal Enthalpies=			-1104.235944
Sum of electronic and thermal Free Energies=			-1104.303820

5''_Os

Os	0.000000000	1.948419095	1.279015727
Os	1.687380435	-0.974209547	1.279015727
Os	-1.687380435	-0.974209547	1.279015727
Os	-1.687380435	-0.974209547	-1.279015727
Os	1.687380435	-0.974209547	-1.279015727
Os	0.000000000	1.948419095	-1.279015727
N	0.000000000	0.000000000	-0.743606570
N	0.000000000	0.000000000	0.743606570
H	0.000000000	-2.895270168	-3.117102535
H	-2.507377513	1.447635084	-3.117102535
H	-2.507377513	1.447635084	3.117102535
H	2.507377513	1.447635084	3.117102535
H	0.000000000	-2.895270168	3.117102535
H	2.507377513	1.447635084	-3.117102535
S	0.000000000	-2.515359702	-1.785294207
S	0.000000000	-2.515359702	1.785294207
S	2.178365401	1.257679851	-1.785294207
S	2.178365401	1.257679851	1.785294207
S	-2.178365401	1.257679851	-1.785294207
S	-2.178365401	1.257679851	1.785294207
Sum of electronic and zero-point Energies=			-3041.973453
Sum of electronic and thermal Energies=			-3041.951573
Sum of electronic and thermal Enthalpies=			-3041.950628
Sum of electronic and thermal Free Energies=			-3042.024138

6''_Os

N	-0.027637000	0.090116000	-0.720484000
N	-0.027549000	-0.090180000	0.720385000
B	-0.957217000	-1.248867000	-2.141855000
B	1.908724000	0.153425000	-1.823454000
B	-0.809642000	-1.763496000	1.885655000
B	1.908630000	-0.150547000	1.823860000
B	-0.959171000	1.247407000	2.141678000
B	-0.812316000	1.762325000	-1.885656000

Os	1.065261000	-1.828801000	1.036142000
Os	0.925966000	-1.601618000	-1.426162000
Os	-2.012699000	0.221942000	-1.325768000
Os	-2.012417000	-0.225025000	1.325655000
Os	1.062524000	1.830404000	-1.036073000
Os	0.923358000	1.603046000	1.426192000
H	-0.592174000	-2.102997000	-3.005537000
H	2.680284000	0.375330000	-2.762081000
H	-0.764817000	-2.630265000	2.769053000
H	2.680267000	-0.370458000	2.762876000
H	-0.594904000	2.102174000	3.005172000
H	-0.768876000	2.629357000	-2.768845000
Sum of electronic and zero-point Energies=			-804.095386
Sum of electronic and thermal Energies=			-804.074838
Sum of electronic and thermal Enthalpies=			-804.073893
Sum of electronic and thermal Free Energies=			-804.146527

7''_Os

Os	-0.000001000	1.987748000	-1.687962000
Os	1.502126000	1.356982000	0.828461000
Os	-1.502126000	1.356981000	0.828462000
H	2.199550000	3.243176000	-0.783632000
H	0.000000000	2.450502000	2.740509000
H	-2.199552000	3.243176000	-0.783631000
N	0.000000000	-0.711296000	-0.240523000
N	0.000000000	0.711296000	-0.240523000
Os	-1.502126000	-1.356982000	0.828461000
Os	1.502126000	-1.356981000	0.828462000
Os	0.000001000	-1.987748000	-1.687962000
H	0.000000000	-2.450502000	2.740509000
H	2.199552000	-3.243176000	-0.783631000
H	-2.199550000	-3.243176000	-0.783632000
N	1.678387000	2.366791000	-0.776317000
N	0.000000000	1.790777000	1.962538000
N	-1.678387000	2.366791000	-0.776315000
N	-1.678387000	-2.366791000	-0.776317000
N	0.000000000	-1.790777000	1.962538000
N	1.678387000	-2.366791000	-0.776315000
Sum of electronic and zero-point Energies=			-985.053030
Sum of electronic and thermal Energies=			-985.035152
Sum of electronic and thermal Enthalpies=			-985.034208
Sum of electronic and thermal Free Energies=			-985.102903