# DFT study on the mechanism of water-assisted dihydrogen elimination in group 6 octahedral metal hydride complexes

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*Received (in XXX, XXX) Xth XXXXXXXXX 20XX, Accepted Xth XXXXXXXXX 20XX*
DOI: 10.1039/b000000x

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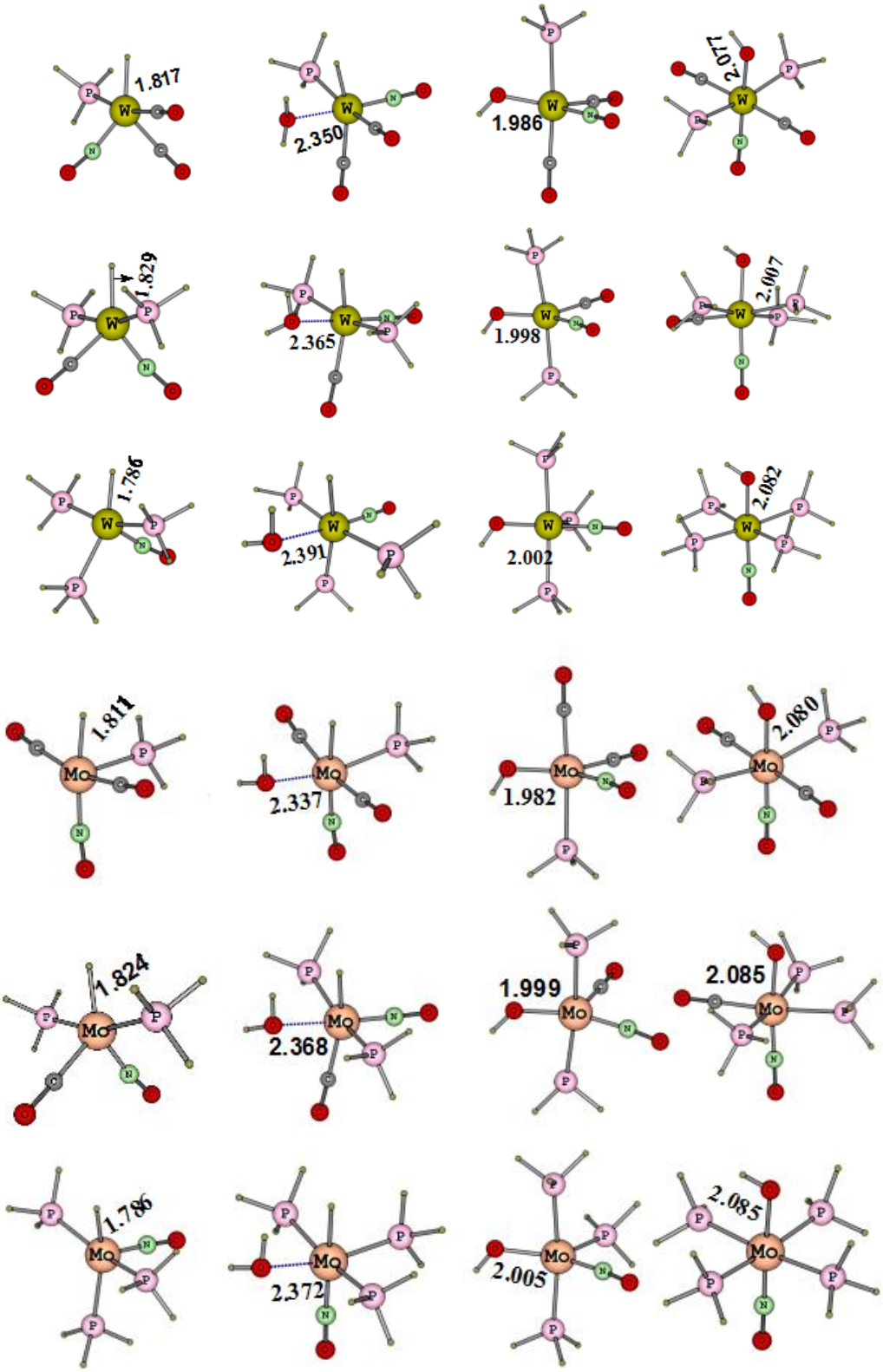
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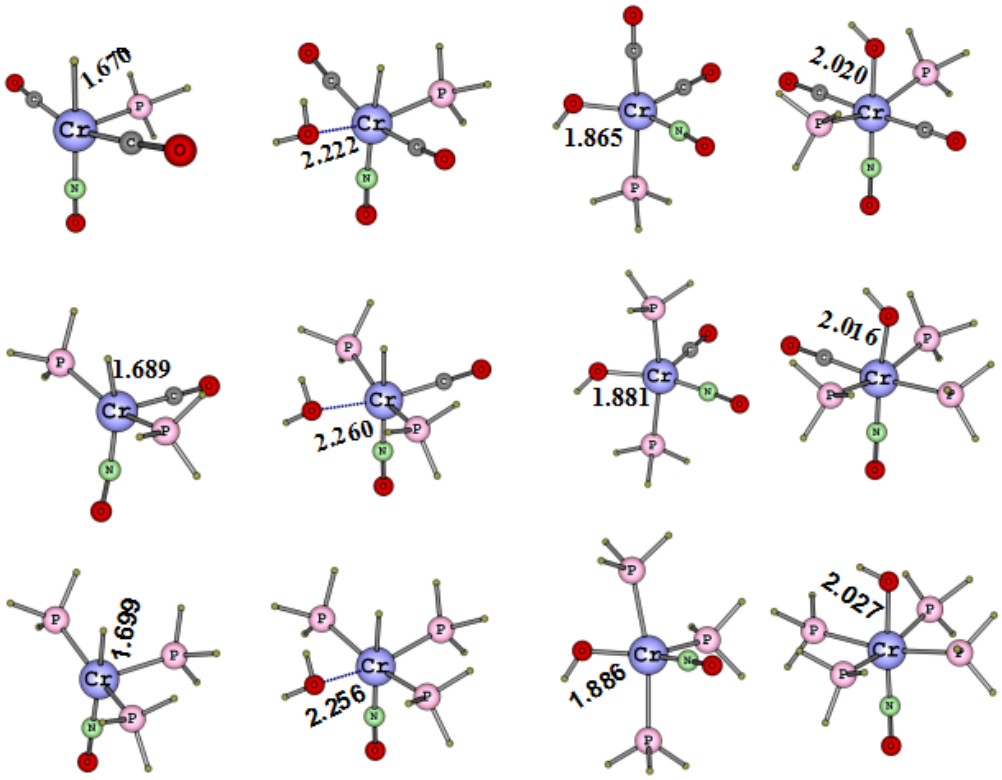
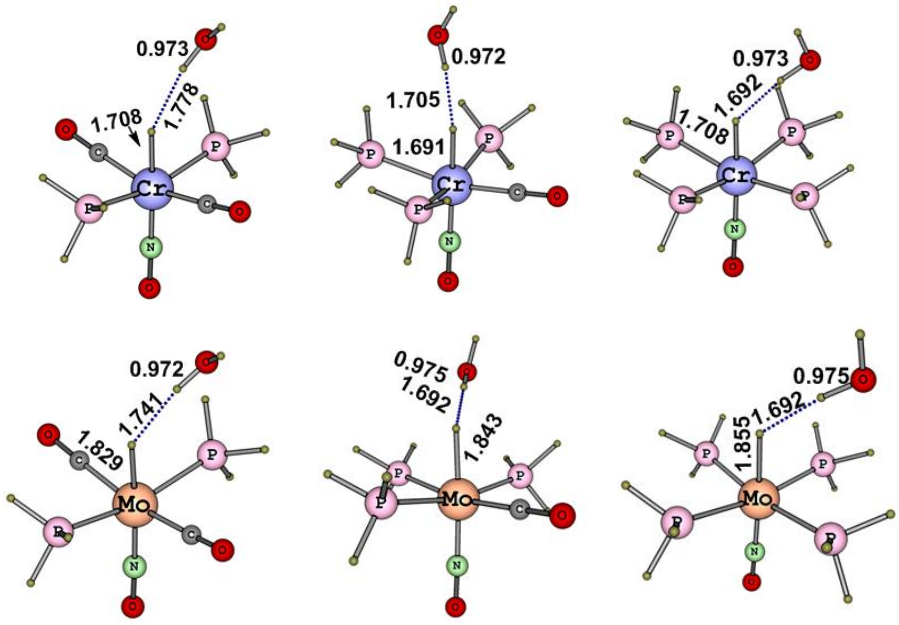
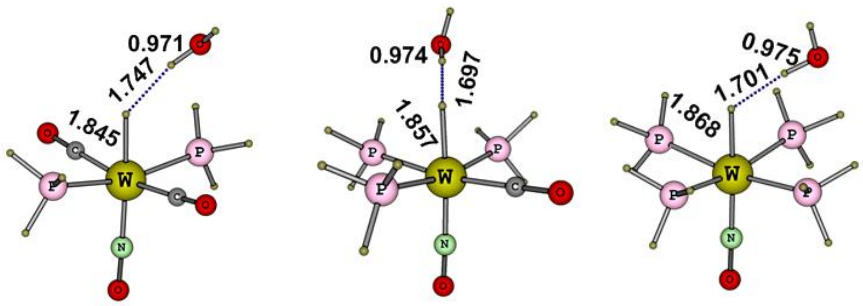
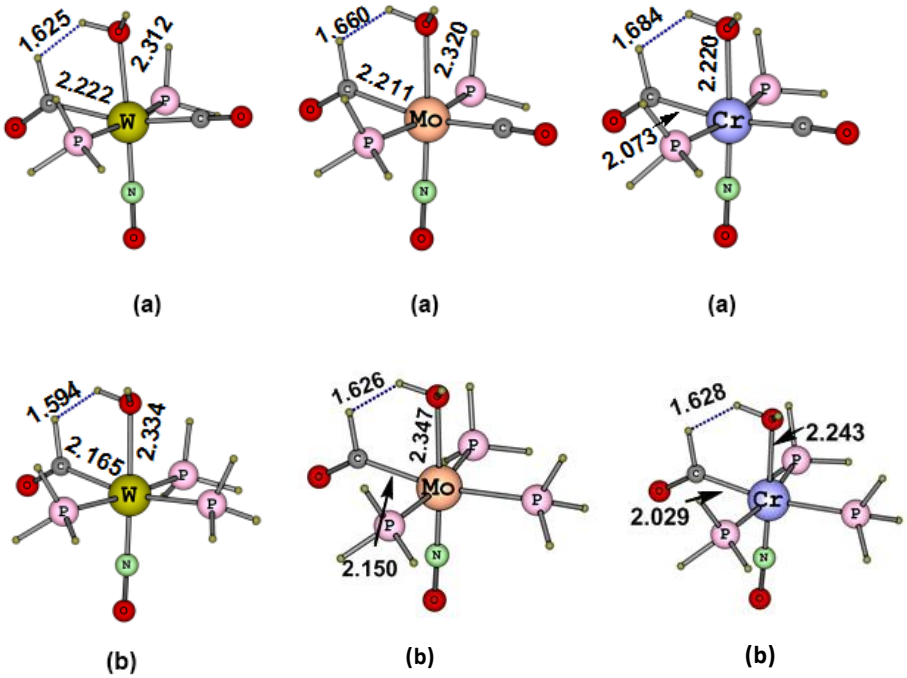



1. Fig. S1 Optimized structures of reactants, intermediates and products obtained through dissociative mechanism for hydrogen elimination, involving $M_{bis}$, $M_{tris}$ and, $M_{tetra}$ systems, studied at B3LYP/def2-TZVPP level. Structures in the 1st, 2nd, 3rd, and 4th columns are **M2**, **M3**, **M4** and **M5**, respectively. Bond distances in Å.

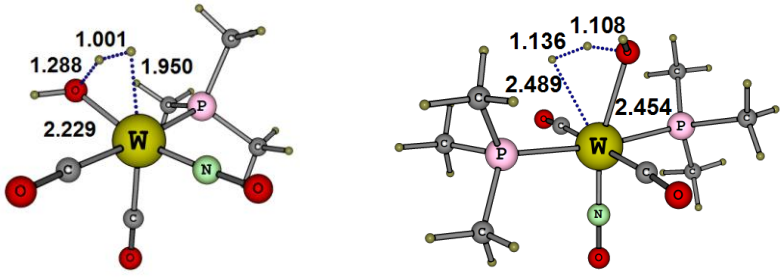


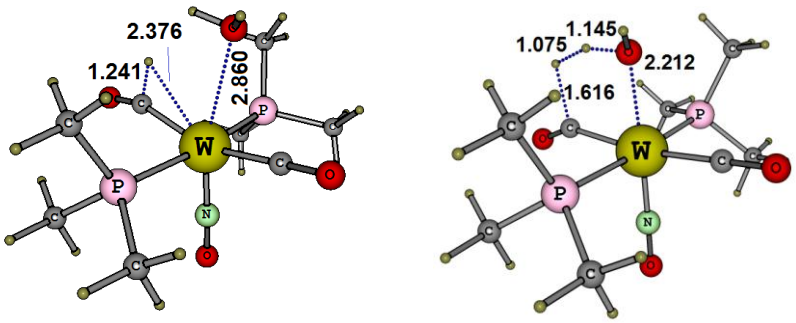



2. Fig. S2 Optimized structures of intermediates (**M6**) through associative mechanism for hydrogen elimination, studied at B3LYP/def2-TZVPP level. Structures in the 1st, 2nd, and 3rd columns are $M_{bis}$, $M_{tris}$ and $M_{tetra}$ systems, respectively. Bond distances in Å.



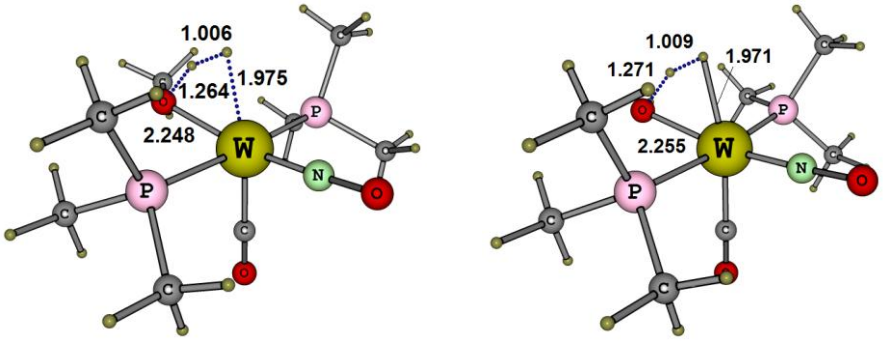

3. Fig. S3 Optimized structures of intermediates (**M7**) through hydride migratory insertion mechanism for hydrogen elimination, involving $M_{bis}$ and $M_{tris}$ systems, studied at B3LYP/def2-TZVPP level. Bond distances in Å.





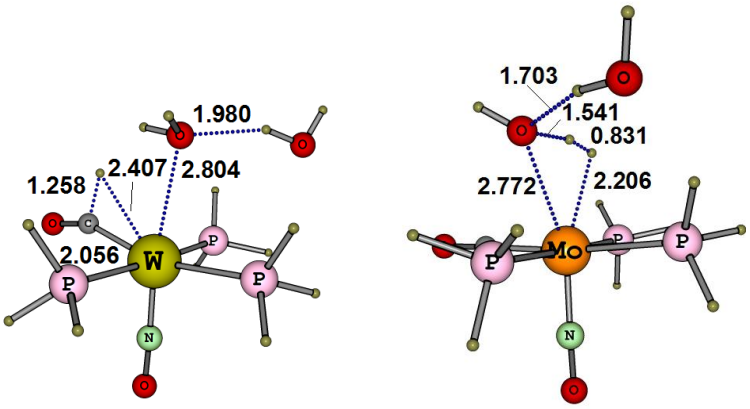

**MTS3** **MTS4**

4. Fig. S4 Optimized transition states, **MTS1**, **MTS2**, **MTS3** and **MTS4** for $WH(CO)_2(NO)(PMe_3)_2$.




**(a)** **(b)**

5. Fig. S5 Optimized transition states, **MTS1** for $WH(CO)_2(NO)(PMe_3)_2$ with **(a)** alcohol and **(b)** water.




**(a)** **(b)**

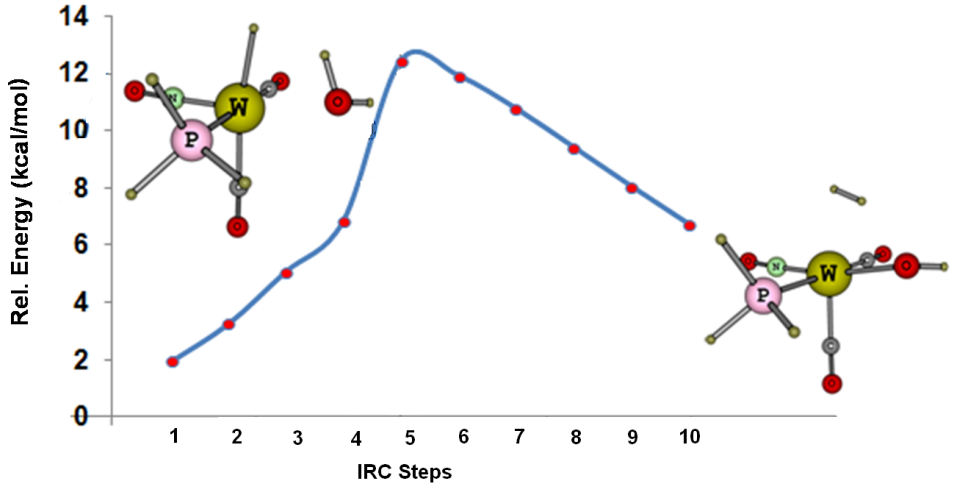
6. Fig. S6 Optimized transition states, **MTS2** and **MTS3** for (a) $W_{tris}$ and (b) $Mo_{tris}$ involving two water molecules.

7. Table S1 Dissociation energy for trimethylphoshine ligand ($\mathbf{E_d}$), binding energies (BSSE corrected) ($\mathbf{E_{b1}}$ and $\mathbf{E_{b2}}$), activation free energy ($\mathbf{G_{act}}$), and Gibbs free energy of reaction ($\mathbf{G_{react}}$) for hydrogen elimination passing through dissociative mechanism. Energies in kcal/mol.

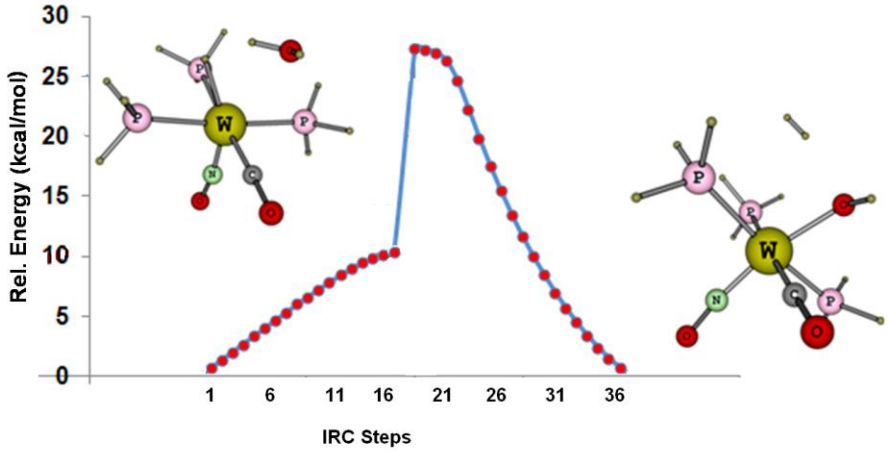
| W complexes | $B_d$ | $E_{b1}$ | $G_{act}$ | $E_{b2}$ | $G_{react}$ |
|---|---|---|---|---|---|
| $WH(CO)_2(NO)(PMe_3)_2$ with $H_2O$ | 29.8 | 13.8 | 7.8 | 11.3 | -8.22 |
| $WH(CO)_2(NO)(PMe_3)_2$ with $CH_3OH$ | 19.4 | 10.6 | 9.0 | 6.9 | 7.9 |

8. Table S2 Dihydrogen interaction distance (**$d_{HH}$**), dihydrogen interaction energy (BSSE corrected) (**$E_{HH}$**) and activation free energy (**$G_{act}$**) for hydrogen elimination through through associative (1 and 3) and migratory mechanism (2 and 4). Distances in Å and energies in kcal/mol.

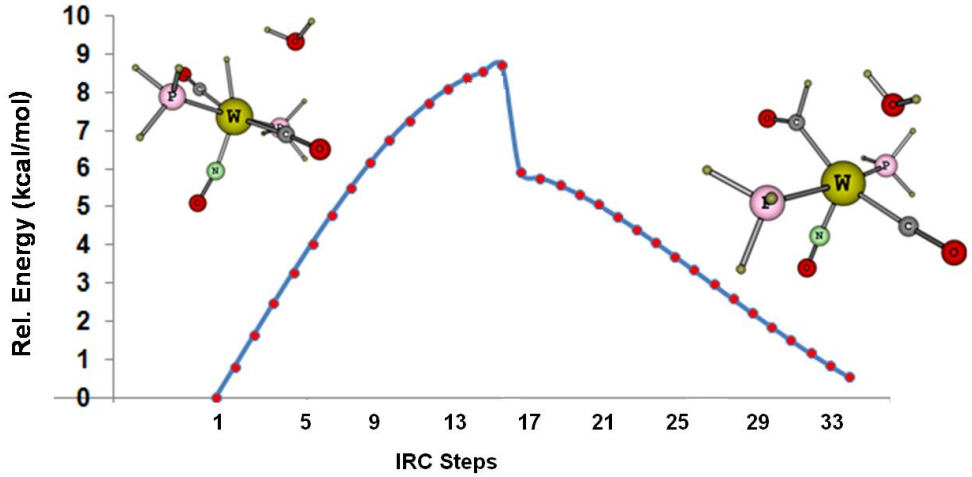
| No | Complexes | $d_{HH}$ | $E_{HH}$ | $G_{act}$ |
|---|---|---|---|---|
| 1 | $WH(CO)_2(NO)(PMe_3)_2$ with $H_2O$ | 1.672 | 4.7 | 32.0 |
| 2 | $WH(CO)_2(NO)(PMe_3)_2$ with $H_2O$ | 1.672 | 4.7 | 29.6 |
| 3 | $MoH(CO)(NO)(PMe_3)_3$ with $2H_2O$ | 1.603 | 10.7 | 28.5 |
| 4 | $WH(CO)(NO)(PMe_3)_3$ with $2H_2O$ | 1.604 | 10.6 | 34.7 |




9. Fig. S4 IRC plot of **MTS1** of dissociative mechanism for $W_{bis}$ systems. Reactant is the water adduct and product is hydroxy complex with hydrogen.




10. Fig. S5 IRC plot of **MTS2** of associative mechanism for $W_{tris}$ systems. Reactant is the water adduct and product is hydroxy complex with hydrogen. Distances in Å.




11. Fig. S6 IRC plot of **MTS3** of migratory insertion mechanism for $W_{bis}$ systems. Reactant is the water adduct and product is formyl complex.

12. Cartesian coordinates (in Å) of all the optimized geometries. Zero point corrected Energy (E-ZPE corrected) and gas phase free energy (G) are also given in a.u.

**M1** complex of $W_{bis}$
E(ZPE- corrected) =-1110.84470
G = -1110.88842

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000009000 | 0.000009000 | -0.081769000 |
| 15 | 2.452969000 | 0.000047000 | -0.478919000 |
| 15 | -2.452968000 | -0.000034000 | -0.478828000 |
| 7 | 0.000086000 | 0.000046000 | 1.774039000 |
| 8 | 0.000095000 | -0.000240000 | 2.950429000 |
| 6 | -0.000033000 | 2.058016000 | -0.277094000 |
| 8 | -0.000183000 | 3.193040000 | -0.423145000 |
| 1 | 3.034198000 | -1.059724000 | -1.203183000 |
| 1 | 3.034189000 | 1.059836000 | -1.203163000 |
| 1 | 3.347507000 | 0.000041000 | 0.611516000 |
| 1 | -3.034167000 | -1.059825000 | -1.203086000 |
| 1 | -3.347494000 | -0.000073000 | 0.611616000 |
| 1 | -3.034227000 | 1.059739000 | -1.203064000 |
| 1 | -0.000081000 | 0.000306000 | -1.917620000 |
| 6 | 0.000027000 | -2.057986000 | -0.277227000 |
| 8 | -0.000059000 | -3.193006000 | -0.423314000 |

**M1** complex of $W_{tris}$
E(ZPE- corrected) = -1340.62154
G = -1340.66527

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000159000 | 0.056622000 | -0.083678000 |
| 15 | 2.443707000 | 0.056782000 | -0.456235000 |
| 15 | -0.010737000 | -2.452804000 | -0.270365000 |
| 15 | -2.443399000 | 0.077372000 | -0.455145000 |
| 7 | 0.001203000 | 0.116766000 | 1.761840000 |
| 8 | 0.001974000 | 0.110079000 | 2.943909000 |
| 6 | 0.008515000 | 2.065499000 | -0.315698000 |
| 8 | 0.013964000 | 3.207101000 | -0.462537000 |
| 1 | 3.106628000 | -1.088365000 | -0.958956000 |
| 1 | 3.327703000 | 0.312144000 | 0.613904000 |
| 1 | 2.987551000 | 0.979221000 | -1.372621000 |
| 1 | -0.013513000 | -3.277494000 | 0.876833000 |

| | | | |
|---|---|---|---|
| 1 | -1.068634000 | -3.098452000 | -0.949221000 |
| 1 | 1.040668000 | -3.107502000 | -0.950609000 |
| 1 | -3.115125000 | -1.061760000 | -0.959777000 |
| 1 | -3.325371000 | 0.337834000 | 0.615459000 |
| 1 | -2.980074000 | 1.005623000 | -1.369885000 |
| 1 | -0.002167000 | -0.159316000 | -1.916487000 |

**M1** complex of $W_{tetra}$
E (ZPE- corrected) = -1570.39194
G = -1570.43550

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000051000 | 0.000056000 | -0.075117000 |
| 15 | -0.082392000 | -2.435633000 | -0.381018000 |
| 15 | -2.436173000 | 0.081895000 | -0.378003000 |
| 15 | 0.082054000 | 2.435868000 | -0.381359000 |
| 7 | -0.000033000 | 0.000121000 | 1.761736000 |
| 8 | 0.000109000 | 0.000465000 | 2.950760000 |
| 1 | -1.156538000 | -3.039490000 | -1.080320000 |
| 1 | -0.110658000 | -3.294510000 | 0.740545000 |
| 1 | 0.944352000 | -3.112438000 | -1.084263000 |
| 1 | -3.292970000 | 0.108798000 | 0.745149000 |
| 1 | -3.042092000 | 1.156041000 | -1.075532000 |
| 1 | -3.113543000 | -0.944813000 | -1.080829000 |
| 1 | -0.944611000 | 3.112099000 | -1.085278000 |
| 1 | 0.109219000 | 3.294823000 | 0.740160000 |
| 1 | 1.156278000 | 3.040235000 | -1.080054000 |
| 1 | -0.000131000 | -0.000162000 | -1.930939000 |
| 15 | 2.436316000 | -0.082535000 | -0.378074000 |
| 1 | 3.041623000 | -1.156771000 | -1.076016000 |
| 1 | 3.114467000 | 0.943966000 | -1.080440000 |
| 1 | 3.293119000 | -0.110422000 | 0.745049000 |

**M1** complex of $Mo_{bis}$
E (ZPE- corrected) =-1111.96075
G = -1112.00407

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.000033000 | 0.000071000 | -0.080635000 |
| 15 | -2.439466000 | -0.001779000 | -0.511411000 |
| 15 | 2.439442000 | 0.001104000 | -0.511096000 |
| 7 | -0.000246000 | 0.000377000 | 1.760402000 |
| 8 | -0.000376000 | 0.000830000 | 2.932182000 |
| 6 | 0.001479000 | -2.046765000 | -0.305998000 |
| 8 | 0.002339000 | -3.176623000 | -0.475986000 |
| 1 | -3.013106000 | 1.055897000 | -1.244592000 |
| 1 | -3.358344000 | -0.002679000 | 0.559589000 |
| 1 | -3.011186000 | -1.060356000 | -1.244778000 |
| 1 | 3.012128000 | 1.059716000 | -1.243670000 |
| 1 | 3.358260000 | 0.000479000 | 0.559958000 |
| 1 | 3.012174000 | -1.056552000 | -1.245000000 |
| 1 | 0.000275000 | 0.000429000 | -1.899168000 |
| 6 | -0.001236000 | 2.046868000 | -0.306539000 |
| 8 | -0.001739000 | 3.176662000 | -0.476900000 |

**M1** complex of $Mo_{tris}$
E (ZPE- corrected) = -1341.73936
G = -1341.78259

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.000047000 | 0.067942000 | -0.082191000 |
| 15 | 2.430793000 | 0.075499000 | -0.491376000 |
| 15 | 0.000679000 | -2.433639000 | -0.283321000 |
| 15 | -2.430935000 | 0.074114000 | -0.491038000 |
| 7 | -0.000085000 | 0.154968000 | 1.746990000 |
| 8 | 0.000558000 | 0.178956000 | 2.923958000 |

| | | | |
|---|---|---|---|
| 6 | -0.000601000 | 2.062045000 | -0.360958000 |
| 8 | -0.001032000 | 3.196888000 | -0.537849000 |
| 1 | 3.082110000 | -1.059041000 | -1.030040000 |
| 1 | 3.342302000 | 0.305992000 | 0.562342000 |
| 1 | 2.963999000 | 1.014711000 | -1.396722000 |
| 1 | 0.000977000 | -3.277341000 | 0.850872000 |
| 1 | -1.052423000 | -3.079795000 | -0.968500000 |
| 1 | 1.054097000 | -3.079181000 | -0.968593000 |
| 1 | -3.081672000 | -1.060786000 | -1.029638000 |
| 1 | -3.342462000 | 0.304093000 | 0.562782000 |
| 1 | -2.964772000 | 1.013036000 | -1.396313000 |
| 1 | -0.000263000 | -0.138657000 | -1.900196000 |

**M1** complex of $Mo_{tetra}$
E (ZPE- corrected) = -1571.51259
G =-1571.55637

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.000009000 | 0.000013000 | -0.073713000 |
| 15 | -2.393203000 | 0.407167000 | -0.408363000 |
| 15 | 0.407208000 | 2.393217000 | -0.408452000 |
| 15 | 2.393217000 | -0.407249000 | -0.408333000 |
| 7 | -0.000019000 | -0.000011000 | 1.746981000 |
| 8 | -0.000039000 | 0.000031000 | 2.930960000 |
| 1 | -2.840134000 | 1.547815000 | -1.118446000 |
| 1 | -3.263722000 | 0.555649000 | 0.695533000 |
| 1 | -3.191762000 | -0.522773000 | -1.117334000 |
| 1 | 0.555658000 | 3.263816000 | 0.695385000 |
| 1 | 1.547930000 | 2.840036000 | -1.118490000 |
| 1 | -0.522632000 | 3.191770000 | -1.117551000 |
| 1 | 3.191855000 | 0.522482000 | -1.117475000 |
| 1 | 3.263744000 | -0.555638000 | 0.695569000 |
| 1 | 2.840018000 | -1.548067000 | -1.118237000 |
| 1 | 0.000037000 | 0.000071000 | -1.915128000 |
| 15 | -0.407212000 | -2.393163000 | -0.408444000 |
| 1 | 0.522588000 | -3.191759000 | -1.117548000 |
| 1 | -0.555660000 | -3.263719000 | 0.695430000 |
| 1 | -1.547973000 | -2.839952000 | -1.118445000 |

**M1** complex of $Cr1_{bis}$
E (ZPE- corrected) = -2088.17874
G = -2088.22026

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.000022000 | -0.000047000 | -0.056702000 |
| 15 | 2.302488000 | 0.000928000 | -0.428381000 |
| 6 | 0.000755000 | -1.875229000 | -0.383223000 |
| 15 | -2.302525000 | -0.000624000 | -0.428367000 |
| 7 | -0.000020000 | -0.000475000 | 1.637681000 |
| 8 | 0.000131000 | -0.000316000 | 2.807382000 |
| 6 | -0.000811000 | 1.875231000 | -0.382572000 |
| 8 | -0.001050000 | 2.991172000 | -0.632970000 |
| 1 | 2.897518000 | -1.055838000 | -1.147474000 |
| 1 | 3.195929000 | 0.000426000 | 0.664891000 |
| 1 | 2.896889000 | 1.059048000 | -1.145995000 |
| 1 | -2.897129000 | -1.058504000 | -1.146174000 |
| 1 | -3.195995000 | -0.000143000 | 0.664884000 |
| 1 | -2.897321000 | 1.056382000 | -1.147294000 |
| 1 | -0.000080000 | 0.000589000 | -1.724212000 |
| 8 | 0.001139000 | -2.991116000 | -0.633855000 |

**M1** complex of $Cr1_{tris}$
E (ZPE- corrected) = -2317.95457
G =-2317.99598

| At. No. | X | Y | Z |
|---|---|---|---|

| | | | |
|---|---|---|---|
| 24 | -0.000002000 | 0.066376000 | -0.060952000 |
| 15 | 2.288524000 | 0.092008000 | -0.454609000 |
| 15 | -0.000242000 | -2.266844000 | -0.343419000 |
| 15 | -2.288505000 | 0.092528000 | -0.454653000 |
| 7 | -0.000027000 | 0.122224000 | 1.625451000 |
| 8 | -0.000032000 | 0.158926000 | 2.800114000 |
| 6 | 0.000243000 | 1.914637000 | -0.374653000 |
| 8 | 0.000406000 | 3.042614000 | -0.589307000 |
| 1 | 2.941894000 | -1.002973000 | -1.069163000 |
| 1 | 3.202925000 | 0.247923000 | 0.612185000 |
| 1 | 2.831324000 | 1.090284000 | -1.289833000 |
| 1 | -0.000172000 | -3.149953000 | 0.762143000 |
| 1 | -1.053460000 | -2.894970000 | -1.046678000 |
| 1 | 1.052718000 | -2.895113000 | -1.046932000 |
| 1 | -2.942015000 | -1.002173000 | -1.069553000 |
| 1 | -3.202918000 | 0.248265000 | 0.612159000 |
| 1 | -2.831133000 | 1.091138000 | -1.289591000 |
| 1 | -0.000019000 | -0.046520000 | -1.738373000 |

**M1** complex of $Cr1_{tera}$
E (ZPE- corrected) = -2547.72609
G = -2547.76778

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.000044000 | 0.000035000 | -0.058964000 |
| 15 | -1.356823000 | -1.842713000 | -0.406206000 |
| 15 | -1.842917000 | 1.356778000 | -0.405779000 |
| 15 | 1.357016000 | 1.842862000 | -0.405832000 |
| 7 | -0.000240000 | -0.000084000 | 1.619365000 |
| 8 | -0.000558000 | -0.000306000 | 2.801727000 |
| 1 | -2.572781000 | -1.725352000 | -1.123370000 |
| 1 | -1.893016000 | -2.567643000 | 0.684695000 |
| 1 | -0.882358000 | -2.970576000 | -1.119968000 |
| 1 | -2.569807000 | 1.889663000 | 0.685434000 |
| 1 | -1.725325000 | 2.574708000 | -1.119604000 |
| 1 | -2.969396000 | 0.883430000 | -1.122428000 |
| 1 | 0.882851000 | 2.970652000 | -1.119903000 |
| 1 | 1.892620000 | 2.567893000 | 0.685284000 |
| 1 | 2.573357000 | 1.725528000 | -1.122360000 |
| 1 | -0.000100000 | -0.000060000 | -1.755139000 |
| 15 | 1.843015000 | -1.356797000 | -0.405574000 |
| 1 | 2.569778000 | -1.889814000 | 0.685650000 |
| 1 | 1.725342000 | -2.574660000 | -1.119494000 |
| 1 | 2.969566000 | -0.883522000 | -1.122162000 |

**M2** complex of $W_{bis}$
E (ZPE- corrected) = -767.65706
G = -767.69597

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.038495000 | -0.050545000 | -0.285811000 |
| 15 | 2.482336000 | 0.011588000 | -0.417850000 |
| 7 | -0.167636000 | -1.181049000 | 1.143973000 |
| 8 | -0.227107000 | -2.064043000 | 1.920770000 |
| 6 | -0.195053000 | 1.523395000 | 0.923502000 |
| 8 | -0.281091000 | 2.467390000 | 1.575400000 |
| 1 | 3.299052000 | 0.096826000 | 0.727817000 |
| 1 | 3.154528000 | -1.044219000 | -1.065838000 |
| 1 | 3.040952000 | 1.075565000 | -1.151424000 |
| 1 | 0.196125000 | -0.150640000 | -2.084569000 |
| 6 | -2.047278000 | -0.039603000 | -0.640898000 |
| 8 | -3.173003000 | -0.034148000 | -0.835127000 |

**M2** complex of $W_{tris}$
E (ZPE- corrected) =-1340.62154
G = -1340.66527

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000002000 | -0.043434000 | -0.256738000 |
| 15 | 2.448374000 | 0.017935000 | -0.577779000 |
| 15 | -2.448368000 | 0.017933000 | -0.577791000 |
| 7 | -0.000004000 | -1.221387000 | 1.129464000 |
| 8 | -0.000012000 | -2.136135000 | 1.884042000 |
| 6 | -0.000001000 | 1.472409000 | 1.004042000 |
| 8 | -0.000019000 | 2.400058000 | 1.696336000 |
| 1 | 3.096587000 | -0.995002000 | -1.318885000 |
| 1 | 3.329870000 | 0.039782000 | 0.522508000 |
| 1 | 2.977034000 | 1.119287000 | -1.281365000 |
| 1 | -3.096574000 | -0.995004000 | -1.318903000 |
| 1 | -3.329870000 | 0.039776000 | 0.522490000 |
| 1 | -2.977025000 | 1.119285000 | -1.281378000 |
| 1 | 0.000003000 | -0.048178000 | -2.085853000 |

**M2** complex of $W_{tetra}$
E (ZPE- corrected) = -1570.39194
G = -1570.43550

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.000636000 | -0.141890000 | -0.246856000 |
| 15 | 0.003609000 | 2.173224000 | 0.482730000 |
| 15 | 2.409182000 | -0.371208000 | -0.521326000 |
| 7 | 0.000413000 | -0.751721000 | 1.424326000 |
| 8 | 0.001180000 | -1.272446000 | 2.509644000 |
| 1 | 0.005158000 | 3.155539000 | -0.546343000 |
| 1 | 1.059913000 | 2.755294000 | 1.241782000 |
| 1 | -1.048731000 | 2.760480000 | 1.243411000 |
| 1 | 3.387365000 | 0.367886000 | 0.202193000 |
| 1 | 2.979397000 | -1.652627000 | -0.313708000 |
| 1 | 2.954824000 | -0.144381000 | -1.810534000 |
| 1 | -0.001202000 | -1.400460000 | -1.513888000 |
| 15 | -2.411060000 | -0.367715000 | -0.519265000 |
| 1 | -2.957053000 | -0.138433000 | -1.807905000 |
| 1 | -2.983312000 | -1.648424000 | -0.312915000 |
| 1 | -3.387618000 | 0.372071000 | 0.205722000 |

**M2** complex of $Mo_{bis}$
E (ZPE- corrected) = -768.76183
G = -768.80099

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.000014000 | 0.088298000 | -0.503509000 |
| 15 | -0.000038000 | -1.384004000 | 1.375066000 |
| 7 | -0.000019000 | 1.571992000 | 0.579565000 |
| 8 | -0.000046000 | 2.425237000 | 1.382417000 |
| 6 | -2.044965000 | -0.126781000 | -0.638591000 |
| 8 | -3.169628000 | -0.306968000 | -0.706999000 |
| 1 | 1.063494000 | -2.293796000 | 1.539475000 |
| 1 | -0.000221000 | -0.833046000 | 2.673488000 |
| 1 | -1.063454000 | -2.293970000 | 1.539241000 |
| 1 | 0.000055000 | -1.500627000 | -1.372974000 |
| 6 | 2.045004000 | -0.126806000 | -0.638503000 |
| 8 | 3.169671000 | -0.306948000 | -0.706946000 |

**M2** complex of $Mo_{tris}$
E (ZPE- corrected) = -998.55506
G = -998.59417

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.000046000 | 0.030805000 | -0.315320000 |
| 15 | -2.431218000 | -0.138726000 | -0.683627000 |
| 15 | 2.431068000 | -0.138695000 | -0.683888000 |

| | | | |
|---|---|---|---|
| 7 | 0.000159000 | 1.382002000 | 0.886065000 |
| 8 | 0.000100000 | 2.395260000 | 1.491863000 |
| 6 | 0.000156000 | -1.278143000 | 1.135352000 |
| 8 | 0.000281000 | -2.077009000 | 1.969169000 |
| 1 | -3.066393000 | 0.681443000 | -1.641841000 |
| 1 | -3.355874000 | 0.055725000 | 0.363982000 |
| 1 | -2.924963000 | -1.371976000 | -1.153005000 |
| 1 | 3.066386000 | 0.681601000 | -1.641910000 |
| 1 | 3.355508000 | 0.055721000 | 0.363910000 |
| 1 | 2.925015000 | -1.371848000 | -1.153320000 |
| 1 | -0.000599000 | -0.414325000 | -2.084450000 |

**M2** complex of $Mo2_{tetra}$
E (ZPE- corrected) = -1228.42
G = -1228.36525

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.000043000 | -0.166998000 | -0.300088000 |
| 15 | -2.406305000 | -0.458721000 | -0.602253000 |
| 15 | -0.000265000 | 2.188064000 | 0.390942000 |
| 15 | 2.406444000 | -0.458414000 | -0.602169000 |
| 7 | 0.000003000 | -0.796700000 | 1.347200000 |
| 8 | 0.000048000 | -1.258156000 | 2.444412000 |
| 1 | -2.923131000 | -0.332249000 | -1.911936000 |
| 1 | -3.431858000 | 0.283755000 | 0.037691000 |
| 1 | -2.940849000 | -1.735576000 | -0.328988000 |
| 1 | 1.046887000 | 2.791140000 | 1.134175000 |
| 1 | -0.000386000 | 3.148390000 | -0.651745000 |
| 1 | -1.047500000 | 2.790942000 | 1.134221000 |
| 1 | 2.923026000 | -0.332492000 | -1.911992000 |
| 1 | 3.432042000 | 0.284441000 | 0.037278000 |
| 1 | 2.941101000 | -1.735102000 | -0.328373000 |
| 1 | 0.000376000 | -1.571097000 | -1.390134000 |

**M2** complex of $Cr2_{bis}$
E (ZPE- corrected)= -1744.98424
G = -1745.02236

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.000006000 | 0.145256000 | -0.506653000 |
| 15 | 0.000131000 | -1.377598000 | 1.228779000 |
| 6 | -1.883778000 | -0.107884000 | -0.735818000 |
| 7 | -0.000056000 | 1.520266000 | 0.483747000 |
| 8 | -0.000439000 | 2.449930000 | 1.191621000 |
| 6 | 1.883833000 | -0.107617000 | -0.735736000 |
| 8 | 2.995938000 | -0.316053000 | -0.880990000 |
| 1 | -1.060414000 | -2.299826000 | 1.343528000 |
| 1 | 0.001219000 | -0.924994000 | 2.565019000 |
| 1 | 1.059806000 | -2.300985000 | 1.342164000 |
| 1 | 0.000170000 | -1.184374000 | -1.516315000 |
| 8 | -2.995854000 | -0.316482000 | -0.881045000 |

**M2** complex of $Cr2_{tris}$
E (ZPE- corrected) = -1974.77120
G = -1974.80967

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.000010000 | 0.018614000 | -0.323565000 |
| 15 | -2.262276000 | -0.262225000 | -0.735454000 |
| 15 | 2.262326000 | -0.262149000 | -0.735413000 |
| 7 | -0.000057000 | 1.458477000 | 0.552920000 |
| 8 | -0.000117000 | 2.515851000 | 1.065535000 |
| 6 | 0.000021000 | -1.025577000 | 1.202653000 |
| 8 | 0.000003000 | -1.683227000 | 2.146761000 |
| 1 | -2.780263000 | 0.148554000 | -1.984509000 |
| 1 | -3.269604000 | 0.316732000 | 0.069540000 |

| | | | |
|---|---|---|---|
| 1 | -2.766866000 | -1.576311000 | -0.758534000 |
| 1 | 2.780360000 | 0.148723000 | -1.984419000 |
| 1 | 3.269615000 | 0.316766000 | 0.069660000 |
| 1 | 2.766938000 | -1.576225000 | -0.758562000 |
| 1 | 0.000024000 | -1.076227000 | -1.609330000 |

**M2** complex of $Cr2_{tetra}$
E (ZPE- corrected) = -2204.53938
G = -2204.57843

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.000002000 | 0.143010000 | -0.367438000 |
| 15 | -2.269934000 | -0.016906000 | -0.799713000 |
| 15 | 2.269893000 | -0.016950000 | -0.799728000 |
| 7 | 0.000010000 | 1.397812000 | 0.746176000 |
| 8 | 0.000107000 | 2.273576000 | 1.542065000 |
| 1 | -2.738771000 | 0.394471000 | -2.070692000 |
| 1 | -3.253709000 | 0.663125000 | -0.043244000 |
| 1 | -2.900752000 | -1.280654000 | -0.805738000 |
| 1 | 2.738607000 | 0.394515000 | -2.070723000 |
| 1 | 3.253881000 | 0.662840000 | -0.043307000 |
| 1 | 2.900491000 | -1.280799000 | -0.805988000 |
| 1 | 0.000276000 | -1.063204000 | -1.564430000 |
| 15 | -0.000018000 | -1.542748000 | 1.177466000 |
| 1 | -0.000562000 | -1.255382000 | 2.561725000 |
| 1 | 1.049094000 | -2.495404000 | 1.215765000 |
| 1 | -1.048621000 | -2.495986000 | 1.215032000 |

**M3** complex of $W3_{bis}$
E (ZPE- corrected) = -844.12695
G = -844.16876

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.047797000 | -0.034892000 | -0.182127000 |
| 15 | 2.486488000 | 0.000996000 | -0.307459000 |
| 7 | -0.148103000 | 1.763290000 | -0.000213000 |
| 8 | -0.212576000 | 2.935950000 | 0.094749000 |
| 6 | -2.051563000 | -0.130579000 | -0.498917000 |
| 8 | -3.180540000 | -0.151550000 | -0.703979000 |
| 1 | 3.348614000 | 0.213406000 | 0.790939000 |
| 1 | 3.133765000 | -1.138736000 | -0.827687000 |
| 1 | 3.045665000 | 0.958585000 | -1.173628000 |
| 1 | 0.236528000 | -0.231022000 | -1.963009000 |
| 6 | -0.198291000 | -0.369587000 | 1.838749000 |
| 8 | -0.274312000 | -0.578938000 | 2.966444000 |
| 8 | 0.112722000 | -2.356185000 | -0.512437000 |
| 1 | -0.526032000 | -2.924571000 | -0.070282000 |
| 1 | -0.025399000 | -2.446872000 | -1.462770000 |

**M3** complex of $W3_{tris}$
E (ZPE- corrected) = -1073.90074
G = -1073.94336

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.000718000 | -0.025195000 | -0.162571000 |
| 15 | -2.459362000 | -0.040304000 | -0.454472000 |
| 15 | 2.450644000 | -0.087394000 | -0.434481000 |
| 7 | 0.036731000 | 1.766460000 | 0.032354000 |
| 8 | 0.065801000 | 2.948670000 | 0.137718000 |
| 6 | -0.026471000 | -0.369553000 | 1.836539000 |
| 8 | -0.040982000 | -0.606957000 | 2.968134000 |
| 1 | -3.012831000 | 0.732359000 | -1.496386000 |
| 1 | -3.356442000 | 0.362214000 | 0.559678000 |
| 1 | -3.090983000 | -1.262497000 | -0.775604000 |
| 1 | 3.025598000 | 0.681728000 | -1.468257000 |
| 1 | 3.350924000 | 0.292093000 | 0.586614000 |

| | | | |
|---|---|---|---|
| 1 | 3.087847000 | -1.309592000 | -0.762975000 |
| 1 | 0.002219000 | -0.278432000 | -1.974443000 |
| 8 | -0.091449000 | -2.365492000 | -0.494754000 |
| 1 | 0.494901000 | -2.950725000 | -0.005792000 |
| 1 | 0.117411000 | -2.444937000 | -1.432804000 |

**M3** complex of $W_{tetra}$
E (ZPE- corrected) = -1304.912342
G = -1304.83388

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.006679000 | -0.025328000 | -0.245141000 |
| 15 | -0.056719000 | -0.442899000 | 2.187584000 |
| 7 | 0.021907000 | 1.743281000 | -0.085725000 |
| 8 | 0.033668000 | 2.929627000 | -0.000960000 |
| 1 | 0.994813000 | -0.091741000 | 3.074557000 |
| 1 | -0.159740000 | -1.786049000 | 2.631287000 |
| 1 | -1.088936000 | 0.054635000 | 3.024640000 |
| 1 | 0.030816000 | -0.184184000 | -2.028479000 |
| 8 | -0.068621000 | -2.370017000 | -0.724384000 |
| 1 | 0.688572000 | -2.913206000 | -0.486108000 |
| 1 | 0.028155000 | -2.144976000 | -1.663092000 |
| 15 | 2.433065000 | -0.059377000 | -0.520499000 |
| 1 | 3.391937000 | 0.170195000 | 0.501823000 |
| 1 | 2.995814000 | 0.840467000 | -1.451669000 |
| 1 | 3.063579000 | -1.224584000 | -1.028704000 |
| 15 | -2.423826000 | -0.043659000 | -0.579401000 |
| 1 | -3.030885000 | -1.202041000 | -1.117897000 |
| 1 | -2.958867000 | 0.878985000 | -1.503296000 |
| 1 | -3.397276000 | 0.175447000 | 0.430430000 |

**M3** complex of $Mo_{bis}$
E (ZPE- corrected) = -845.23373
G = -845.27581

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.002102000 | -0.241438000 | -0.149449000 |
| 15 | 0.018173000 | 2.162435000 | -0.455582000 |
| 7 | -0.003275000 | -0.121083000 | 1.681328000 |
| 8 | -0.006697000 | 0.077841000 | 2.839277000 |
| 6 | 2.038834000 | -0.204438000 | -0.344847000 |
| 8 | 3.172692000 | -0.130573000 | -0.486693000 |
| 1 | 0.063172000 | 3.007117000 | 0.674119000 |
| 1 | -1.051334000 | 2.798024000 | -1.120609000 |
| 1 | 1.063621000 | 2.767092000 | -1.183970000 |
| 1 | -0.014862000 | -0.180177000 | -1.975957000 |
| 8 | -0.070577000 | -2.547860000 | -0.521487000 |
| 1 | 0.698135000 | -3.029874000 | -0.202238000 |
| 1 | -0.068884000 | -2.631263000 | -1.481709000 |
| 6 | -2.057363000 | -0.197697000 | -0.344202000 |
| 8 | -3.187927000 | -0.120242000 | -0.485354000 |

**M3** complex of $Mo_{tris}$
E (ZPE- corrected) = -1075.01983
G = -1075.06216

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.000433000 | -0.046159000 | -0.184665000 |
| 15 | 2.443037000 | -0.112493000 | -0.496812000 |
| 15 | -2.450031000 | -0.071610000 | -0.522534000 |
| 7 | 0.033963000 | 1.733871000 | -0.079578000 |
| 8 | 0.061584000 | 2.914157000 | -0.025864000 |
| 6 | -0.028901000 | -0.282148000 | 1.831634000 |
| 8 | -0.045693000 | -0.436583000 | 2.973401000 |
| 1 | 3.066352000 | -1.319677000 | -0.897282000 |
| 1 | 3.384483000 | 0.217307000 | 0.505870000 |

| | | | |
|---|---|---|---|
| 1 | 2.988956000 | 0.698235000 | -1.512830000 |
| 1 | -3.061386000 | -1.276044000 | -0.935148000 |
| 1 | -3.392451000 | 0.261488000 | 0.477126000 |
| 1 | -2.976105000 | 0.755704000 | -1.535020000 |
| 1 | 0.005568000 | -0.318927000 | -1.980197000 |
| 8 | -0.089745000 | -2.396652000 | -0.459516000 |
| 1 | 0.541109000 | -2.964671000 | -0.007756000 |
| 1 | 0.093066000 | -2.444798000 | -1.405583000 |

**M3** complex of $Mo_{tetra}$
E (ZPE- corrected) = -1304.78390
G =-1304.82689

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.002666000 | -0.186765000 | -0.129744000 |
| 15 | 0.039815000 | 2.184477000 | -0.454491000 |
| 7 | 0.002634000 | -0.049166000 | 1.676261000 |
| 8 | 0.011265000 | 0.089669000 | 2.855761000 |
| 1 | 1.081887000 | 2.819125000 | -1.179945000 |
| 1 | 0.084382000 | 3.039330000 | 0.670128000 |
| 1 | -1.010047000 | 2.861889000 | -1.128254000 |
| 1 | -0.003175000 | -0.330971000 | -1.988047000 |
| 8 | -0.120166000 | -2.532628000 | -0.461812000 |
| 1 | 0.637860000 | -3.027365000 | -0.136915000 |
| 1 | -0.028177000 | -2.482035000 | -1.422494000 |
| 15 | 2.424935000 | -0.244438000 | -0.366507000 |
| 1 | 3.254502000 | 0.062671000 | 0.736095000 |
| 1 | 3.070190000 | 0.597320000 | -1.302722000 |
| 1 | 3.131536000 | -1.420250000 | -0.749075000 |
| 15 | -2.448624000 | -0.194451000 | -0.356573000 |
| 1 | -3.147599000 | -1.350004000 | -0.788118000 |
| 1 | -3.082657000 | 0.702481000 | -1.247113000 |
| 1 | -3.265850000 | 0.075947000 | 0.763870000 |

**M3** complex of $Cr_{bis}$
E (ZPE- corrected) = -1821.45186
G = -1821.49252

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.001234000 | -0.242782000 | -0.143014000 |
| 15 | 0.008018000 | 2.065838000 | -0.260921000 |
| 7 | -0.001099000 | -0.318399000 | 1.548104000 |
| 8 | 0.004475000 | -0.270313000 | 2.720027000 |
| 6 | 1.880202000 | -0.198712000 | -0.440467000 |
| 8 | 3.000927000 | -0.120319000 | -0.661510000 |
| 1 | 1.060518000 | 2.731370000 | -0.924196000 |
| 1 | 0.026387000 | 2.836195000 | 0.923204000 |
| 1 | -1.053898000 | 2.742425000 | -0.897797000 |
| 1 | 0.004635000 | -0.035343000 | -1.810592000 |
| 8 | -0.076758000 | -2.409728000 | -0.627708000 |
| 1 | 0.606500000 | -2.922579000 | -0.186272000 |
| 1 | 0.092124000 | -2.480530000 | -1.572652000 |
| 6 | -1.898503000 | -0.199814000 | -0.436644000 |
| 8 | -3.017323000 | -0.126188000 | -0.650758000 |

**M3** complex of $Cr_{tris}$
E (ZPE- corrected) = -2051.23285
G = -2051.27406

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.002280000 | -0.176046000 | -0.117278000 |
| 15 | 0.035291000 | 2.106269000 | -0.308210000 |
| 7 | 0.010941000 | -0.218422000 | 1.557594000 |
| 8 | 0.032272000 | -0.174768000 | 2.744151000 |

| | | | |
|---|---|---|---|
| 1 | 1.080097000 | 2.770370000 | -1.000868000 |
| 1 | 0.067733000 | 2.933670000 | 0.840285000 |
| 1 | -1.013155000 | 2.800162000 | -0.964365000 |
| 1 | 0.002634000 | -0.053474000 | -1.826640000 |
| 8 | -0.135463000 | -2.387449000 | -0.562749000 |
| 1 | 0.475494000 | -2.923051000 | -0.048867000 |
| 1 | 0.139620000 | -2.450333000 | -1.482883000 |
| 15 | -2.312312000 | -0.204023000 | -0.424803000 |
| 1 | -3.207075000 | -0.125190000 | 0.668762000 |
| 1 | -2.927199000 | -1.317267000 | -1.047713000 |
| 1 | -2.944927000 | 0.782736000 | -1.215385000 |
| 15 | 2.284088000 | -0.256091000 | -0.450620000 |
| 1 | 2.906154000 | -1.397605000 | -1.030957000 |
| 1 | 3.199768000 | -0.140188000 | 0.623493000 |
| 1 | 2.918508000 | 0.679651000 | -1.300076000 |

**M3** complex of $Cr_{tetra}$
E (ZPE- corrected) = -2281.00056
G = -2281.04214

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.002280000 | -0.176046000 | -0.117278000 |
| 15 | 0.035291000 | 2.106269000 | -0.308210000 |
| 7 | 0.010941000 | -0.218422000 | 1.557594000 |
| 8 | 0.032272000 | -0.174768000 | 2.744151000 |
| 1 | 1.080097000 | 2.770370000 | -1.000868000 |
| 1 | 0.067733000 | 2.933670000 | 0.840285000 |
| 1 | -1.013155000 | 2.800162000 | -0.964365000 |
| 1 | 0.002634000 | -0.053474000 | -1.826640000 |
| 8 | -0.135463000 | -2.387449000 | -0.562749000 |
| 1 | 0.475494000 | -2.923051000 | -0.048867000 |
| 1 | 0.139620000 | -2.450333000 | -1.482883000 |
| 15 | -2.312312000 | -0.204023000 | -0.424803000 |
| 1 | -3.207075000 | -0.125190000 | 0.668762000 |
| 1 | -2.927199000 | -1.317267000 | -1.047713000 |
| 1 | -2.944927000 | 0.782736000 | -1.215385000 |
| 15 | 2.284088000 | -0.256091000 | -0.450620000 |
| 1 | 2.906154000 | -1.397605000 | -1.030957000 |
| 1 | 3.199768000 | -0.140188000 | 0.623493000 |
| 1 | 2.918508000 | 0.679651000 | -1.300076000 |

**M4** complex of $W_{bis}$
E (ZPE- corrected) = -842.97246
G = -843.01358

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.046046000 | -0.214374000 | -0.044906000 |
| 15 | 2.549771000 | -0.010330000 | -0.024241000 |
| 7 | -0.249464000 | 1.259406000 | -1.117195000 |
| 8 | -0.353424000 | 2.113076000 | -1.922474000 |
| 6 | -0.327391000 | 0.967806000 | 1.527128000 |
| 8 | -0.484762000 | 1.604337000 | 2.473342000 |
| 1 | 3.159880000 | 1.245049000 | -0.200460000 |
| 1 | 3.240373000 | -0.418814000 | 1.133081000 |
| 1 | 3.296895000 | -0.746674000 | -0.965507000 |
| 6 | -2.047478000 | -0.532443000 | -0.123875000 |
| 8 | -3.183685000 | -0.665103000 | -0.178698000 |
| 8 | 0.472868000 | -2.130814000 | 0.014567000 |
| 1 | -0.148832000 | -2.860912000 | 0.026522000 |

**M4** complex of $W_{tris}$
E (ZPE- corrected) = -1072.74875
G = -1072.79103

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.046046000 | -0.214374000 | -0.044906000 |

| | | | |
|---|---|---|---|
| 15 | 2.549771000 | -0.010330000 | -0.024241000 |
| 7 | -0.249464000 | 1.259406000 | -1.117195000 |
| 8 | -0.353424000 | 2.113076000 | -1.922474000 |
| 6 | -0.327391000 | 0.967806000 | 1.527128000 |
| 8 | -0.484762000 | 1.604337000 | 2.473342000 |
| 1 | 3.159880000 | 1.245049000 | -0.200460000 |
| 1 | 3.240373000 | -0.418814000 | 1.133081000 |
| 1 | 3.296895000 | -0.746674000 | -0.965507000 |
| 6 | -2.047478000 | -0.532443000 | -0.123875000 |
| 8 | -3.183685000 | -0.665103000 | -0.178698000 |
| 8 | 0.472868000 | -2.130814000 | 0.014567000 |
| 1 | -0.148832000 | -2.860912000 | 0.026522000 |

**M4** complex of $W_{tetra}$
E (ZPE- corrected) = -1302.51125
G = -1302.55408

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.009107000 | -0.220203000 | 0.023276000 |
| 15 | 0.082031000 | 1.488572000 | -1.627081000 |
| 15 | 2.438963000 | -0.435951000 | 0.132138000 |
| 7 | 0.062067000 | 1.047367000 | 1.327009000 |
| 8 | 0.120949000 | 1.754684000 | 2.291003000 |
| 1 | 0.001516000 | 1.063171000 | -2.975620000 |
| 1 | 1.208470000 | 2.338047000 | -1.793761000 |
| 1 | -0.889654000 | 2.518508000 | -1.722297000 |
| 1 | 3.325150000 | 0.391055000 | -0.603149000 |
| 1 | 3.054049000 | -0.247970000 | 1.390413000 |
| 1 | 3.073871000 | -1.662429000 | -0.194648000 |
| 15 | -2.499976000 | -0.281479000 | 0.141338000 |
| 1 | -3.175532000 | -1.385577000 | -0.422922000 |
| 1 | -3.110440000 | -0.312612000 | 1.416000000 |
| 1 | -3.316976000 | 0.737723000 | -0.399925000 |
| 8 | -0.217595000 | -2.165352000 | -0.400904000 |
| 1 | 0.526888000 | -2.758250000 | -0.522311000 |

**M4** complex of $Mo_{bis}$
E (ZPE- corrected) = -844.08169
G = -844.12239

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.076592000 | -0.288976000 | -0.077607000 |
| 15 | -2.491671000 | -0.144108000 | -0.062470000 |
| 7 | 0.170040000 | 1.234535000 | -1.060617000 |
| 8 | 0.178605000 | 2.144173000 | -1.804230000 |
| 6 | 0.230261000 | 0.820867000 | 1.550006000 |
| 8 | 0.314239000 | 1.432951000 | 2.518309000 |
| 1 | -3.279528000 | -1.264125000 | -0.410661000 |
| 1 | -3.094894000 | 0.792210000 | -0.924662000 |
| 1 | -3.188332000 | 0.203808000 | 1.112648000 |
| 8 | -0.083379000 | -2.264205000 | -0.065504000 |
| 1 | -0.902522000 | -2.760843000 | -0.024747000 |
| 6 | 2.119914000 | -0.467456000 | -0.159839000 |
| 8 | 3.257053000 | -0.492251000 | -0.207665000 |

**M4** complex of $Mo_{tris}$
E (ZPE- corrected) = -1073.86540
G = -1073.90754

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.014781000 | -0.231516000 | -0.064794000 |
| 15 | -2.462548000 | -0.485273000 | -0.090563000 |
| 15 | 2.536408000 | -0.263735000 | -0.097414000 |
| 7 | -0.097813000 | 1.247266000 | -1.091053000 |
| 8 | -0.193435000 | 2.132507000 | -1.869566000 |
| 6 | -0.075732000 | 0.929688000 | 1.508949000 |

| | | | |
|---|---|---|---|
| 8 | -0.130195000 | 1.577612000 | 2.463526000 |
| 1 | -3.090548000 | -1.602063000 | -0.693675000 |
| 1 | -3.199262000 | 0.520161000 | -0.745804000 |
| 1 | -3.206057000 | -0.512948000 | 1.109293000 |
| 1 | 3.217236000 | -0.956054000 | -1.122465000 |
| 1 | 3.260750000 | 0.941749000 | -0.157673000 |
| 1 | 3.209056000 | -0.850291000 | 0.993431000 |
| 8 | 0.277953000 | -2.212270000 | -0.004970000 |
| 1 | -0.415366000 | -2.873548000 | 0.029640000 |

**M4** complex of $Mo_{tera}$
E (ZPE- corrected) = -1303.63154
G = -1303.67389

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.009291000 | 0.266499000 | -0.067756000 |
| 15 | 0.072576000 | -1.305621000 | 1.706543000 |
| 7 | 0.068684000 | -1.085711000 | -1.253408000 |
| 8 | 0.133181000 | -1.875578000 | -2.144709000 |
| 1 | -0.038583000 | -0.802132000 | 3.025532000 |
| 1 | 1.206131000 | -2.125364000 | 1.944862000 |
| 1 | -0.887300000 | -2.338914000 | 1.845117000 |
| 8 | -0.228823000 | 2.229859000 | 0.274164000 |
| 1 | 0.510772000 | 2.831686000 | 0.380969000 |
| 15 | 2.437503000 | 0.502333000 | -0.158034000 |
| 1 | 3.079737000 | 0.289470000 | -1.398734000 |
| 1 | 3.323096000 | -0.291738000 | 0.611658000 |
| 1 | 3.050616000 | 1.744885000 | 0.141145000 |
| 15 | -2.506201000 | 0.342422000 | -0.169772000 |
| 1 | -3.134777000 | 0.493176000 | -1.427406000 |
| 1 | -3.166842000 | 1.398326000 | 0.492503000 |
| 1 | -3.326449000 | -0.713640000 | 0.287282000 |

**M4** complex of $Cr_{bis}$
E (ZPE- corrected) = -1820.29248
G = -1820.33268

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.090125000 | -0.261437000 | -0.137217000 |
| 15 | -2.350575000 | -0.219616000 | -0.148427000 |
| 7 | 0.146903000 | 1.285350000 | -0.811549000 |
| 8 | 0.166871000 | 2.305763000 | -1.384177000 |
| 6 | 0.200236000 | 0.396695000 | 1.611257000 |
| 8 | 0.263726000 | 0.780864000 | 2.687199000 |
| 1 | -3.066246000 | -1.437491000 | -0.160552000 |
| 1 | -2.997399000 | 0.386373000 | -1.245648000 |
| 1 | -3.088720000 | 0.418110000 | 0.869638000 |
| 8 | 0.015364000 | -2.097686000 | -0.452431000 |
| 1 | -0.813449000 | -2.581420000 | -0.446219000 |
| 6 | 2.014943000 | -0.437495000 | -0.263575000 |
| 8 | 3.146793000 | -0.485129000 | -0.338447000 |

**M4** complex of $Cr_{tris}$
E (ZPE- corrected) = -2050.07798
G = -2050.11889

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.001296000 | -0.210118000 | -0.082182000 |
| 15 | -2.346320000 | -0.505286000 | -0.165918000 |
| 15 | 2.404584000 | -0.344432000 | -0.156530000 |
| 7 | -0.075737000 | 1.205309000 | -0.980381000 |
| 8 | -0.122693000 | 2.135012000 | -1.702520000 |
| 6 | -0.056677000 | 0.724806000 | 1.517869000 |
| 8 | -0.092626000 | 1.291238000 | 2.517958000 |
| 1 | -2.966225000 | -0.701270000 | -1.420817000 |
| 1 | -3.220367000 | 0.493849000 | 0.307568000 |

| | | | |
|---|---|---|---|
| 1 | -2.946829000 | -1.603095000 | 0.491644000 |
| 1 | 2.987531000 | -1.037419000 | -1.237476000 |
| 1 | 3.238944000 | 0.792209000 | -0.178871000 |
| 1 | 3.046748000 | -1.043423000 | 0.883779000 |
| 8 | 0.250920000 | -2.074332000 | -0.098748000 |
| 1 | -0.459465000 | -2.713597000 | -0.014806000 |

**M4** complex of $Cr_{tetra}$
E (ZPE- corrected) = -2279.84738
G = -2279.88958

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.000421000 | -0.265518000 | 0.038262000 |
| 15 | 0.051417000 | 1.458193000 | -1.472539000 |
| 7 | 0.080746000 | 0.720776000 | 1.387799000 |
| 8 | 0.138189000 | 1.305744000 | 2.420903000 |
| 1 | -0.141025000 | 1.153671000 | -2.841492000 |
| 1 | 1.198109000 | 2.271868000 | -1.654149000 |
| 1 | -0.874955000 | 2.526271000 | -1.413669000 |
| 8 | -0.257258000 | -2.002284000 | -0.650551000 |
| 1 | 0.477286000 | -2.568051000 | -0.898331000 |
| 15 | -2.389383000 | -0.417835000 | 0.136964000 |
| 1 | -2.928607000 | -1.259623000 | 1.134796000 |
| 1 | -3.089846000 | -0.971359000 | -0.954423000 |
| 1 | -3.240969000 | 0.684990000 | 0.370489000 |
| 15 | 2.329609000 | -0.567723000 | 0.075529000 |
| 1 | 2.923629000 | -1.706227000 | -0.524412000 |
| 1 | 2.954353000 | -0.698503000 | 1.336275000 |
| 1 | 3.244807000 | 0.376777000 | -0.450089000 |

**M5** complex of $W_{bis}$
E (ZPE- corrected) = -1186.13538
G = -1186.18173

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.000008000 | -0.001688000 | -0.067831000 |
| 15 | -2.505185000 | 0.021889000 | -0.315694000 |
| 15 | 2.505176000 | 0.022079000 | -0.315605000 |
| 7 | -0.000058000 | -0.033568000 | 1.771219000 |
| 8 | -0.000128000 | -0.090471000 | 2.955044000 |
| 6 | 0.000037000 | -2.069674000 | -0.050321000 |
| 8 | 0.000296000 | -3.212516000 | 0.020127000 |
| 1 | -3.117644000 | 1.117589000 | -0.956233000 |
| 1 | -3.322292000 | -0.032227000 | 0.830017000 |
| 1 | -3.130692000 | -0.999148000 | -1.060159000 |
| 1 | 3.117613000 | 1.117916000 | -0.955931000 |
| 1 | 3.322262000 | -0.032213000 | 0.830113000 |
| 1 | 3.130729000 | -0.998802000 | -1.060244000 |
| 8 | 0.000034000 | 0.098012000 | -2.142160000 |
| 1 | 0.000045000 | -0.701013000 | -2.670061000 |
| 6 | -0.000155000 | 2.085070000 | -0.006463000 |
| 8 | 0.000026000 | 3.221965000 | 0.101196000 |

**M5** complex of $W_{tris}$
E (ZPE- corrected) = -1415.91625
G = -1415.96308

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000050000 | -0.053084000 | -0.066222000 |
| 15 | -2.500032000 | -0.067048000 | -0.185664000 |
| 15 | -0.003262000 | 2.511621000 | 0.079172000 |
| 15 | 2.500114000 | -0.060610000 | -0.186090000 |
| 7 | 0.000619000 | -0.299910000 | 1.751523000 |
| 8 | 0.001007000 | -0.478487000 | 2.929224000 |
| 6 | 0.002736000 | -2.045503000 | -0.337799000 |
| 8 | 0.004403000 | -3.191107000 | -0.465605000 |

| | | | |
|---|---|---|---|
| 1 | -3.293259000 | 1.050123000 | 0.172162000 |
| 1 | -3.209504000 | -1.021441000 | 0.570196000 |
| 1 | -3.093077000 | -0.309623000 | -1.442335000 |
| 1 | -1.056457000 | 3.214783000 | 0.705293000 |
| 1 | 1.049899000 | 3.217703000 | 0.702073000 |
| 1 | -0.006067000 | 3.199224000 | -1.150902000 |
| 1 | 3.290390000 | 1.058667000 | 0.171710000 |
| 1 | 3.212080000 | -1.013135000 | 0.569772000 |
| 1 | 3.093896000 | -0.301630000 | -1.442726000 |
| 8 | -0.001034000 | 0.389618000 | -2.095450000 |
| 1 | 0.000365000 | -0.313696000 | -2.745348000 |

**M5** complex of $W_{tetra}$
E (ZPE- corrected) = -1645.68566
G = -1645.73231

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000360000 | -0.002147000 | -0.055503000 |
| 15 | -2.054584000 | 1.397711000 | -0.090301000 |
| 15 | 1.370316000 | 2.068366000 | -0.097690000 |
| 15 | 2.060746000 | -1.352365000 | -0.225217000 |
| 7 | 0.020840000 | -0.114743000 | 1.768259000 |
| 8 | 0.040255000 | -0.214391000 | 2.962757000 |
| 1 | -2.526223000 | 1.815255000 | -1.353738000 |
| 1 | -2.102554000 | 2.653956000 | 0.559501000 |
| 1 | -3.284549000 | 0.924770000 | 0.427670000 |
| 1 | 0.940163000 | 3.256593000 | 0.540563000 |
| 1 | 2.686281000 | 2.099203000 | 0.423745000 |
| 1 | 1.651718000 | 2.618773000 | -1.365927000 |
| 1 | 3.277101000 | -0.902946000 | 0.346457000 |
| 1 | 2.134335000 | -2.664315000 | 0.302896000 |
| 1 | 2.578505000 | -1.654401000 | -1.507489000 |
| 8 | -0.041681000 | 0.223164000 | -2.124648000 |
| 1 | 0.095113000 | -0.515853000 | -2.718671000 |
| 15 | -1.390853000 | -2.037831000 | -0.235244000 |
| 1 | -1.744420000 | -2.507537000 | -1.522448000 |
| 1 | -0.961201000 | -3.280504000 | 0.290948000 |
| 1 | -2.689754000 | -2.089309000 | 0.327779000 |

**M5** complex of $Mo_{bis}$
E (ZPE- corrected) = -1187.24874
G = -1187.29451

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.000015000 | -0.002193000 | -0.056487000 |
| 15 | -2.494910000 | 0.021693000 | -0.358116000 |
| 15 | 2.494939000 | 0.021411000 | -0.358238000 |
| 7 | -0.000021000 | -0.033600000 | 1.763404000 |
| 8 | 0.000199000 | -0.094588000 | 2.941466000 |
| 6 | -0.000109000 | -2.063704000 | -0.064506000 |
| 8 | -0.000331000 | -3.205421000 | -0.021601000 |
| 1 | -3.076178000 | 1.115295000 | -1.029301000 |
| 1 | -3.372027000 | -0.026819000 | 0.744398000 |
| 1 | -3.088538000 | -1.000086000 | -1.126204000 |
| 1 | 3.076376000 | 1.115092000 | -1.029149000 |
| 1 | 3.372123000 | -0.027568000 | 0.744202000 |
| 1 | 3.088323000 | -1.000260000 | -1.126656000 |
| 8 | -0.000068000 | 0.092382000 | -2.134695000 |
| 1 | -0.000200000 | -0.717779000 | -2.646324000 |
| 6 | 0.000106000 | 2.083945000 | -0.022385000 |
| 8 | 0.000105000 | 3.220305000 | 0.060366000 |

**M5** complex of $Mo_{tris}$
E (ZPE- corrected) = -1417.03218

G = -1417.07991

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.000006000 | -0.074412000 | -0.052472000 |
| 15 | -2.494639000 | -0.072932000 | -0.257034000 |
| 15 | 2.494614000 | -0.073959000 | -0.257151000 |
| 7 | 0.000016000 | -0.379035000 | 1.733090000 |
| 8 | 0.000048000 | -0.581795000 | 2.900636000 |
| 6 | -0.000502000 | -2.046483000 | -0.382297000 |
| 8 | -0.000822000 | -3.185285000 | -0.545634000 |
| 1 | -3.251114000 | 1.119881000 | -0.346788000 |
| 1 | -3.281897000 | -0.704814000 | 0.726844000 |
| 1 | -3.049878000 | -0.702191000 | -1.389860000 |
| 1 | 3.251570000 | 1.118601000 | -0.346241000 |
| 1 | 3.281631000 | -0.706741000 | 0.726341000 |
| 1 | 3.049512000 | -0.702814000 | -1.390367000 |
| 8 | 0.000018000 | 0.500542000 | -2.057122000 |
| 1 | 0.000538000 | -0.158781000 | -2.752119000 |
| 15 | 0.000479000 | 2.500941000 | 0.133783000 |
| 1 | -0.002773000 | 3.162834000 | 1.379697000 |
| 1 | -1.052880000 | 3.226519000 | -0.462170000 |
| 1 | 1.057169000 | 3.226487000 | -0.456366000 |

**M5** complex of $Mo_{tetra}$
E (ZPE- corrected) = -1646.80408
G = -1646.85053

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.001284000 | -0.000719000 | -0.053788000 |
| 15 | 0.001541000 | 2.485654000 | -0.113673000 |
| 15 | 0.031024000 | -2.460190000 | -0.256042000 |
| 7 | -0.084993000 | -0.086099000 | 1.749367000 |
| 8 | -0.161489000 | -0.165406000 | 2.937668000 |
| 1 | 0.171720000 | 3.084663000 | -1.379318000 |
| 1 | 0.956035000 | 3.253670000 | 0.594141000 |
| 1 | -1.120381000 | 3.244699000 | 0.301064000 |
| 1 | 1.128046000 | -3.223743000 | 0.214662000 |
| 1 | -0.966208000 | -3.265966000 | 0.343000000 |
| 1 | -0.028616000 | -3.041420000 | -1.544112000 |
| 8 | 0.161931000 | 0.161588000 | -2.126024000 |
| 1 | -0.368685000 | -0.383302000 | -2.708703000 |
| 15 | 2.484725000 | 0.025063000 | -0.107180000 |
| 1 | 3.237763000 | 0.980286000 | 0.615615000 |
| 1 | 3.091729000 | 0.215176000 | -1.366298000 |
| 1 | 3.252245000 | -1.093608000 | 0.300479000 |
| 15 | -2.461984000 | 0.007055000 | -0.249346000 |
| 1 | -3.238916000 | 1.094061000 | 0.222108000 |
| 1 | -3.048511000 | -0.064529000 | -1.534473000 |
| 1 | -3.250493000 | -1.000279000 | 0.355846000 |

**M5** complex of $Cr_{bis}$
E (ZPE- corrected) = -2163.45340
G = -2163.49644

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.000026000 | -0.011231000 | 0.029108000 |
| 15 | -2.328704000 | 0.031775000 | -0.431474000 |
| 15 | 2.328783000 | 0.027702000 | -0.431235000 |
| 7 | -0.000221000 | -0.043863000 | 1.713238000 |
| 8 | -0.000467000 | -0.093998000 | 2.884759000 |
| 6 | -0.001710000 | -1.931656000 | -0.051709000 |
| 8 | -0.002701000 | -3.073007000 | -0.076768000 |
| 1 | -2.792271000 | 1.120382000 | -1.191713000 |
| 1 | -3.346676000 | 0.023066000 | 0.549988000 |
| 1 | -2.837680000 | -1.001619000 | -1.241107000 |
| 1 | 2.794335000 | 1.115692000 | -1.191147000 |

| | | | |
|---|---|---|---|
| 1 | 3.346553000 | 0.017081000 | 0.550415000 |
| 1 | 2.836176000 | -1.006372000 | -1.240996000 |
| 8 | 0.000057000 | 0.107515000 | -1.987892000 |
| 1 | -0.000387000 | -0.726743000 | -2.461191000 |
| 6 | 0.001880000 | 1.936173000 | 0.002595000 |
| 8 | 0.003099000 | 3.073971000 | 0.026126000 |

**M5** complex of $Cr_{tris}$
E (ZPE- corrected) =-2393.23658
G = -2393.28126

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.000067000 | 0.099017000 | 0.016171000 |
| 15 | 2.348970000 | 0.063379000 | -0.334191000 |
| 15 | 0.001364000 | -2.338607000 | 0.109172000 |
| 15 | -2.349255000 | 0.060357000 | -0.333212000 |
| 7 | 0.000411000 | 0.335878000 | 1.675921000 |
| 8 | 0.000934000 | 0.503790000 | 2.842477000 |
| 6 | -0.001546000 | 1.946909000 | -0.312889000 |
| 8 | -0.002495000 | 3.080923000 | -0.490789000 |
| 1 | 2.978743000 | -1.124572000 | -0.767317000 |
| 1 | 3.291041000 | 0.414816000 | 0.659600000 |
| 1 | 2.841730000 | 0.897838000 | -1.357166000 |
| 1 | 0.002628000 | -3.072615000 | 1.316188000 |
| 1 | -1.053783000 | -3.029677000 | -0.522844000 |
| 1 | 1.056370000 | -3.028476000 | -0.524378000 |
| 1 | -2.978411000 | -1.129026000 | -0.763369000 |
| 1 | -3.291324000 | 0.413433000 | 0.659985000 |
| 1 | -2.842844000 | 0.892033000 | -1.358050000 |
| 8 | 0.000282000 | -0.422889000 | -1.931010000 |
| 1 | -0.002109000 | 0.285719000 | -2.576831000 |

**M5** complex of $Cr_{tetra}$
E (ZPE- corrected) = -2623.00845
G = -2623.05444

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.010202000 | -0.000310000 | 0.024912000 |
| 15 | 1.680344000 | 1.664675000 | -0.089043000 |
| 15 | 1.686923000 | -1.658117000 | -0.088680000 |
| 15 | -1.627218000 | -1.668061000 | -0.351988000 |
| 7 | -0.207486000 | -0.003587000 | 1.678848000 |
| 8 | -0.373873000 | -0.007235000 | 2.854979000 |
| 1 | 2.868661000 | 1.365500000 | -0.790559000 |
| 1 | 2.284884000 | 2.241310000 | 1.052458000 |
| 1 | 1.405709000 | 2.877141000 | -0.763593000 |
| 1 | 2.297972000 | -2.224656000 | 1.054283000 |
| 1 | 1.416057000 | -2.876072000 | -0.755171000 |
| 1 | 2.871337000 | -1.356282000 | -0.795700000 |
| 1 | -1.263475000 | -2.953880000 | -0.823791000 |
| 1 | -2.457075000 | -2.109537000 | 0.702701000 |
| 1 | -2.661701000 | -1.467249000 | -1.299688000 |
| 8 | 0.382309000 | 0.005327000 | -1.962704000 |
| 1 | -0.335162000 | 0.004631000 | -2.598575000 |
| 15 | -1.633042000 | 1.663522000 | -0.342820000 |
| 1 | -1.273466000 | 2.946628000 | -0.825563000 |
| 1 | -2.679550000 | 1.460098000 | -1.276996000 |
| 1 | -2.449539000 | 2.109908000 | 0.720138000 |

**M6** complex of $W_{bis}$
E (ZPE- corrected) = -1187.29548
G = -1187.34542

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.159663000 | -0.004960000 | 0.020709000 |
| 15 | 2.033359000 | -0.522430000 | 1.131827000 |

| | | | |
|---|---|---|---|
| 15 | -1.993898000 | 0.540422000 | -1.567241000 |
| 7 | -1.216375000 | -0.173573000 | 1.530439000 |
| 8 | -1.918823000 | -0.273250000 | 2.468589000 |
| 6 | 0.201643000 | 2.013780000 | 0.281641000 |
| 8 | 0.421341000 | 3.130157000 | 0.401144000 |
| 1 | 2.882013000 | -1.492575000 | 0.572856000 |
| 1 | 1.968642000 | -1.023923000 | 2.447140000 |
| 1 | 2.988098000 | 0.488263000 | 1.339797000 |
| 1 | -2.217250000 | -0.294760000 | -2.680078000 |
| 1 | -3.323792000 | 0.603829000 | -1.102689000 |
| 1 | -1.973565000 | 1.767605000 | -2.260138000 |
| 1 | 0.793703000 | 0.183558000 | -1.547833000 |
| 8 | 3.487484000 | 0.201190000 | -1.658354000 |
| 1 | 2.524328000 | 0.225787000 | -1.780839000 |
| 1 | 3.818945000 | 0.989146000 | -2.096130000 |
| 6 | -0.307497000 | -1.995216000 | -0.526333000 |
| 8 | -0.376028000 | -3.088869000 | -0.853657000 |

**M6** complex of $W_{tris}$
E (ZPE- corrected) = -1417.07365
G = -1187.34542

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.185552000 | 0.047307000 | -0.015876000 |
| 15 | 1.610466000 | 1.650000000 | 0.627636000 |
| 15 | 1.246617000 | -1.877896000 | 0.799893000 |
| 15 | -1.697764000 | -1.551926000 | -1.147337000 |
| 7 | -1.164628000 | 0.212336000 | 1.535151000 |
| 8 | -1.801108000 | 0.286425000 | 2.528260000 |
| 6 | -1.148412000 | 1.559618000 | -0.945471000 |
| 8 | -1.694422000 | 2.418276000 | -1.483770000 |
| 1 | 2.853090000 | 1.228126000 | 1.147365000 |
| 1 | 1.301284000 | 2.603690000 | 1.618919000 |
| 1 | 2.114396000 | 2.531510000 | -0.346969000 |
| 1 | 1.013832000 | -2.429078000 | 2.078286000 |
| 1 | 1.261223000 | -3.092728000 | 0.080378000 |
| 1 | 2.643924000 | -1.722457000 | 0.906268000 |
| 1 | -1.319881000 | -2.897175000 | -1.374373000 |
| 1 | -2.969048000 | -1.819189000 | -0.596708000 |
| 1 | -2.116548000 | -1.274495000 | -2.464385000 |
| 1 | 0.779170000 | -0.231862000 | -1.577432000 |
| 8 | 3.432981000 | -0.233563000 | -1.490487000 |
| 1 | 2.473870000 | -0.231636000 | -1.662128000 |
| 1 | 3.848995000 | -0.081281000 | -2.342517000 |

**M6** complex of $W_{tetra}$
E (ZPE- corrected) = -1646.84416
G = -1646.89446

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.155940000 | 0.001023000 | 0.018524000 |
| 15 | -1.305767000 | 1.867279000 | 0.714947000 |
| 15 | 1.572729000 | 1.599906000 | -1.197460000 |
| 15 | 1.320163000 | -1.848881000 | -1.102531000 |
| 7 | 1.174343000 | -0.032664000 | 1.540395000 |
| 8 | 1.850657000 | -0.058245000 | 2.517625000 |
| 1 | -1.372759000 | 3.055058000 | -0.052534000 |
| 1 | -1.079209000 | 2.481368000 | 1.965785000 |
| 1 | -2.701607000 | 1.688223000 | 0.844379000 |
| 1 | 2.730829000 | 2.120683000 | -0.578995000 |
| 1 | 2.181919000 | 1.246797000 | -2.427278000 |
| 1 | 1.051753000 | 2.838042000 | -1.649028000 |
| 1 | 1.960751000 | -1.653204000 | -2.351322000 |
| 1 | 2.401804000 | -2.487924000 | -0.457039000 |
| 1 | 0.629959000 | -3.026719000 | -1.481872000 |
| 1 | -0.820540000 | 0.031953000 | -1.573210000 |

| | | | |
|---|---|---|---|
| 8 | -3.489424000 | 0.026595000 | -1.585199000 |
| 1 | -2.518552000 | 0.030568000 | -1.669854000 |
| 1 | -3.823261000 | -0.034722000 | -2.483373000 |
| 15 | -1.538064000 | -1.597677000 | 0.851522000 |
| 1 | -1.803621000 | -2.799972000 | 0.153471000 |
| 1 | -1.335622000 | -2.174257000 | 2.123935000 |
| 1 | -2.887563000 | -1.219120000 | 1.026787000 |

**M6** complex of $Mo_{bis}$
E (ZPE- corrected) = -1188.41143
G = -1188.46074

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.206885000 | -0.009525000 | 0.041699000 |
| 15 | 1.978198000 | -0.567824000 | 1.139533000 |
| 15 | -1.996286000 | 0.588585000 | -1.564237000 |
| 7 | -1.272748000 | -0.198150000 | 1.523435000 |
| 8 | -1.988145000 | -0.308154000 | 2.444667000 |
| 6 | 0.186784000 | 1.992689000 | 0.324147000 |
| 8 | 0.427573000 | 3.101979000 | 0.450029000 |
| 1 | 2.828499000 | -1.521297000 | 0.554729000 |
| 1 | 1.917488000 | -1.111665000 | 2.438671000 |
| 1 | 2.937677000 | 0.430537000 | 1.383052000 |
| 1 | -2.205816000 | -0.218119000 | -2.700292000 |
| 1 | -3.338793000 | 0.659886000 | -1.136197000 |
| 1 | -1.948825000 | 1.829162000 | -2.231143000 |
| 1 | 0.749122000 | 0.204465000 | -1.503378000 |
| 8 | 3.437681000 | 0.232943000 | -1.641867000 |
| 1 | 2.471978000 | 0.259568000 | -1.745158000 |
| 1 | 3.763447000 | 1.012394000 | -2.098643000 |
| 6 | -0.352041000 | -1.972462000 | -0.572293000 |
| 8 | -0.416300000 | -3.050595000 | -0.942532000 |

**M6** complex of $Mo_{tris}$
E (ZPE- corrected) = -1418.190812
G = -1418.193312

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.191393000 | 0.063639000 | 0.051916000 |
| 15 | 1.948849000 | -0.445446000 | 1.228752000 |
| 15 | -1.943326000 | 0.595472000 | -1.600659000 |
| 7 | -1.256247000 | 0.074899000 | 1.535118000 |
| 8 | -1.972014000 | 0.055308000 | 2.469045000 |
| 6 | 0.262879000 | 2.021199000 | 0.156888000 |
| 8 | 0.534959000 | 3.135591000 | 0.210312000 |
| 1 | 2.735956000 | -1.557162000 | 0.864244000 |
| 1 | 1.881188000 | -0.709356000 | 2.613312000 |
| 1 | 2.985895000 | 0.504003000 | 1.261645000 |
| 1 | -2.381165000 | -0.362457000 | -2.545405000 |
| 1 | -3.223916000 | 1.006843000 | -1.171944000 |
| 1 | -1.715141000 | 1.638624000 | -2.520346000 |
| 1 | 0.771520000 | -0.047967000 | -1.512545000 |
| 8 | 3.441899000 | 0.052002000 | -1.706976000 |
| 1 | 2.470214000 | 0.070799000 | -1.751281000 |
| 1 | 3.725501000 | 0.895008000 | -2.069432000 |
| 15 | -0.440719000 | -2.382592000 | -0.485353000 |
| 1 | -1.176314000 | -3.251341000 | 0.351335000 |
| 1 | 0.710059000 | -3.191311000 | -0.604131000 |
| 1 | -1.039649000 | -2.774743000 | -1.703249000 |

**M6** complex of $Mo_{tetra}$
E (ZPE- corrected) = -1647.96483
G = -1648.01500

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.198767000 | 0.000800000 | 0.037726000 |

| | | | |
|---|---|---|---|
| 15 | -1.317282000 | 1.810655000 | 0.757560000 |
| 15 | 1.384666000 | -1.794729000 | -1.134771000 |
| 7 | 1.222769000 | -0.025086000 | 1.535498000 |
| 8 | 1.912636000 | -0.044694000 | 2.497391000 |
| 1 | -1.436400000 | 2.998089000 | -0.002488000 |
| 1 | -1.101995000 | 2.432846000 | 2.006960000 |
| 1 | -2.703655000 | 1.584311000 | 0.905337000 |
| 1 | 2.011141000 | -1.556609000 | -2.382336000 |
| 1 | 2.482934000 | -2.440075000 | -0.522952000 |
| 1 | 0.709902000 | -2.971973000 | -1.539132000 |
| 1 | -0.768626000 | 0.025554000 | -1.545345000 |
| 8 | -3.430076000 | 0.018185000 | -1.593409000 |
| 1 | -2.457078000 | 0.022599000 | -1.659789000 |
| 1 | -3.746479000 | -0.013445000 | -2.499428000 |
| 15 | 1.538296000 | 1.650564000 | -1.185347000 |
| 1 | 2.687657000 | 2.218304000 | -0.590716000 |
| 1 | 0.966120000 | 2.868574000 | -1.626088000 |
| 1 | 2.141600000 | 1.322559000 | -2.423895000 |
| 15 | -1.457891000 | -1.649210000 | 0.835206000 |
| 1 | -2.815471000 | -1.302608000 | 1.010837000 |
| 1 | -1.696343000 | -2.844247000 | 0.116566000 |
| 1 | -1.258209000 | -2.249005000 | 2.097894000 |

**M6** complex of $Cr_{bis}$
E (ZPE- corrected) = -1418.19158
G = -1418.24036

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.270583000 | -0.002862000 | 0.075768000 |
| 15 | 1.704805000 | -0.182733000 | 1.352594000 |
| 15 | -1.822653000 | 0.192819000 | -1.655551000 |
| 7 | -1.366507000 | -0.092001000 | 1.361911000 |
| 8 | -2.140044000 | -0.152103000 | 2.236414000 |
| 6 | -0.022214000 | 1.886099000 | 0.024779000 |
| 8 | 0.156361000 | 3.013217000 | -0.043275000 |
| 1 | 2.636287000 | -1.201081000 | 1.082231000 |
| 1 | 1.554256000 | -0.409536000 | 2.736577000 |
| 1 | 2.611322000 | 0.890673000 | 1.427196000 |
| 1 | -1.846414000 | -0.769220000 | -2.685797000 |
| 1 | -3.205172000 | 0.187262000 | -1.369340000 |
| 1 | -1.814432000 | 1.335494000 | -2.481686000 |
| 1 | 0.754073000 | 0.090377000 | -1.248627000 |
| 8 | 3.463269000 | 0.041954000 | -1.459723000 |
| 1 | 2.501701000 | 0.065718000 | -1.577023000 |
| 1 | 3.802879000 | 0.750226000 | -2.012561000 |
| 6 | -0.124907000 | -1.863442000 | -0.321912000 |
| 8 | -0.015151000 | -2.967372000 | -0.595367000 |

**M6** complex of $Cr_{tris}$
E (ZPE- corrected) = -2394.40553
G = -2394.45349

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.283054000 | 0.065632000 | 0.028539000 |
| 15 | -1.381524000 | 1.539053000 | 0.779331000 |
| 15 | 1.555991000 | -1.413916000 | -1.235349000 |
| 7 | 1.352543000 | 0.264441000 | 1.314940000 |
| 8 | 2.115635000 | 0.397577000 | 2.198250000 |
| 1 | -1.898737000 | 2.507328000 | -0.103584000 |
| 1 | -1.057608000 | 2.414134000 | 1.838659000 |
| 1 | -2.621589000 | 1.092741000 | 1.286403000 |
| 1 | 1.874494000 | -1.080582000 | -2.568111000 |
| 1 | 2.863887000 | -1.763300000 | -0.829012000 |
| 1 | 1.109438000 | -2.730132000 | -1.501355000 |
| 1 | -0.745787000 | -0.190879000 | -1.288996000 |
| 8 | -3.401630000 | -0.289933000 | -1.369128000 |

| | | | |
|---|---|---|---|
| 1 | -2.437033000 | -0.253883000 | -1.485787000 |
| 1 | -3.771379000 | -0.101098000 | -2.235156000 |
| 6 | 0.944872000 | 1.460224000 | -1.033863000 |
| 8 | 1.340091000 | 2.308289000 | -1.699203000 |
| 15 | -0.954750000 | -1.757708000 | 0.901524000 |
| 1 | -2.344903000 | -1.637095000 | 1.108229000 |
| 1 | -0.996588000 | -2.985104000 | 0.203323000 |
| 1 | -0.633046000 | -2.298633000 | 2.167103000 |

**M6** complex of $Cr_{tetra}$
E (ZPE- corrected) = -2624.17726
G =-2624.22582

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.245470000 | 0.000034000 | 0.064755000 |
| 15 | 1.199209000 | -1.636295000 | 0.893165000 |
| 15 | -1.290549000 | -1.628128000 | -1.209806000 |
| 15 | -1.290814000 | 1.627932000 | -1.209936000 |
| 7 | -1.323318000 | -0.000044000 | 1.347422000 |
| 8 | -2.097985000 | -0.000147000 | 2.240214000 |
| 1 | 1.436112000 | -2.830353000 | 0.171133000 |
| 1 | 0.904020000 | -2.252719000 | 2.130509000 |
| 1 | 2.557433000 | -1.353775000 | 1.162615000 |
| 1 | -2.469609000 | -2.258561000 | -0.747237000 |
| 1 | -1.770004000 | -1.337783000 | -2.510686000 |
| 1 | -0.611188000 | -2.816578000 | -1.572857000 |
| 1 | -1.769791000 | 1.337464000 | -2.510962000 |
| 1 | -2.470266000 | 2.257832000 | -0.747641000 |
| 1 | -0.611872000 | 2.816704000 | -1.572725000 |
| 1 | 0.794582000 | -0.000002000 | -1.289932000 |
| 8 | 3.448028000 | 0.000028000 | -1.442745000 |
| 1 | 2.475352000 | 0.000084000 | -1.482221000 |
| 1 | 3.738930000 | -0.000197000 | -2.357870000 |
| 15 | 1.199053000 | 1.636534000 | 0.893109000 |
| 1 | 2.557330000 | 1.354160000 | 1.162446000 |
| 1 | 1.435761000 | 2.830656000 | 0.171116000 |
| 1 | 0.903890000 | 2.252871000 | 2.130502000 |

**M7** complex of $W_{bis}$
E (ZPE- corrected) = -1187.26088
G = -1187.30664

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.006462000 | 0.073821000 | -0.040962000 |
| 15 | 2.471514000 | -0.271570000 | -0.043378000 |
| 15 | -2.475046000 | 0.067488000 | -0.088180000 |
| 7 | -0.028346000 | 0.040360000 | 1.764367000 |
| 8 | -0.056482000 | -0.005382000 | 2.946068000 |
| 6 | 0.161798000 | 2.112505000 | -0.158706000 |
| 8 | 0.246758000 | 3.259653000 | -0.224107000 |
| 1 | 3.141657000 | -0.442524000 | -1.274595000 |
| 1 | 2.978866000 | -1.410110000 | 0.615783000 |
| 1 | 3.350048000 | 0.679703000 | 0.515940000 |
| 1 | -3.164761000 | -0.050995000 | -1.318505000 |
| 1 | -3.136224000 | -0.977745000 | 0.589988000 |
| 1 | -3.233948000 | 1.138648000 | 0.429298000 |
| 1 | -0.202686000 | -2.289870000 | -1.672507000 |
| 8 | 0.099320000 | -0.022577000 | -2.348818000 |
| 1 | -0.079851000 | -0.956491000 | -2.592814000 |
| 1 | -0.433072000 | 0.548880000 | -2.909941000 |
| 6 | -0.158070000 | -2.095312000 | -0.496114000 |
| 8 | -0.223240000 | -3.110034000 | 0.151893000 |

**M7** complex of $W_{tris}$
E (ZPE- corrected) = -1417.03226

G = -1417.07799

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.012199000 | -0.016520000 | -0.040340000 |
| 15 | -1.690194000 | 1.798376000 | -0.055645000 |
| 15 | 1.914933000 | -1.549402000 | -0.077552000 |
| 7 | 0.114172000 | 0.088706000 | 1.750847000 |
| 8 | 0.216790000 | 0.173593000 | 2.933274000 |
| 1 | -2.012140000 | 2.440986000 | -1.273104000 |
| 1 | -1.382180000 | 2.952415000 | 0.694682000 |
| 1 | -3.021926000 | 1.645103000 | 0.404609000 |
| 1 | 2.565866000 | -1.842319000 | -1.301940000 |
| 1 | 3.061650000 | -1.146334000 | 0.640081000 |
| 1 | 1.880624000 | -2.885212000 | 0.396095000 |
| 1 | 1.504429000 | 1.613940000 | -1.765870000 |
| 8 | -0.122313000 | -0.014460000 | -2.372036000 |
| 1 | 0.562777000 | 0.648407000 | -2.615752000 |
| 1 | 0.070347000 | -0.821194000 | -2.859646000 |
| 6 | 1.418022000 | 1.518200000 | -0.576170000 |
| 8 | 2.142889000 | 2.286257000 | 0.010242000 |
| 15 | -1.742998000 | -1.823602000 | -0.038058000 |
| 1 | -3.016363000 | -1.627503000 | 0.553510000 |
| 1 | -2.238548000 | -2.348238000 | -1.258280000 |
| 1 | -1.504196000 | -3.081387000 | 0.568845000 |

**M7** complex of $Mo_{bis}$
E (ZPE- corrected) = -1188.38065
G = -1188.42640

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.006341000 | 0.103665000 | -0.057988000 |
| 15 | 2.469985000 | -0.244257000 | -0.066811000 |
| 15 | -2.473498000 | 0.033302000 | -0.100114000 |
| 7 | -0.022709000 | 0.037837000 | 1.727580000 |
| 8 | -0.046569000 | -0.023895000 | 2.903542000 |
| 6 | 0.136371000 | 2.149695000 | -0.136232000 |
| 8 | 0.208337000 | 3.296015000 | -0.152774000 |
| 1 | 3.120345000 | -0.531098000 | -1.286902000 |
| 1 | 2.973860000 | -1.328715000 | 0.679339000 |
| 1 | 3.378625000 | 0.733025000 | 0.393003000 |
| 1 | -3.156864000 | -0.199449000 | -1.317242000 |
| 1 | -3.098492000 | -0.983491000 | 0.650403000 |
| 1 | -3.281724000 | 1.105323000 | 0.337152000 |
| 1 | -0.163223000 | -2.258705000 | -1.659218000 |
| 8 | 0.093493000 | 0.023746000 | -2.374521000 |
| 1 | -0.071685000 | -0.909101000 | -2.621143000 |
| 1 | -0.448121000 | 0.584908000 | -2.936872000 |
| 6 | -0.125653000 | -2.060968000 | -0.487249000 |
| 8 | -0.176724000 | -3.070805000 | 0.167336000 |

**M7** complex of $Mo_{tris}$
E (ZPE- corrected) = -1418.15564
G = -1418.20158

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.023703000 | -0.018144000 | -0.054349000 |
| 15 | -1.277067000 | 2.112033000 | -0.075485000 |
| 15 | 1.561771000 | -1.902789000 | -0.094106000 |
| 7 | 0.146714000 | 0.078278000 | 1.714100000 |
| 8 | 0.278188000 | 0.149843000 | 2.889403000 |
| 1 | -1.423609000 | 2.820363000 | -1.290000000 |
| 1 | -0.743618000 | 3.167309000 | 0.692919000 |
| 1 | -2.620229000 | 2.256919000 | 0.353021000 |
| 1 | 2.156386000 | -2.306835000 | -1.315203000 |
| 1 | 2.759334000 | -1.738632000 | 0.633804000 |
| 1 | 1.271907000 | -3.212993000 | 0.363434000 |
| 1 | 1.779395000 | 1.265456000 | -1.758726000 |

| | | | |
|---|---|---|---|
| 8 | -0.147803000 | -0.011126000 | -2.397697000 |
| 1 | 0.653570000 | 0.497432000 | -2.644877000 |
| 1 | -0.120761000 | -0.839923000 | -2.885180000 |
| 6 | 1.679163000 | 1.187653000 | -0.573563000 |
| 8 | 2.543189000 | 1.789749000 | 0.015365000 |
| 15 | -2.092326000 | -1.451385000 | 0.000188000 |
| 1 | -2.704258000 | -1.922315000 | -1.188538000 |
| 1 | -3.294400000 | -0.989137000 | 0.590777000 |
| 1 | -2.094396000 | -2.705098000 | 0.658370000 |

**M7** complex of $Cr7_{bis}$
E (ZPE- corrected) = -2164.59292
G = -2164.63731

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.009054000 | 0.132395000 | -0.061709000 |
| 15 | 2.325352000 | -0.300105000 | -0.112087000 |
| 15 | -2.339704000 | 0.116342000 | -0.137328000 |
| 7 | -0.030301000 | -0.102231000 | 1.585755000 |
| 8 | -0.060396000 | -0.300380000 | 2.741070000 |
| 6 | 0.196624000 | 2.029199000 | 0.037756000 |
| 8 | 0.313729000 | 3.163314000 | 0.171579000 |
| 1 | 2.928594000 | -0.738547000 | -1.311600000 |
| 1 | 2.779093000 | -1.338311000 | 0.725226000 |
| 1 | 3.308767000 | 0.654742000 | 0.232370000 |
| 1 | -3.018339000 | -0.191440000 | -1.341269000 |
| 1 | -2.972974000 | -0.844327000 | 0.676096000 |
| 1 | -3.151561000 | 1.217561000 | 0.219887000 |
| 1 | -0.211360000 | -2.000773000 | -1.754925000 |
| 8 | 0.124417000 | 0.305999000 | -2.271457000 |
| 1 | -0.092880000 | -0.571823000 | -2.637441000 |
| 1 | -0.394291000 | 0.962298000 | -2.745111000 |
| 6 | -0.176376000 | -1.865088000 | -0.585008000 |
| 8 | -0.263555000 | -2.898867000 | 0.026586000 |

**M7** complex of $Cr7_{tris}$
E (ZPE- corrected) = -2394.36595
G = -2394.41078

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.038730000 | -0.026697000 | -0.064106000 |
| 15 | -1.096290000 | 2.066421000 | -0.102597000 |
| 15 | 1.383369000 | -1.878221000 | -0.135392000 |
| 7 | 0.216376000 | 0.108009000 | 1.568893000 |
| 8 | 0.425490000 | 0.221785000 | 2.725406000 |
| 1 | -1.141063000 | 2.819152000 | -1.298748000 |
| 1 | -0.517348000 | 3.053895000 | 0.719652000 |
| 1 | -2.443095000 | 2.304653000 | 0.275531000 |
| 1 | 1.977731000 | -2.294759000 | -1.353356000 |
| 1 | 2.576285000 | -1.748084000 | 0.605045000 |
| 1 | 1.056454000 | -3.185492000 | 0.310668000 |
| 1 | 1.685591000 | 1.082561000 | -1.810000000 |
| 8 | -0.336147000 | -0.086334000 | -2.286579000 |
| 1 | 0.468807000 | 0.361833000 | -2.615646000 |
| 1 | -0.382361000 | -0.937952000 | -2.730981000 |
| 6 | 1.612662000 | 1.007447000 | -0.629431000 |
| 8 | 2.527239000 | 1.550207000 | -0.059426000 |
| 15 | -2.051028000 | -1.264728000 | 0.138451000 |
| 1 | -2.755602000 | -1.806706000 | -0.967446000 |
| 1 | -2.066612000 | -2.454093000 | 0.905318000 |
| 1 | -3.193285000 | -0.692367000 | 0.750712000 |

**MTS1** complex of $W_{bis}$
E (ZPE- corrected) = -844.11327
G = -844.15517

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.054630000 | -0.127476000 | -0.170327000 |
| 15 | 2.509977000 | 0.025449000 | -0.135598000 |
| 7 | -0.269907000 | 1.640008000 | -0.558912000 |
| 8 | -0.406490000 | 2.767896000 | -0.862127000 |
| 6 | -2.069708000 | -0.395887000 | -0.253242000 |
| 8 | -3.207459000 | -0.512124000 | -0.295780000 |
| 1 | 3.129681000 | 1.081961000 | 0.557905000 |
| 1 | 3.207869000 | -1.052982000 | 0.441096000 |
| 1 | 3.244181000 | 0.123146000 | -1.334792000 |
| 1 | 0.165586000 | -0.929379000 | -1.930991000 |
| 6 | -0.177438000 | 0.276770000 | 1.813280000 |
| 8 | -0.250797000 | 0.500847000 | 2.935872000 |
| 8 | 0.379218000 | -2.295724000 | -0.177617000 |
| 1 | -0.347819000 | -2.902062000 | -0.013029000 |
| 1 | 0.249928000 | -1.721677000 | -1.332655000 |

**MTS1** complex of $W_{tris}$
E (ZPE- corrected) = -1073.88982
G = -1073.93204

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.000784000 | -0.110264000 | -0.156345000 |
| 15 | -2.497379000 | -0.146782000 | -0.226541000 |
| 15 | 2.477973000 | -0.273463000 | -0.201396000 |
| 7 | 0.077857000 | 1.657661000 | -0.551255000 |
| 8 | 0.134677000 | 2.801270000 | -0.855336000 |
| 6 | -0.010599000 | 0.308467000 | 1.803707000 |
| 8 | -0.009965000 | 0.539244000 | 2.934291000 |
| 1 | -3.204942000 | -0.128374000 | -1.448681000 |
| 1 | -3.208081000 | 0.886536000 | 0.413872000 |
| 1 | -3.153274000 | -1.250403000 | 0.355751000 |
| 1 | 3.189114000 | -0.026424000 | -1.396692000 |
| 1 | 3.247521000 | 0.552463000 | 0.641866000 |
| 1 | 3.103985000 | -1.500169000 | 0.121103000 |
| 1 | -0.002967000 | -0.983472000 | -1.914263000 |
| 8 | -0.200909000 | -2.329009000 | -0.146781000 |
| 1 | 0.559877000 | -2.865955000 | 0.089243000 |
| 1 | -0.053959000 | -1.767493000 | -1.294433000 |

**MTS1** complex of $W_{tetra}$
E (ZPE- corrected) = -1303.65749
G = -1303.69967

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.000784000 | -0.089524000 | -0.209785000 |
| 15 | -0.011841000 | 0.064844000 | 2.217636000 |
| 15 | -2.473026000 | -0.107366000 | -0.318657000 |
| 7 | 0.067343000 | 1.705796000 | -0.412679000 |
| 8 | 0.123108000 | 2.882070000 | -0.604759000 |
| 1 | -0.070474000 | -1.152986000 | 2.937500000 |
| 1 | -1.039817000 | 0.729105000 | 2.935082000 |
| 1 | 1.059150000 | 0.639119000 | 2.949661000 |
| 1 | -3.271197000 | 0.474534000 | 0.695479000 |
| 1 | -3.132482000 | 0.505543000 | -1.407743000 |
| 1 | -3.132010000 | -1.354835000 | -0.376558000 |
| 1 | -0.027402000 | -0.723746000 | -2.024424000 |
| 15 | 2.453683000 | -0.216134000 | -0.304972000 |
| 1 | 3.094136000 | -1.476803000 | -0.400468000 |
| 1 | 3.146809000 | 0.403206000 | -1.370501000 |
| 1 | 3.273242000 | 0.296809000 | 0.730656000 |
| 8 | -0.173525000 | -2.304205000 | -0.435695000 |
| 1 | 0.623856000 | -2.828827000 | -0.326583000 |
| 1 | -0.066052000 | -1.569984000 | -1.515705000 |

**MTS1** complex of $Mo_{bis}$

E (ZPE- corrected) = -845.21542
G =-845.25644

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.009741000 | -0.268651000 | -0.164869000 |
| 15 | 0.108755000 | 2.138488000 | -0.638865000 |
| 7 | -0.003138000 | 0.016625000 | 1.624991000 |
| 8 | 0.001019000 | 0.225335000 | 2.778525000 |
| 6 | 2.044862000 | -0.335562000 | -0.186727000 |
| 8 | 3.187040000 | -0.334797000 | -0.165866000 |
| 1 | 1.053403000 | 2.938283000 | 0.036626000 |
| 1 | -1.001370000 | 2.994747000 | -0.471309000 |
| 1 | 0.437763000 | 2.525279000 | -1.954584000 |
| 1 | -0.033041000 | -0.673954000 | -2.105744000 |
| 8 | -0.198545000 | -2.398711000 | -0.663119000 |
| 1 | 0.623179000 | -2.890798000 | -0.587745000 |
| 1 | -0.083036000 | -1.531456000 | -1.701435000 |
| 6 | -2.093282000 | -0.203829000 | -0.191813000 |
| 8 | -3.227839000 | -0.121342000 | -0.176042000 |

**MTS1** complex of $Mo_{tris}$
E (ZPE- corrected) = -1075.009368
G = -1075.051256

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.000134000 | -0.134246000 | -0.196761000 |
| 15 | 2.478612000 | -0.317809000 | -0.241475000 |
| 15 | -2.497204000 | -0.184836000 | -0.273179000 |
| 7 | 0.081498000 | 1.613665000 | -0.597351000 |
| 8 | 0.141020000 | 2.751904000 | -0.900030000 |
| 6 | -0.015037000 | 0.295359000 | 1.757893000 |
| 8 | -0.015809000 | 0.541442000 | 2.881594000 |
| 1 | 3.090705000 | -1.566143000 | 0.015073000 |
| 1 | 3.269034000 | 0.451125000 | 0.636564000 |
| 1 | 3.187303000 | -0.019762000 | -1.425486000 |
| 1 | -3.142651000 | -1.282244000 | 0.330711000 |
| 1 | -3.228990000 | 0.850973000 | 0.340104000 |
| 1 | -3.200094000 | -0.202460000 | -1.497300000 |
| 1 | 0.005997000 | -1.005776000 | -1.947002000 |
| 8 | -0.211110000 | -2.350273000 | -0.176057000 |
| 1 | 0.555377000 | -2.883950000 | 0.048057000 |
| 1 | -0.056502000 | -1.776151000 | -1.326883000 |

**MTS1** complex of $Mo_{tetra}$
E (ZPE- corrected) = -1304.89851
G = -1304.82263

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.000177000 | -0.098681000 | -0.265571000 |
| 15 | -0.017079000 | -0.026912000 | 2.172438000 |
| 7 | 0.071719000 | 1.682216000 | -0.416110000 |
| 8 | 0.131195000 | 2.858592000 | -0.570870000 |
| 1 | 1.054386000 | 0.510940000 | 2.928906000 |
| 1 | -0.089293000 | -1.266205000 | 2.851946000 |
| 1 | -1.041720000 | 0.619914000 | 2.907792000 |
| 1 | -0.023257000 | -0.665341000 | -2.094677000 |
| 8 | -0.182121000 | -2.302315000 | -0.560713000 |
| 1 | 0.618775000 | -2.827195000 | -0.485345000 |
| 1 | -0.071178000 | -1.517212000 | -1.614781000 |
| 15 | 2.454989000 | -0.234771000 | -0.370887000 |
| 1 | 3.289318000 | 0.214070000 | 0.681982000 |
| 1 | 3.141445000 | 0.438711000 | -1.406207000 |
| 1 | 3.089382000 | -1.489361000 | -0.542810000 |
| 15 | -2.473333000 | -0.117569000 | -0.387063000 |
| 1 | -3.124825000 | -1.362591000 | -0.518073000 |
| 1 | -3.123428000 | 0.546724000 | -1.450456000 |

| | | | |
|---|---|---|---|
| 1 | -3.290311000 | 0.405187000 | 0.643824000 |

**MTS1** complex of $Cr_{bis}$
E (ZPE- corrected) = -1821.42750
G =-1821.46776

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.010961000 | -0.248468000 | -0.214618000 |
| 15 | 0.124683000 | 2.090856000 | -0.387862000 |
| 7 | -0.005839000 | -0.281779000 | 1.470320000 |
| 8 | 0.004071000 | -0.269641000 | 2.636983000 |
| 6 | 1.908302000 | -0.361415000 | -0.270167000 |
| 8 | 3.047222000 | -0.421754000 | -0.256643000 |
| 1 | 0.871679000 | 2.667297000 | -1.436459000 |
| 1 | 0.719523000 | 2.794683000 | 0.678505000 |
| 1 | -1.021446000 | 2.904572000 | -0.523711000 |
| 1 | -0.015339000 | -0.237637000 | -2.062856000 |
| 8 | -0.238394000 | -2.195415000 | -0.911218000 |
| 1 | 0.579179000 | -2.697682000 | -0.872710000 |
| 1 | -0.078284000 | -1.102656000 | -1.831611000 |
| 6 | -1.964294000 | -0.200784000 | -0.255849000 |
| 8 | -3.098608000 | -0.161006000 | -0.233940000 |

**MTS1** complex of $Cr_{tris}$
E (ZPE- corrected) = -2051.21693
G = -2051.25834

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.001786000 | -0.146526000 | -0.163759000 |
| 15 | 2.341240000 | -0.414140000 | -0.264146000 |
| 15 | -2.378441000 | -0.174432000 | -0.238948000 |
| 7 | 0.025040000 | 0.193246000 | 1.477372000 |
| 8 | 0.069221000 | 0.455386000 | 2.619830000 |
| 6 | 0.124785000 | 1.655905000 | -0.632688000 |
| 8 | 0.193340000 | 2.767101000 | -0.917955000 |
| 1 | 2.932331000 | -1.700626000 | -0.213572000 |
| 1 | 3.114791000 | 0.176803000 | 0.754601000 |
| 1 | 3.083976000 | 0.065615000 | -1.363470000 |
| 1 | -3.006034000 | -1.251527000 | 0.416661000 |
| 1 | -3.125711000 | 0.881046000 | 0.321523000 |
| 1 | -3.072385000 | -0.260065000 | -1.463344000 |
| 1 | 0.011760000 | -0.601039000 | -1.942784000 |
| 8 | -0.336031000 | -2.229107000 | -0.428818000 |
| 1 | 0.429370000 | -2.786140000 | -0.265860000 |
| 1 | -0.103437000 | -1.414039000 | -1.497056000 |

**MTS1** complex of $Cr_{tetra}$
E (ZPE- corrected) = -2280.98651
G = -2281.02863

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.017003000 | -0.181394000 | -0.157622000 |
| 15 | 0.247630000 | 2.070882000 | -0.615593000 |
| 7 | 0.053191000 | 0.036766000 | 1.493026000 |
| 8 | 0.150523000 | 0.226551000 | 2.657279000 |
| 1 | 1.009099000 | 2.515618000 | -1.723502000 |
| 1 | 0.877107000 | 2.884047000 | 0.353415000 |
| 1 | -0.846745000 | 2.944282000 | -0.848177000 |
| 1 | -0.027833000 | -0.481152000 | -1.985988000 |
| 8 | -0.486190000 | -2.210447000 | -0.628457000 |
| 1 | 0.238916000 | -2.830022000 | -0.513036000 |
| 1 | -0.196835000 | -1.325568000 | -1.607643000 |
| 15 | -2.395383000 | -0.177832000 | -0.164132000 |
| 1 | -2.981182000 | -0.987945000 | 0.828397000 |
| 1 | -3.105880000 | -0.695838000 | -1.266431000 |
| 1 | -3.199233000 | 0.968787000 | 0.034721000 |

| | | | |
|---|---|---|---|
| 15 | 2.280835000 | -0.609072000 | -0.249922000 |
| 1 | 2.743934000 | -1.944681000 | -0.381354000 |
| 1 | 3.059673000 | -0.274770000 | 0.878224000 |
| 1 | 3.153823000 | -0.065183000 | -1.222742000 |

**MTS2** complex of $W_{bis}$
E (ZPE- corrected) = -1187.24877
G = -1187.29357

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.024958000 | -0.003448000 | -0.033536000 |
| 15 | -2.432941000 | 0.589106000 | 0.029299000 |
| 15 | 2.455442000 | -0.499350000 | -0.389868000 |
| 7 | 0.145028000 | -0.034296000 | 1.767035000 |
| 8 | 0.191213000 | -0.055257000 | 2.949479000 |
| 6 | -0.437131000 | -2.018116000 | -0.021021000 |
| 8 | -0.698772000 | -3.131105000 | 0.038453000 |
| 1 | -2.917229000 | 1.699441000 | -0.689284000 |
| 1 | -3.000235000 | 0.893864000 | 1.282574000 |
| 1 | -3.390562000 | -0.348526000 | -0.404451000 |
| 1 | 3.324525000 | 0.563780000 | -0.683809000 |
| 1 | 3.200582000 | -1.091286000 | 0.663520000 |
| 1 | 2.837240000 | -1.383002000 | -1.413763000 |
| 1 | 1.220365000 | 0.615378000 | -2.134805000 |
| 8 | -0.850221000 | -0.084527000 | -2.285786000 |
| 1 | 0.192143000 | 0.283364000 | -2.443745000 |
| 1 | -0.923903000 | -0.948924000 | -2.707308000 |
| 6 | 0.526802000 | 2.023684000 | -0.102254000 |
| 8 | 0.822712000 | 3.124808000 | -0.103187000 |

**MTS2** complex of $W_{tris}$
E (ZPE- corrected) = -1417.029631
G = -1417.074102

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.011624000 | -0.060875000 | -0.019072000 |
| 15 | -2.199962000 | 1.175534000 | 0.020866000 |
| 15 | 1.290851000 | 2.139665000 | 0.034713000 |
| 15 | 2.195413000 | -1.174636000 | -0.320151000 |
| 7 | -0.025321000 | -0.270985000 | 1.765377000 |
| 8 | -0.054842000 | -0.398060000 | 2.945999000 |
| 6 | -1.004270000 | -1.805993000 | -0.213183000 |
| 8 | -1.584352000 | -2.799305000 | -0.279228000 |
| 1 | -2.341674000 | 2.495164000 | -0.466800000 |
| 1 | -2.779867000 | 1.384546000 | 1.287886000 |
| 1 | -3.328121000 | 0.635097000 | -0.629446000 |
| 1 | 1.268312000 | 2.982758000 | 1.179743000 |
| 1 | 2.686286000 | 2.094385000 | -0.141155000 |
| 1 | 0.992836000 | 3.132569000 | -0.916432000 |
| 1 | 3.365621000 | -0.391043000 | -0.375167000 |
| 1 | 2.629853000 | -2.121231000 | 0.642335000 |
| 1 | 2.425306000 | -1.958453000 | -1.465255000 |
| 1 | 1.514406000 | 0.626155000 | -1.907264000 |
| 8 | -0.641069000 | 0.242162000 | -2.367095000 |
| 1 | 0.389011000 | 0.451548000 | -2.431243000 |
| 1 | -0.811332000 | -0.560723000 | -2.873206000 |

**MTS2** complex of $W_{tetra}$
E (ZPE- corrected) = -1646.79974
G = -1646.84506

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.018785000 | -0.007424000 | -0.009955000 |
| 15 | -1.741461000 | 1.748685000 | 0.055256000 |
| 15 | 1.801773000 | 1.717701000 | -0.036717000 |
| 15 | 1.840567000 | -1.647718000 | -0.363769000 |

| | | | |
|---|---|---|---|
| 7 | 0.016664000 | -0.190169000 | 1.766990000 |
| 8 | -0.011767000 | -0.324025000 | 2.955778000 |
| 1 | -1.619227000 | 2.956537000 | -0.669476000 |
| 1 | -2.046996000 | 2.317565000 | 1.309247000 |
| 1 | -3.071776000 | 1.468262000 | -0.345087000 |
| 1 | 2.044481000 | 2.484248000 | 1.133452000 |
| 1 | 3.135861000 | 1.334467000 | -0.293633000 |
| 1 | 1.739124000 | 2.796865000 | -0.941367000 |
| 1 | 3.163350000 | -1.185797000 | -0.540807000 |
| 1 | 2.108277000 | -2.615257000 | 0.639135000 |
| 1 | 1.816774000 | -2.540937000 | -1.455763000 |
| 1 | 1.526484000 | 0.239404000 | -2.042419000 |
| 8 | -0.669145000 | 0.373707000 | -2.364572000 |
| 1 | 0.407543000 | 0.337383000 | -2.442280000 |
| 1 | -1.013849000 | -0.351397000 | -2.897869000 |
| 15 | -1.734716000 | -1.750853000 | -0.148838000 |
| 1 | -1.686693000 | -2.873165000 | -1.016095000 |
| 1 | -1.965546000 | -2.470289000 | 1.041650000 |
| 1 | -3.089711000 | -1.431998000 | -0.429599000 |

**MTS2** complex of $Mo_{bis}$
E (ZPE- corrected) = -1188.36598
G = -1188.41041

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.009741000 | -0.268651000 | -0.164869000 |
| 15 | 0.108755000 | 2.138488000 | -0.638865000 |
| 7 | -0.003138000 | 0.016625000 | 1.624991000 |
| 8 | 0.001019000 | 0.225335000 | 2.778525000 |
| 6 | 2.044862000 | -0.335562000 | -0.186727000 |
| 8 | 3.187040000 | -0.334797000 | -0.165866000 |
| 1 | 1.053403000 | 2.938283000 | 0.036626000 |
| 1 | -1.001370000 | 2.994747000 | -0.471309000 |
| 1 | 0.437763000 | 2.525279000 | -1.954584000 |
| 1 | -0.033041000 | -0.673954000 | -2.105744000 |
| 8 | -0.198545000 | -2.398711000 | -0.663119000 |
| 1 | 0.623179000 | -2.890798000 | -0.587745000 |
| 1 | -0.083036000 | -1.531456000 | -1.701435000 |
| 6 | -2.093282000 | -0.203829000 | -0.191813000 |
| 8 | -3.227839000 | -0.121342000 | -0.176042000 |

**MTS2** complex of $Mo_{tris}$
E (ZPE- corrected) = -1418.149317
G = -1418.193312

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.015981000 | 0.079488000 | -0.010953000 |
| 15 | 2.229125000 | -1.116585000 | 0.030510000 |
| 15 | -2.213450000 | 1.124893000 | -0.361665000 |
| 7 | 0.013957000 | 0.327132000 | 1.749747000 |
| 8 | 0.026707000 | 0.485725000 | 2.920708000 |
| 6 | 0.960345000 | 1.839325000 | -0.242904000 |
| 8 | 1.513032000 | 2.842902000 | -0.328995000 |
| 1 | 2.388165000 | -2.415591000 | -0.501147000 |
| 1 | 2.817803000 | -1.362485000 | 1.287764000 |
| 1 | 3.352134000 | -0.539960000 | -0.596426000 |
| 1 | -3.363895000 | 0.314452000 | -0.405634000 |
| 1 | -2.686110000 | 2.085648000 | 0.571586000 |
| 1 | -2.448226000 | 1.879632000 | -1.524213000 |
| 1 | -1.514725000 | -0.667641000 | -1.910203000 |
| 8 | 0.653965000 | -0.273962000 | -2.361144000 |
| 1 | -0.373732000 | -0.493842000 | -2.407727000 |
| 1 | 0.804982000 | 0.513201000 | -2.896631000 |
| 15 | -1.236652000 | -2.150855000 | 0.063623000 |
| 1 | -1.197640000 | -2.991677000 | 1.211163000 |
| 1 | -0.912500000 | -3.142129000 | -0.880028000 |

| | | | |
|---|---|---|---|
| 1 | -2.632220000 | -2.143092000 | -0.110863000 |

**MTS2** complex of $Mo_{tetra}$
E (ZPE- corrected) = -1647.92282
G = -1647.96786

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.016459000 | -0.010717000 | 0.001991000 |
| 15 | -1.733482000 | 1.757469000 | 0.035542000 |
| 15 | 1.838992000 | -1.649003000 | -0.355638000 |
| 7 | 0.012044000 | -0.179370000 | 1.761153000 |
| 8 | -0.011108000 | -0.302935000 | 2.944966000 |
| 1 | -1.591060000 | 2.945931000 | -0.715001000 |
| 1 | -2.048155000 | 2.362916000 | 1.270771000 |
| 1 | -3.063471000 | 1.483505000 | -0.366212000 |
| 1 | 3.163294000 | -1.190776000 | -0.514307000 |
| 1 | 2.102287000 | -2.635027000 | 0.633462000 |
| 1 | 1.814878000 | -2.529446000 | -1.456333000 |
| 1 | 1.575320000 | 0.209957000 | -2.040568000 |
| 8 | -0.632845000 | 0.366647000 | -2.369583000 |
| 1 | 0.437678000 | 0.318625000 | -2.431689000 |
| 1 | -0.973045000 | -0.351202000 | -2.914988000 |
| 15 | 1.799147000 | 1.713975000 | -0.046694000 |
| 1 | 2.033080000 | 2.513987000 | 1.104646000 |
| 1 | 1.738461000 | 2.771534000 | -0.975155000 |
| 1 | 3.135749000 | 1.329543000 | -0.278090000 |
| 15 | -1.722331000 | -1.767651000 | -0.157393000 |
| 1 | -3.084232000 | -1.462593000 | -0.411933000 |
| 1 | -1.662774000 | -2.857310000 | -1.062585000 |
| 1 | -1.936865000 | -2.535507000 | 1.005971000 |

**MTS2** complex of $Cr_{tris}$
E (ZPE- corrected) = -2394.352682
G = -2394.395175

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.000422000 | 0.095985000 | 0.052823000 |
| 15 | 2.185987000 | -0.865315000 | 0.108715000 |
| 15 | -0.962371000 | -2.111576000 | 0.009161000 |
| 15 | -2.153344000 | 0.890620000 | -0.486818000 |
| 7 | -0.127159000 | 0.316745000 | 1.688315000 |
| 8 | -0.222920000 | 0.463241000 | 2.849828000 |
| 6 | 0.750261000 | 1.812460000 | -0.191599000 |
| 8 | 1.216828000 | 2.855495000 | -0.283418000 |
| 1 | 2.455717000 | -2.095015000 | -0.528027000 |
| 1 | 2.751373000 | -1.181664000 | 1.363024000 |
| 1 | 3.282559000 | -0.151281000 | -0.413215000 |
| 1 | -0.859122000 | -2.935973000 | 1.170647000 |
| 1 | -2.342437000 | -2.272432000 | -0.201310000 |
| 1 | -0.474368000 | -3.065042000 | -0.901027000 |
| 1 | -3.247266000 | 0.011688000 | -0.577714000 |
| 1 | -2.745899000 | 1.841731000 | 0.393656000 |
| 1 | -2.353402000 | 1.622342000 | -1.669695000 |
| 1 | -1.347503000 | -0.805523000 | -1.920009000 |
| 8 | 0.817595000 | -0.209179000 | -2.303163000 |
| 1 | -0.170476000 | -0.514928000 | -2.358220000 |
| 1 | 0.903398000 | 0.568088000 | -2.866307000 |

**MTS2** complex of $Cr_{tetra}$
E (ZPE- corrected) = -2624.12680
G = -2624.17017

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.021065000 | -0.016190000 | 0.065551000 |
| 15 | -1.705215000 | 1.607949000 | 0.067096000 |
| 15 | 1.621294000 | 1.708461000 | -0.144106000 |

| | | | |
|---|---|---|---|
| 15 | 1.780165000 | -1.516817000 | -0.402011000 |
| 7 | 0.103145000 | -0.138023000 | 1.705645000 |
| 8 | 0.160525000 | -0.230295000 | 2.884339000 |
| 1 | -1.613924000 | 2.768186000 | -0.732261000 |
| 1 | -2.018941000 | 2.255517000 | 1.282694000 |
| 1 | -3.031659000 | 1.271834000 | -0.292819000 |
| 1 | 1.820559000 | 2.577015000 | 0.969135000 |
| 1 | 2.976898000 | 1.410196000 | -0.379688000 |
| 1 | 1.457910000 | 2.724296000 | -1.105087000 |
| 1 | 3.094960000 | -1.047235000 | -0.582598000 |
| 1 | 2.083957000 | -2.523101000 | 0.563143000 |
| 1 | 1.719138000 | -2.388862000 | -1.506631000 |
| 1 | 1.512899000 | 0.217373000 | -2.031028000 |
| 8 | -0.730556000 | 0.305294000 | -2.314012000 |
| 1 | 0.320482000 | 0.284147000 | -2.381688000 |
| 1 | -1.058880000 | -0.387710000 | -2.897573000 |
| 15 | -1.552794000 | -1.764675000 | -0.097251000 |
| 1 | -2.936054000 | -1.524090000 | -0.293701000 |
| 1 | -1.454453000 | -2.794188000 | -1.065768000 |
| 1 | -1.691985000 | -2.612402000 | 1.022619000 |

**MTS3** complex of $W_{bis}$
E (ZPE- corrected) = -1187.25074
G = -1187.29861

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.016082000 | 0.006341000 | 0.025924000 |
| 15 | -2.373010000 | 0.607156000 | 0.392239000 |
| 15 | 2.434865000 | -0.404745000 | -0.420863000 |
| 7 | 0.338539000 | -0.049990000 | 1.788996000 |
| 8 | 0.591282000 | -0.053179000 | 2.947472000 |
| 6 | -0.444755000 | -2.018632000 | -0.100352000 |
| 8 | -0.691442000 | -3.140475000 | -0.125941000 |
| 1 | -3.238963000 | 0.694886000 | -0.717078000 |
| 1 | -2.687213000 | 1.846775000 | 0.985904000 |
| 1 | -3.184490000 | -0.206394000 | 1.208833000 |
| 1 | 3.276034000 | 0.643983000 | -0.850494000 |
| 1 | 3.182722000 | -0.815047000 | 0.699971000 |
| 1 | 2.903147000 | -1.382492000 | -1.327361000 |
| 1 | 0.221826000 | 1.519746000 | -1.738553000 |
| 8 | -0.945641000 | -0.467414000 | -2.548518000 |
| 1 | -0.557845000 | 0.280264000 | -3.025558000 |
| 1 | -0.723187000 | -1.261534000 | -3.047612000 |
| 6 | 0.378860000 | 1.971805000 | -0.586152000 |
| 8 | 0.635257000 | 3.136728000 | -0.533141000 |

**MTS3** complex of $W_{tris}$
E (ZPE- corrected) = -1417.02541
G = -1417.07428

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.044493000 | 0.029658000 | 0.007732000 |
| 15 | -1.413969000 | 2.034805000 | -0.035271000 |
| 15 | 1.708205000 | -1.799185000 | -0.006249000 |
| 7 | 0.240648000 | 0.183846000 | 1.774010000 |
| 8 | 0.408387000 | 0.314336000 | 2.948714000 |
| 1 | -1.261058000 | 3.000064000 | -1.054090000 |
| 1 | -1.277891000 | 2.896280000 | 1.071361000 |
| 1 | -2.831459000 | 2.003186000 | -0.064045000 |
| 1 | 2.646879000 | -1.899569000 | -1.057832000 |
| 1 | 2.626387000 | -1.771986000 | 1.062685000 |
| 1 | 1.415439000 | -3.186489000 | 0.058698000 |
| 1 | 1.084924000 | 0.943480000 | -1.893356000 |
| 8 | -0.715333000 | -0.565948000 | -2.585029000 |
| 1 | -0.058895000 | 0.061099000 | -2.936196000 |
| 1 | -0.471738000 | -1.425400000 | -2.946674000 |

| | | | |
|---|---|---|---|
| 6 | 1.512412000 | 1.241705000 | -0.758325000 |
| 8 | 2.439723000 | 1.998117000 | -0.751758000 |
| 15 | -1.982398000 | -1.541205000 | 0.152292000 |
| 1 | -3.288902000 | -1.144318000 | -0.225984000 |
| 1 | -2.055464000 | -2.817254000 | -0.461904000 |
| 1 | -2.319490000 | -1.979196000 | 1.450041000 |

**MTS3** complex of $Mo_{bis}$
E (ZPE- corrected) = -1188.37236
G = -1188.42022

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.020671000 | 0.018968000 | 0.026599000 |
| 15 | 2.326988000 | -0.720020000 | 0.407231000 |
| 15 | -2.428779000 | 0.443289000 | -0.442467000 |
| 7 | -0.385648000 | -0.060520000 | 1.762950000 |
| 8 | -0.658852000 | -0.157950000 | 2.907068000 |
| 6 | 0.489518000 | 2.046563000 | 0.044166000 |
| 8 | 0.757033000 | 3.157312000 | 0.120875000 |
| 1 | 3.006360000 | -1.399123000 | -0.624722000 |
| 1 | 2.537051000 | -1.663171000 | 1.432082000 |
| 1 | 3.371699000 | 0.164547000 | 0.752677000 |
| 1 | -3.078478000 | -0.251120000 | -1.485045000 |
| 1 | -3.310210000 | 0.093415000 | 0.599415000 |
| 1 | -2.978025000 | 1.714994000 | -0.722987000 |
| 1 | -0.169181000 | -1.431364000 | -1.795406000 |
| 8 | 1.037185000 | 0.602525000 | -2.520239000 |
| 1 | 0.676124000 | -0.124962000 | -3.044971000 |
| 1 | 0.886002000 | 1.409229000 | -3.025102000 |
| 6 | -0.397120000 | -1.896888000 | -0.682829000 |
| 8 | -0.685508000 | -3.055957000 | -0.655606000 |

**MTS3** complex of $Mo_{tris}$
E (ZPE- corrected) = -1418.15071
G = -1418.19976

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.055377000 | 0.023344000 | 0.005454000 |
| 15 | -1.122918000 | 2.202869000 | 0.046573000 |
| 15 | 1.489135000 | -1.990355000 | -0.101356000 |
| 7 | 0.391983000 | 0.156935000 | 1.736229000 |
| 8 | 0.663679000 | 0.271443000 | 2.887048000 |
| 1 | -1.044715000 | 3.069983000 | -1.064767000 |
| 1 | -0.688373000 | 3.116820000 | 1.027141000 |
| 1 | -2.514103000 | 2.361981000 | 0.267179000 |
| 1 | 2.234611000 | -2.264892000 | -1.269901000 |
| 1 | 2.565600000 | -2.008782000 | 0.808364000 |
| 1 | 1.069179000 | -3.327134000 | 0.117814000 |
| 1 | 1.143551000 | 0.777842000 | -1.927614000 |
| 8 | -0.967662000 | -0.354909000 | -2.564049000 |
| 1 | -0.227604000 | 0.141848000 | -2.949734000 |
| 1 | -0.967159000 | -1.209664000 | -3.008511000 |
| 6 | 1.623272000 | 1.022730000 | -0.820465000 |
| 8 | 2.642801000 | 1.649814000 | -0.824474000 |
| 15 | -2.152503000 | -1.303063000 | 0.275615000 |
| 1 | -2.535947000 | -2.409234000 | -0.522683000 |
| 1 | -3.426525000 | -0.683762000 | 0.246786000 |
| 1 | -2.334097000 | -1.952955000 | 1.515342000 |

**MTS3** complex of $Cr_{bis}$
E (ZPE- corrected) = -2164.58714
G = -2164.63372

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.023234000 | 0.035803000 | 0.072827000 |
| 15 | 2.079937000 | -1.002220000 | 0.252908000 |

| | | | |
|---|---|---|---|
| 15 | -2.185251000 | 0.812893000 | -0.408618000 |
| 7 | -0.483192000 | -0.464231000 | 1.584726000 |
| 8 | -0.821872000 | -0.864924000 | 2.635564000 |
| 6 | 0.654936000 | 1.777853000 | 0.544756000 |
| 8 | 1.039010000 | 2.797871000 | 0.898191000 |
| 1 | 2.701917000 | -1.508923000 | -0.906791000 |
| 1 | 2.127734000 | -2.176305000 | 1.030137000 |
| 1 | 3.220091000 | -0.371767000 | 0.798958000 |
| 1 | -2.644701000 | 0.847279000 | -1.743601000 |
| 1 | -3.245913000 | 0.061107000 | 0.134921000 |
| 1 | -2.659372000 | 2.091852000 | -0.038582000 |
| 1 | -0.172229000 | -0.996647000 | -2.052381000 |
| 8 | 1.185997000 | 1.065875000 | -2.287318000 |
| 1 | 0.808284000 | 0.538866000 | -3.002404000 |
| 1 | 1.219634000 | 1.973666000 | -2.607087000 |
| 6 | -0.520609000 | -1.503726000 | -1.044407000 |
| 8 | -0.983351000 | -2.608028000 | -1.136505000 |

**MTS3** complex of $Cr_{tris}$
E (ZPE- corrected) = -2394.36193
G = -2394.40793

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.044928000 | 0.003651000 | 0.038051000 |
| 15 | -0.805434000 | 2.189363000 | 0.088178000 |
| 15 | 1.147661000 | -2.041185000 | -0.245925000 |
| 7 | 0.634973000 | 0.143865000 | 1.571628000 |
| 8 | 1.099779000 | 0.263491000 | 2.652059000 |
| 1 | -0.832435000 | 2.967613000 | -1.090138000 |
| 1 | -0.092134000 | 3.096940000 | 0.896105000 |
| 1 | -2.104835000 | 2.543718000 | 0.532490000 |
| 1 | 1.608699000 | -2.430208000 | -1.524575000 |
| 1 | 2.379592000 | -2.145214000 | 0.430733000 |
| 1 | 0.650704000 | -3.319367000 | 0.118952000 |
| 1 | 1.002978000 | 0.605928000 | -2.053685000 |
| 8 | -1.321837000 | -0.182535000 | -2.398572000 |
| 1 | -0.541364000 | 0.182433000 | -2.844630000 |
| 1 | -1.538766000 | -0.990350000 | -2.875749000 |
| 6 | 1.511178000 | 0.751764000 | -0.981773000 |
| 8 | 2.606357000 | 1.247280000 | -0.992959000 |
| 15 | -2.080596000 | -1.000758000 | 0.557408000 |
| 1 | -3.287367000 | -0.263217000 | 0.650635000 |
| 1 | -2.648095000 | -2.077268000 | -0.168628000 |
| 1 | -2.185967000 | -1.613447000 | 1.825359000 |

**MTS4** complex of $W_{bis}$
E (ZPE- corrected) = -1187.25647
G = -1187.30186

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.002807000 | -0.054517000 | -0.052709000 |
| 15 | -2.504287000 | 0.100367000 | -0.076913000 |
| 15 | 2.490021000 | -0.071538000 | -0.156925000 |
| 7 | 0.045613000 | -0.098527000 | 1.762400000 |
| 8 | 0.085352000 | -0.104535000 | 2.943735000 |
| 6 | -0.084741000 | -2.086606000 | -0.210571000 |
| 8 | -0.131922000 | -3.232743000 | -0.284605000 |
| 1 | -3.144598000 | 1.190373000 | 0.547601000 |
| 1 | -3.278852000 | -0.926637000 | 0.498325000 |
| 1 | -3.153233000 | 0.171132000 | -1.326538000 |
| 1 | 3.219378000 | 0.999376000 | 0.400835000 |
| 1 | 3.206330000 | -1.122586000 | 0.449796000 |
| 1 | 3.138559000 | -0.102007000 | -1.412116000 |
| 1 | 0.103132000 | 2.308773000 | -1.825379000 |
| 8 | -0.125526000 | 0.198145000 | -2.224727000 |
| 1 | 0.015931000 | 1.352249000 | -2.255458000 |

| | | | |
|---|---|---|---|
| 1 | 0.452920000 | -0.244450000 | -2.852266000 |
| 6 | 0.078039000 | 2.133998000 | -0.234901000 |
| 8 | 0.119973000 | 3.186753000 | 0.255505000 |

**MTS4** complex of $W_{tris}$
E (ZPE- corrected) = -1417.02854
G = -1417.07360

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000690000 | -0.005638000 | -0.047495000 |
| 15 | -2.288675000 | 0.965409000 | -0.061354000 |
| 15 | 2.349253000 | -0.781357000 | -0.142470000 |
| 7 | 0.073410000 | 0.054486000 | 1.758062000 |
| 8 | 0.135916000 | 0.117035000 | 2.943929000 |
| 1 | -2.800587000 | 1.471098000 | -1.275288000 |
| 1 | -2.534720000 | 2.092532000 | 0.749006000 |
| 1 | -3.434180000 | 0.226788000 | 0.322559000 |
| 1 | 3.311717000 | -0.064669000 | 0.599145000 |
| 1 | 2.748732000 | -2.075435000 | 0.272118000 |
| 1 | 3.036409000 | -0.787384000 | -1.379153000 |
| 1 | 0.744012000 | 2.081308000 | -1.930830000 |
| 8 | -0.103489000 | 0.114972000 | -2.254671000 |
| 1 | 0.357970000 | 1.176082000 | -2.321636000 |
| 1 | 0.390019000 | -0.480635000 | -2.826137000 |
| 6 | 0.741499000 | 1.975376000 | -0.348207000 |
| 8 | 1.136537000 | 2.984100000 | 0.087618000 |
| 15 | -0.905611000 | -2.329449000 | -0.112202000 |
| 1 | -1.146858000 | -2.975206000 | -1.347195000 |
| 1 | -2.161218000 | -2.631086000 | 0.468239000 |
| 1 | -0.201474000 | -3.397724000 | 0.491987000 |

**MTS4** complex of $Mo_{bis}$
E (ZPE- corrected) = -1188.37424
G = -1188.41945

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | 0.001580000 | 0.070224000 | -0.063291000 |
| 15 | 2.506197000 | -0.050615000 | -0.106070000 |
| 15 | -2.490969000 | 0.041484000 | -0.176701000 |
| 7 | -0.041810000 | 0.099541000 | 1.733687000 |
| 8 | -0.078349000 | 0.101324000 | 2.909932000 |
| 6 | 0.048217000 | 2.100595000 | -0.203813000 |
| 8 | 0.077404000 | 3.245412000 | -0.257454000 |
| 1 | 3.168877000 | -1.106726000 | 0.552160000 |
| 1 | 3.285356000 | 1.003446000 | 0.412484000 |
| 1 | 3.136881000 | -0.167145000 | -1.360905000 |
| 1 | -3.208769000 | -1.061899000 | 0.330234000 |
| 1 | -3.234697000 | 1.052454000 | 0.464594000 |
| 1 | -3.131630000 | 0.110971000 | -1.433610000 |
| 1 | -0.067296000 | -2.287884000 | -1.862799000 |
| 8 | 0.123383000 | -0.164250000 | -2.234717000 |
| 1 | 0.002718000 | -1.326876000 | -2.264061000 |
| 1 | -0.467286000 | 0.261851000 | -2.862251000 |
| 6 | -0.040570000 | -2.116213000 | -0.227932000 |
| 8 | -0.063959000 | -3.169200000 | 0.254563000 |

**MTS4** complex of $Mo_{tris}$
E (ZPE- corrected) = -1418.14954
G = -1418.19492

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.000391000 | 0.009052000 | -0.056465000 |
| 15 | 2.367493000 | -0.759848000 | -0.075589000 |
| 15 | -2.412354000 | 0.561571000 | -0.161283000 |
| 7 | -0.080369000 | -0.091373000 | 1.727800000 |
| 8 | -0.147469000 | -0.178186000 | 2.906637000 |

| | | | |
|---|---|---|---|
| 1 | 2.911933000 | -1.221537000 | -1.292112000 |
| 1 | 2.712256000 | -1.864386000 | 0.729779000 |
| 1 | 3.454288000 | 0.064952000 | 0.302254000 |
| 1 | -3.091693000 | 0.504162000 | -1.400037000 |
| 1 | -3.307589000 | -0.243742000 | 0.572909000 |
| 1 | -2.938478000 | 1.809353000 | 0.252669000 |
| 1 | -0.530589000 | -2.105918000 | -1.997528000 |
| 8 | 0.125467000 | -0.055005000 | -2.262365000 |
| 1 | -0.232718000 | -1.161578000 | -2.344962000 |
| 1 | -0.418918000 | 0.494012000 | -2.834110000 |
| 6 | -0.552370000 | -2.022363000 | -0.363486000 |
| 8 | -0.855463000 | -3.067237000 | 0.048574000 |
| 15 | 0.689535000 | 2.411924000 | -0.083426000 |
| 1 | -0.141920000 | 3.419845000 | 0.459591000 |
| 1 | 0.955761000 | 3.071301000 | -1.305067000 |
| 1 | 1.870497000 | 2.825875000 | 0.576144000 |

**MTS4** complex of $Cr_{bis}$
E (ZPE- corrected) = -2164.58310
G = -2164.62717

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | -0.001492000 | 0.084763000 | -0.053334000 |
| 15 | 2.379564000 | -0.114370000 | -0.122859000 |
| 15 | -2.362633000 | 0.139773000 | -0.249636000 |
| 7 | -0.072784000 | -0.043146000 | 1.610780000 |
| 8 | -0.108770000 | -0.149115000 | 2.777436000 |
| 6 | 0.104703000 | 1.983582000 | -0.046164000 |
| 8 | 0.176811000 | 3.125124000 | 0.001818000 |
| 1 | 2.952047000 | -1.012876000 | -1.044790000 |
| 1 | 3.058578000 | -0.545834000 | 1.034116000 |
| 1 | 3.197735000 | 0.996591000 | -0.416977000 |
| 1 | -3.129033000 | -0.986011000 | 0.118277000 |
| 1 | -3.100058000 | 1.101344000 | 0.471327000 |
| 1 | -2.959965000 | 0.359973000 | -1.510664000 |
| 1 | -0.084599000 | -2.053404000 | -2.004803000 |
| 8 | 0.214506000 | 0.079399000 | -2.118754000 |
| 1 | 0.038531000 | -1.080752000 | -2.281690000 |
| 1 | -0.344223000 | 0.601547000 | -2.701557000 |
| 6 | -0.107966000 | -1.949341000 | -0.324099000 |
| 8 | -0.197311000 | -3.017828000 | 0.108291000 |

**MTS4** complex of $Cr_{tris}$
E (ZPE- corrected) = -2394.35774
G = -2394.40259

| At. No. | X | Y | Z |
|---|---|---|---|
| 24 | 0.003227000 | 0.015240000 | -0.058229000 |
| 15 | 2.263064000 | -0.712149000 | -0.092305000 |
| 15 | -2.295938000 | 0.524248000 | -0.206260000 |
| 7 | -0.110159000 | -0.170818000 | 1.591125000 |
| 8 | -0.201258000 | -0.326231000 | 2.757286000 |
| 1 | 2.777662000 | -1.257767000 | -1.285882000 |
| 1 | 2.630521000 | -1.754481000 | 0.782813000 |
| 1 | 3.358594000 | 0.138041000 | 0.198041000 |
| 1 | -2.956770000 | 0.494105000 | -1.456089000 |
| 1 | -3.185247000 | -0.321189000 | 0.488842000 |
| 1 | -2.857114000 | 1.746138000 | 0.239538000 |
| 1 | -0.438639000 | -1.954617000 | -2.089105000 |
| 8 | 0.210756000 | 0.109411000 | -2.142651000 |
| 1 | -0.137486000 | -0.998339000 | -2.328686000 |
| 1 | -0.333779000 | 0.693999000 | -2.677580000 |
| 6 | -0.507045000 | -1.890705000 | -0.419804000 |
| 8 | -0.826274000 | -2.937967000 | -0.033274000 |
| 15 | 0.630673000 | 2.297208000 | 0.033460000 |
| 1 | 0.627587000 | 3.116801000 | -1.118698000 |
| 1 | 1.913084000 | 2.685951000 | 0.489887000 |
| 1 | -0.095245000 | 3.184239000 | 0.861065000 |

**M1** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -1346.713475
G = -1346.768221

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.000004000 | 0.006572000 | 0.068474000 |
| 15 | -2.478797000 | -0.006587000 | -0.359319000 |
| 15 | 2.478812000 | -0.006774000 | -0.359280000 |
| 7 | -0.000114000 | 0.019657000 | 1.919858000 |
| 8 | -0.000193000 | 0.034360000 | 3.103497000 |
| 6 | -0.000138000 | -2.048664000 | -0.055797000 |
| 8 | -0.000310000 | -3.195027000 | -0.135489000 |
| 1 | 0.000023000 | 0.009666000 | -1.776707000 |
| 6 | -3.544891000 | -0.141853000 | 1.128805000 |
| 1 | -4.603327000 | -0.134442000 | 0.863664000 |
| 1 | -3.313389000 | -1.065769000 | 1.656920000 |
| 1 | -3.336334000 | 0.689256000 | 1.801115000 |
| 6 | -3.102260000 | -1.369101000 | -1.418795000 |
| 1 | -2.591041000 | -1.333690000 | -2.379588000 |
| 1 | -2.882542000 | -2.328533000 | -0.952575000 |
| 1 | -4.178531000 | -1.286640000 | -1.576846000 |
| 6 | -3.175152000 | 1.464325000 | -1.207831000 |
| 1 | -2.672340000 | 1.596222000 | -2.164840000 |
| 1 | -4.247241000 | 1.353313000 | -1.376414000 |
| 1 | -2.998761000 | 2.354486000 | -0.605643000 |
| 6 | 3.175220000 | 1.463945000 | -1.208080000 |
| 1 | 2.998982000 | 2.354217000 | -0.606013000 |
| 1 | 4.247281000 | 1.352801000 | -1.376753000 |
| 1 | 2.672327000 | 1.595744000 | -2.165060000 |
| 6 | 3.102328000 | -1.369513000 | -1.418428000 |
| 1 | 4.178602000 | -1.287059000 | -1.576454000 |
| 1 | 2.882610000 | -2.328850000 | -0.952010000 |
| 1 | 2.591151000 | -1.334325000 | -2.379252000 |
| 6 | 3.544788000 | -0.141723000 | 1.128958000 |
| 1 | 3.336246000 | 0.689604000 | 1.801004000 |
| 1 | 3.313130000 | -1.065460000 | 1.657314000 |
| 1 | 4.603253000 | -0.134492000 | 0.863926000 |
| 6 | 0.000249000 | 2.061868000 | -0.081975000 |
| 8 | 0.000491000 | 3.206258000 | -0.178510000 |

**M2** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -885.593958
G = -885.639166

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.525375000 | -0.048357000 | -0.259984000 |
| 15 | 2.010832000 | 0.005118000 | -0.170450000 |
| 7 | -0.751201000 | -1.196600000 | 1.139152000 |
| 8 | -0.848807000 | -2.092210000 | 1.904179000 |
| 6 | -0.779984000 | 1.506059000 | 0.949399000 |
| 8 | -0.909304000 | 2.445306000 | 1.605916000 |
| 1 | -0.143569000 | -0.124442000 | -2.038461000 |
| 6 | 2.789189000 | 0.079077000 | 1.486972000 |
| 1 | 2.461801000 | 0.982320000 | 2.000170000 |
| 1 | 2.466066000 | -0.778630000 | 2.075851000 |
| 1 | 3.877909000 | 0.078427000 | 1.419289000 |
| 6 | 2.833545000 | -1.438970000 | -0.945958000 |
| 1 | 3.919498000 | -1.344687000 | -0.903009000 |
| 1 | 2.536997000 | -2.350710000 | -0.427998000 |
| 1 | 2.516766000 | -1.517258000 | -1.984730000 |
| 6 | 2.757840000 | 1.427948000 | -1.052031000 |
| 1 | 3.847097000 | 1.385346000 | -1.011843000 |
| 1 | 2.433819000 | 1.417708000 | -2.091500000 |
| 1 | 2.422522000 | 2.359255000 | -0.596903000 |
| 6 | -2.503541000 | -0.037416000 | -0.787978000 |
| 8 | -3.610334000 | -0.034301000 | -1.075321000 |

**M3** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -962.061312
G = -962.108838

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.518399000 | -0.037715000 | -0.170580000 |
| 15 | 2.034232000 | -0.040123000 | -0.111442000 |
| 7 | -0.552075000 | 1.759093000 | 0.017715000 |
| 8 | -0.555001000 | 2.937468000 | 0.120784000 |
| 6 | -0.783896000 | -0.371118000 | 1.831655000 |
| 8 | -0.924670000 | -0.587745000 | 2.954027000 |
| 1 | -0.145635000 | -0.271097000 | -1.936135000 |
| 8 | -0.445309000 | -2.377114000 | -0.489976000 |
| 1 | -1.174890000 | -2.885148000 | -0.120658000 |
| 1 | -0.523724000 | -2.416881000 | -1.451231000 |
| 6 | 2.747767000 | 1.201747000 | -1.253702000 |
| 1 | 3.837791000 | 1.205162000 | -1.210274000 |
| 1 | 2.420142000 | 0.981603000 | -2.267938000 |
| 1 | 2.374829000 | 2.190104000 | -0.986945000 |
| 6 | 2.881017000 | -1.590084000 | -0.611974000 |
| 1 | 2.598328000 | -2.401275000 | 0.057786000 |
| 1 | 2.576835000 | -1.857951000 | -1.622894000 |
| 1 | 3.964608000 | -1.468714000 | -0.587195000 |
| 6 | 2.862809000 | 0.367685000 | 1.476119000 |
| 1 | 2.608063000 | -0.380924000 | 2.225507000 |
| 1 | 3.947468000 | 0.411290000 | 1.366351000 |
| 1 | 2.501285000 | 1.332922000 | 1.829412000 |
| 6 | -2.512454000 | -0.069460000 | -0.597324000 |
| 8 | -3.630523000 | -0.046684000 | -0.859066000 |

**MTS1** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -962.049712
G = -962.096382

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.529180000 | -0.128767000 | -0.165280000 |
| 15 | 2.043458000 | -0.019163000 | -0.061151000 |
| 7 | -0.687955000 | 1.637941000 | -0.563537000 |
| 8 | -0.772410000 | 2.772752000 | -0.875119000 |
| 6 | -0.697689000 | 0.281903000 | 1.807452000 |
| 8 | -0.789692000 | 0.510967000 | 2.930240000 |
| 1 | -0.267550000 | -0.943342000 | -1.917103000 |
| 8 | -0.149256000 | -2.324750000 | -0.167333000 |
| 1 | -0.910639000 | -2.897315000 | -0.041337000 |
| 1 | -0.221150000 | -1.739520000 | -1.312542000 |
| 6 | 2.922073000 | -0.150502000 | -1.665225000 |
| 1 | 4.002584000 | -0.078678000 | -1.534539000 |
| 1 | 2.678495000 | -1.104037000 | -2.131685000 |
| 1 | 2.586954000 | 0.645835000 | -2.328726000 |
| 6 | 2.717039000 | 1.530229000 | 0.646662000 |
| 1 | 2.362964000 | 1.646232000 | 1.670057000 |
| 1 | 3.807761000 | 1.527083000 | 0.642714000 |
| 1 | 2.359329000 | 2.380635000 | 0.067210000 |
| 6 | 2.822447000 | -1.334136000 | 0.946489000 |
| 1 | 2.513083000 | -1.225803000 | 1.985432000 |
| 1 | 2.476354000 | -2.303320000 | 0.591407000 |
| 1 | 3.910445000 | -1.285002000 | 0.889788000 |
| 6 | -2.553961000 | -0.369224000 | -0.313235000 |
| 8 | -3.693010000 | -0.461686000 | -0.390387000 |

**M4** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -960.909412
G = -960.956400

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.524307000 | -0.206311000 | -0.042904000 |
| 15 | 2.059401000 | -0.013580000 | -0.005736000 |

| | | | |
|---|---|---|---|
| 7 | -0.721500000 | 1.267284000 | -1.109749000 |
| 8 | -0.808599000 | 2.126814000 | -1.916476000 |
| 6 | -0.837445000 | 0.959399000 | 1.529306000 |
| 8 | -1.005017000 | 1.591111000 | 2.479833000 |
| 8 | 0.003502000 | -2.134451000 | 0.011856000 |
| 1 | -0.638899000 | -2.846369000 | -0.000087000 |
| 6 | 2.841422000 | -0.877736000 | 1.405762000 |
| 1 | 2.483886000 | -1.906396000 | 1.419053000 |
| 1 | 3.929363000 | -0.867965000 | 1.328537000 |
| 1 | 2.545180000 | -0.398661000 | 2.338384000 |
| 6 | 2.865950000 | -0.784557000 | -1.459783000 |
| 1 | 3.953241000 | -0.754395000 | -1.377203000 |
| 1 | 2.535119000 | -1.819630000 | -1.532914000 |
| 1 | 2.563556000 | -0.261199000 | -2.366501000 |
| 6 | 2.774710000 | 1.669735000 | 0.044530000 |
| 1 | 3.864610000 | 1.641096000 | 0.017937000 |
| 1 | 2.410301000 | 2.244479000 | -0.806304000 |
| 1 | 2.452388000 | 2.174595000 | 0.954421000 |
| 6 | -2.532293000 | -0.565483000 | -0.149425000 |
| 8 | -3.666713000 | -0.710220000 | -0.221273000 |

**M5** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -1422.006490
G = -1422.062850

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000000000 | -0.018308000 | 0.049912000 |
| 15 | -2.523494000 | 0.024514000 | -0.248609000 |
| 15 | 2.523529000 | 0.024369000 | -0.248561000 |
| 7 | -0.000092000 | -0.054735000 | 1.884393000 |
| 8 | -0.000170000 | -0.112093000 | 3.073988000 |
| 6 | -0.000136000 | -2.080695000 | 0.085356000 |
| 8 | -0.000232000 | -3.225224000 | 0.183351000 |
| 6 | -3.527483000 | 0.167994000 | 1.276562000 |
| 1 | -4.594936000 | 0.186432000 | 1.052803000 |
| 1 | -3.311091000 | -0.673573000 | 1.933464000 |
| 1 | -3.254304000 | 1.080739000 | 1.804283000 |
| 6 | -3.255429000 | -1.434597000 | -1.088338000 |
| 1 | -2.767669000 | -1.566627000 | -2.053579000 |
| 1 | -3.081750000 | -2.328867000 | -0.491118000 |
| 1 | -4.327883000 | -1.311303000 | -1.245616000 |
| 6 | -3.121580000 | 1.401238000 | -1.299296000 |
| 1 | -2.562611000 | 1.380144000 | -2.234149000 |
| 1 | -4.189826000 | 1.319210000 | -1.504180000 |
| 1 | -2.924213000 | 2.351774000 | -0.805044000 |
| 6 | 3.121485000 | 1.400604000 | -1.299953000 |
| 1 | 2.924009000 | 2.351371000 | -0.806187000 |
| 1 | 4.189742000 | 1.318574000 | -1.504771000 |
| 1 | 2.562496000 | 1.378981000 | -2.234780000 |
| 6 | 3.255513000 | -1.435128000 | -1.087568000 |
| 1 | 4.327944000 | -1.311861000 | -1.245020000 |
| 1 | 3.081932000 | -2.329102000 | -0.489876000 |
| 1 | 2.767662000 | -1.567673000 | -2.052693000 |
| 6 | 3.527469000 | 0.168688000 | 1.276554000 |
| 1 | 3.254144000 | 1.081642000 | 1.803841000 |
| 1 | 3.311149000 | -0.672603000 | 1.933835000 |
| 1 | 4.594929000 | 0.187160000 | 1.052839000 |
| 8 | 0.000096000 | 0.073209000 | -2.046113000 |
| 1 | -0.000177000 | -0.742280000 | -2.548063000 |
| 6 | 0.000197000 | 2.054392000 | 0.152226000 |
| 8 | 0.000350000 | 3.191309000 | 0.303036000 |

**M6** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -1423.166250
G = -1423.226376

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.088820000 | -0.176926000 | 0.058208000 |

| | | | |
|---|---|---|---|
| 15 | -2.450167000 | -0.143680000 | -0.008251000 |
| 15 | 2.535691000 | 0.380297000 | -0.159425000 |
| 7 | 0.293645000 | -1.852437000 | 0.803956000 |
| 8 | 0.458140000 | -2.922713000 | 1.281236000 |
| 6 | 0.089233000 | -0.899279000 | -1.871313000 |
| 8 | 0.088676000 | -1.297880000 | -2.948039000 |
| 1 | -0.008067000 | 1.513774000 | -0.697138000 |
| 8 | -1.852744000 | 3.386454000 | -0.948834000 |
| 1 | -1.110274000 | 2.761908000 | -0.853457000 |
| 1 | -1.458474000 | 4.210161000 | -1.245107000 |
| 6 | 0.052537000 | 0.770787000 | 1.889882000 |
| 8 | 0.036087000 | 1.300488000 | 2.907602000 |
| 6 | -3.303729000 | 1.023458000 | 1.117898000 |
| 1 | -4.386833000 | 0.930300000 | 1.025446000 |
| 1 | -3.014904000 | 0.821357000 | 2.148462000 |
| 1 | -3.010015000 | 2.040800000 | 0.861635000 |
| 6 | -3.219180000 | 0.262010000 | -1.621806000 |
| 1 | -2.869232000 | -0.431081000 | -2.385592000 |
| 1 | -4.306885000 | 0.204325000 | -1.557840000 |
| 1 | -2.931377000 | 1.273979000 | -1.903808000 |
| 6 | 3.154861000 | 0.697331000 | -1.857756000 |
| 1 | 2.585078000 | 1.512634000 | -2.301244000 |
| 1 | 4.213637000 | 0.960285000 | -1.850139000 |
| 1 | 3.012617000 | -0.189759000 | -2.473473000 |
| 6 | 3.115947000 | 1.879229000 | 0.726940000 |
| 1 | 2.547006000 | 2.741931000 | 0.383296000 |
| 1 | 2.944430000 | 1.764339000 | 1.796316000 |
| 1 | 4.178342000 | 2.055590000 | 0.552665000 |
| 6 | -3.215596000 | -1.755558000 | 0.418258000 |
| 1 | -2.905647000 | -2.053044000 | 1.418954000 |
| 1 | -4.304318000 | -1.695232000 | 0.380926000 |
| 1 | -2.873937000 | -2.518519000 | -0.279804000 |
| 6 | 3.691740000 | -0.908681000 | 0.447755000 |
| 1 | 4.731170000 | -0.601156000 | 0.323950000 |
| 1 | 3.497407000 | -1.104173000 | 1.501440000 |
| 1 | 3.523059000 | -1.834633000 | -0.100311000 |

**MTS2** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -1423.118981
G = -1423.175332

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.014098000 | 0.006627000 | 0.022515000 |
| 15 | -2.525625000 | 0.032198000 | -0.121627000 |
| 15 | 2.538258000 | 0.023139000 | -0.189573000 |
| 7 | 0.054402000 | 0.060197000 | 1.818502000 |
| 8 | 0.073055000 | 0.085991000 | 3.010120000 |
| 6 | 0.020635000 | -2.054996000 | 0.160836000 |
| 8 | 0.014717000 | -3.188877000 | 0.349029000 |
| 1 | 0.563533000 | 1.287686000 | -2.039406000 |
| 8 | -0.457248000 | -0.636758000 | -2.297759000 |
| 1 | 0.068522000 | 0.332675000 | -2.404930000 |
| 1 | 0.102929000 | -1.326194000 | -2.671735000 |
| 6 | 3.362364000 | 1.659873000 | -0.218873000 |
| 1 | 3.141093000 | 2.193667000 | 0.704511000 |
| 1 | 4.443517000 | 1.558103000 | -0.322234000 |
| 1 | 2.970572000 | 2.239482000 | -1.053384000 |
| 6 | 3.240541000 | -0.783605000 | -1.681384000 |
| 1 | 4.330913000 | -0.751689000 | -1.670269000 |
| 1 | 2.917728000 | -1.823529000 | -1.727201000 |
| 1 | 2.877221000 | -0.265343000 | -2.567655000 |
| 6 | 3.404760000 | -0.832156000 | 1.182811000 |
| 1 | 3.122338000 | -1.884215000 | 1.194398000 |
| 1 | 4.488099000 | -0.753555000 | 1.082411000 |
| 1 | 3.098430000 | -0.391833000 | 2.131113000 |
| 6 | -3.348812000 | -1.560087000 | -0.506145000 |
| 1 | -2.968145000 | -1.926578000 | -1.458146000 |

| | | | |
|---|---|---|---|
| 1 | -3.113072000 | -2.292636000 | 0.264782000 |
| 1 | -4.431627000 | -1.443398000 | -0.569885000 |
| 6 | -3.241997000 | 1.148029000 | -1.387235000 |
| 1 | -2.922302000 | 2.171861000 | -1.197480000 |
| 1 | -2.869115000 | 0.850422000 | -2.365916000 |
| 1 | -4.332167000 | 1.104649000 | -1.383381000 |
| 6 | -3.351635000 | 0.562609000 | 1.424941000 |
| 1 | -4.437243000 | 0.529022000 | 1.325200000 |
| 1 | -3.043423000 | -0.085824000 | 2.244022000 |
| 1 | -3.046753000 | 1.579149000 | 1.670518000 |
| 6 | 0.000207000 | 2.090637000 | -0.100018000 |
| 8 | -0.016895000 | 3.236447000 | -0.081713000 |

**MTS3** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -1423.121304
G =-1423.179204

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.008400000 | 0.057213000 | -0.038477000 |
| 15 | -2.509697000 | -0.097503000 | -0.025078000 |
| 15 | 2.516457000 | -0.087828000 | 0.049766000 |
| 7 | 0.063206000 | -0.152687000 | -1.813038000 |
| 8 | 0.103572000 | -0.342773000 | -2.992053000 |
| 1 | 0.047562000 | -1.292297000 | 1.916975000 |
| 8 | -0.364096000 | 1.016934000 | 2.629816000 |
| 1 | -0.112219000 | 0.174170000 | 3.037346000 |
| 1 | 0.216550000 | 1.689013000 | 3.003013000 |
| 6 | 0.003483000 | -1.853526000 | 0.811150000 |
| 8 | -0.003943000 | -3.053522000 | 0.864868000 |
| 6 | 3.326695000 | -0.068712000 | 1.700403000 |
| 1 | 4.408412000 | -0.176998000 | 1.610426000 |
| 1 | 3.109494000 | 0.871343000 | 2.207056000 |
| 1 | 2.938122000 | -0.886443000 | 2.306694000 |
| 6 | 3.178123000 | -1.624872000 | -0.699014000 |
| 1 | 2.842026000 | -1.684653000 | -1.733806000 |
| 1 | 4.268599000 | -1.649826000 | -0.671879000 |
| 1 | 2.777725000 | -2.487319000 | -0.168281000 |
| 6 | 3.445993000 | 1.210201000 | -0.856398000 |
| 1 | 3.236445000 | 2.185425000 | -0.419044000 |
| 1 | 4.521064000 | 1.025402000 | -0.828338000 |
| 1 | 3.113933000 | 1.226582000 | -1.893898000 |
| 6 | -3.109475000 | -1.466493000 | -1.084952000 |
| 1 | -2.758067000 | -1.310323000 | -2.104344000 |
| 1 | -2.691183000 | -2.405605000 | -0.725411000 |
| 1 | -4.198777000 | -1.526352000 | -1.083711000 |
| 6 | -3.326693000 | -0.439792000 | 1.583040000 |
| 1 | -2.943436000 | -1.373937000 | 1.992292000 |
| 1 | -3.102684000 | 0.360682000 | 2.286480000 |
| 1 | -4.407713000 | -0.521515000 | 1.461390000 |
| 6 | -3.470310000 | 1.336209000 | -0.651240000 |
| 1 | -3.277501000 | 2.205040000 | -0.023168000 |
| 1 | -3.146827000 | 1.572013000 | -1.664406000 |
| 1 | -4.541452000 | 1.127695000 | -0.657751000 |
| 6 | 0.019013000 | 2.125394000 | -0.084755000 |
| 8 | 0.031152000 | 3.277170000 | -0.126230000 |

**MTS4** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -1423.126527
G =-1423.183805

| | | | |
|---|---|---|---|
| 74 | -0.000767000 | -0.048720000 | -0.032487000 |
| 15 | -2.536992000 | 0.023571000 | -0.070752000 |
| 15 | 2.525012000 | -0.025095000 | -0.092158000 |
| 7 | 0.037795000 | -0.099144000 | 1.774599000 |
| 8 | 0.072661000 | -0.114087000 | 2.964911000 |
| 1 | 0.093368000 | 2.306658000 | -1.821567000 |
| 8 | -0.107505000 | 0.187543000 | -2.228799000 |
| 1 | 0.018707000 | 1.325087000 | -2.253147000 |

| | | | |
|---|---|---|---|
| 1 | 0.514113000 | -0.236548000 | -2.826681000 |
| 6 | 0.054209000 | 2.134084000 | -0.215607000 |
| 8 | 0.079539000 | 3.194430000 | 0.265504000 |
| 6 | 3.335949000 | -1.461739000 | 0.710005000 |
| 1 | 3.049418000 | -2.378682000 | 0.196752000 |
| 1 | 4.422760000 | -1.365534000 | 0.700653000 |
| 1 | 2.992014000 | -1.531073000 | 1.741440000 |
| 6 | 3.337084000 | 0.025741000 | -1.741437000 |
| 1 | 3.055148000 | -0.852376000 | -2.323046000 |
| 1 | 3.015714000 | 0.917489000 | -2.279196000 |
| 1 | 4.423334000 | 0.044269000 | -1.645392000 |
| 6 | 3.315023000 | 1.385457000 | 0.774766000 |
| 1 | 4.402785000 | 1.302147000 | 0.764230000 |
| 1 | 3.018936000 | 2.320516000 | 0.301781000 |
| 1 | 2.967263000 | 1.407874000 | 1.807019000 |
| 6 | -3.340355000 | -0.487662000 | -1.638291000 |
| 1 | -3.001097000 | 0.158078000 | -2.446372000 |
| 1 | -3.048327000 | -1.508992000 | -1.879373000 |
| 1 | -4.426848000 | -0.432566000 | -1.560121000 |
| 6 | -3.311124000 | -1.077088000 | 1.174022000 |
| 1 | -3.025985000 | -2.109131000 | 0.974742000 |
| 1 | -2.945051000 | -0.810891000 | 2.165064000 |
| 1 | -4.398736000 | -0.994223000 | 1.157333000 |
| 6 | -3.349619000 | 1.632337000 | 0.279395000 |
| 1 | -4.436569000 | 1.537457000 | 0.282804000 |
| 1 | -3.019845000 | 2.002514000 | 1.249405000 |
| 1 | -3.055615000 | 2.361584000 | -0.474696000 |
| 6 | -0.064880000 | -2.070448000 | -0.199505000 |
| 8 | -0.107363000 | -3.221086000 | -0.284892000 |

**M7** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -1423.130173
G = -1423.187358

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000241000 | 0.127026000 | -0.048795000 |
| 15 | 2.515334000 | -0.064764000 | -0.027923000 |
| 15 | -2.506938000 | -0.074804000 | -0.037662000 |
| 7 | -0.028312000 | 0.099302000 | 1.749168000 |
| 8 | -0.056590000 | 0.054402000 | 2.940774000 |
| 1 | -0.036040000 | -2.211735000 | -1.710867000 |
| 8 | 0.073984000 | 0.069865000 | -2.375195000 |
| 1 | -0.035106000 | -0.878243000 | -2.607615000 |
| 1 | -0.559756000 | 0.580390000 | -2.887222000 |
| 6 | 0.014143000 | -2.036513000 | -0.525056000 |
| 8 | 0.054967000 | -3.076964000 | 0.090953000 |
| 6 | -3.370235000 | -0.471293000 | -1.616906000 |
| 1 | -4.442786000 | -0.591265000 | -1.458852000 |
| 1 | -3.220069000 | 0.329893000 | -2.341651000 |
| 1 | -2.972686000 | -1.397443000 | -2.031593000 |
| 6 | -3.098339000 | -1.406251000 | 1.074145000 |
| 1 | -2.743665000 | -1.203549000 | 2.084242000 |
| 1 | -4.187564000 | -1.467622000 | 1.080176000 |
| 1 | -2.676282000 | -2.359468000 | 0.760359000 |
| 6 | -3.464974000 | 1.373372000 | 0.560617000 |
| 1 | -3.301470000 | 2.220985000 | -0.103835000 |
| 1 | -4.533215000 | 1.157118000 | 0.616153000 |
| 1 | -3.104204000 | 1.649162000 | 1.550904000 |
| 6 | 3.097637000 | -1.326005000 | 1.166259000 |
| 1 | 2.771927000 | -1.043788000 | 2.166979000 |
| 1 | 2.643563000 | -2.286502000 | 0.927684000 |
| 1 | 4.184830000 | -1.416467000 | 1.153606000 |
| 6 | 3.348091000 | -0.566075000 | -1.588121000 |
| 1 | 2.968639000 | -1.536817000 | -1.905961000 |
| 1 | 3.136095000 | 0.158657000 | -2.373312000 |
| 1 | 4.427713000 | -0.636378000 | -1.450042000 |

| | | | |
|---|---|---|---|
| 6 | 3.481877000 | 1.416142000 | 0.467880000 |
| 1 | 3.314984000 | 2.218235000 | -0.250123000 |
| 1 | 3.132971000 | 1.757963000 | 1.441599000 |
| 1 | 4.549991000 | 1.199737000 | 0.525778000 |
| 6 | 0.004709000 | 2.160933000 | -0.185389000 |
| 8 | 0.010024000 | 3.313916000 | -0.276098000 |

**MTS4** complex of $WH(NO)(CO)_2(PMe_3)_2$
E (ZPE- corrected) = -1423.126527
G = -1423.183805

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.000767000 | -0.048720000 | -0.032487000 |
| 15 | -2.536992000 | 0.023571000 | -0.070752000 |
| 15 | 2.525012000 | -0.025095000 | -0.092158000 |
| 7 | 0.037795000 | -0.099144000 | 1.774599000 |
| 8 | 0.072661000 | -0.114087000 | 2.964911000 |
| 1 | 0.093368000 | 2.306658000 | -1.821567000 |
| 8 | -0.107505000 | 0.187543000 | -2.228799000 |
| 1 | 0.018707000 | 1.325087000 | -2.253147000 |
| 1 | 0.514113000 | -0.236548000 | -2.826681000 |
| 6 | 0.054209000 | 2.134084000 | -0.215607000 |
| 8 | 0.079539000 | 3.194430000 | 0.265504000 |
| 6 | 3.335949000 | -1.461739000 | 0.710005000 |
| 1 | 3.049418000 | -2.378682000 | 0.196752000 |
| 1 | 4.422760000 | -1.365534000 | 0.700653000 |
| 1 | 2.992014000 | -1.531073000 | 1.741440000 |
| 6 | 3.337084000 | 0.025741000 | -1.741437000 |
| 1 | 3.055148000 | -0.852376000 | -2.323046000 |
| 1 | 3.015714000 | 0.917489000 | -2.279196000 |
| 1 | 4.423334000 | 0.044269000 | -1.645392000 |
| 6 | 3.315023000 | 1.385457000 | 0.774766000 |
| 1 | 4.402785000 | 1.302147000 | 0.764230000 |
| 1 | 3.018936000 | 2.320516000 | 0.301781000 |
| 1 | 2.967263000 | 1.407874000 | 1.807019000 |
| 6 | -3.340355000 | -0.487662000 | -1.638291000 |
| 1 | -3.001097000 | 0.158078000 | -2.446372000 |
| 1 | -3.048327000 | -1.508992000 | -1.879373000 |
| 1 | -4.426848000 | -0.432566000 | -1.560121000 |
| 6 | -3.311124000 | -1.077088000 | 1.174022000 |
| 1 | -3.025985000 | -2.109131000 | 0.974742000 |
| 1 | -2.945051000 | -0.810891000 | 2.165064000 |
| 1 | -4.398736000 | -0.994223000 | 1.157333000 |
| 6 | -3.349619000 | 1.632337000 | 0.279395000 |
| 1 | -4.436569000 | 1.537457000 | 0.282804000 |
| 1 | -3.019845000 | 2.002514000 | 1.249405000 |
| 1 | -3.055615000 | 2.361584000 | -0.474696000 |
| 6 | -0.064880000 | -2.070448000 | -0.199505000 |
| 8 | -0.107363000 | -3.221086000 | -0.284892000 |

**M1** complex of $WH(NO)(CO)(PMe_3)_3$
E (ZPE- corrected) = -1694.409334
G = -1694.469473

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.001272000 | -0.337329000 | 0.081554000 |
| 15 | -2.448424000 | -0.537513000 | -0.406241000 |
| 15 | -0.003283000 | 2.230832000 | -0.110795000 |
| 15 | 2.453958000 | -0.534350000 | -0.405476000 |
| 7 | 0.000351000 | -0.054025000 | 1.899852000 |
| 8 | -0.003287000 | 0.197281000 | 3.068256000 |
| 6 | -0.003411000 | -2.331811000 | 0.307265000 |
| 8 | -0.007865000 | -3.476940000 | 0.484077000 |
| 1 | -0.005182000 | -0.433881000 | -1.771653000 |
| 6 | -3.593189000 | -0.424417000 | 1.030394000 |

| | | | |
|---|---|---|---|
| 1 | -4.628293000 | -0.606104000 | 0.735964000 |
| 1 | -3.297556000 | -1.160617000 | 1.776646000 |
| 1 | -3.519863000 | 0.560659000 | 1.489183000 |
| 6 | -2.939128000 | -2.149502000 | -1.140267000 |
| 1 | -2.377641000 | -2.304980000 | -2.060292000 |
| 1 | -2.693054000 | -2.957416000 | -0.453506000 |
| 1 | -4.007791000 | -2.175340000 | -1.358771000 |
| 6 | -3.242317000 | 0.603554000 | -1.617831000 |
| 1 | -2.707590000 | 0.531578000 | -2.564006000 |
| 1 | -4.290117000 | 0.343866000 | -1.777025000 |
| 1 | -3.187932000 | 1.634044000 | -1.271715000 |
| 6 | 1.426163000 | 3.094852000 | 0.672045000 |
| 1 | 1.524045000 | 2.745699000 | 1.699448000 |
| 1 | 2.349650000 | 2.865745000 | 0.144602000 |
| 1 | 1.284466000 | 4.176858000 | 0.674921000 |
| 6 | -0.086213000 | 3.054818000 | -1.753154000 |
| 1 | 0.755573000 | 2.730428000 | -2.363001000 |
| 1 | -0.998634000 | 2.752831000 | -2.264909000 |
| 1 | -0.068467000 | 4.142014000 | -1.662001000 |
| 6 | -1.362270000 | 3.068931000 | 0.811458000 |
| 1 | -2.330638000 | 2.805918000 | 0.391163000 |
| 1 | -1.338291000 | 2.730197000 | 1.847097000 |
| 1 | -1.252076000 | 4.154342000 | 0.787607000 |
| 6 | 3.222001000 | 0.541631000 | -1.691329000 |
| 1 | 3.159748000 | 1.591020000 | -1.409402000 |
| 1 | 4.271247000 | 0.283815000 | -1.844405000 |
| 1 | 2.678989000 | 0.406653000 | -2.625753000 |
| 6 | 2.968466000 | -2.180452000 | -1.042099000 |
| 1 | 4.036937000 | -2.202499000 | -1.262119000 |
| 1 | 2.737089000 | -2.948700000 | -0.306429000 |
| 1 | 2.408233000 | -2.402225000 | -1.949238000 |
| 6 | 3.605109000 | -0.318651000 | 1.013823000 |
| 1 | 3.524137000 | 0.693080000 | 1.408924000 |
| 1 | 3.320344000 | -1.008731000 | 1.806921000 |
| 1 | 4.640247000 | -0.508727000 | 0.725016000 |

**M2** complex for $WH(NO)(CO)(PMe_3)_2$
E (ZPE- corrected) = -1233.306286
G = -1233.357714

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.000012000 | 0.032015000 | -0.085275000 |
| 15 | -2.475022000 | -0.057605000 | -0.390394000 |
| 15 | 2.475062000 | -0.057581000 | -0.390362000 |
| 7 | -0.000049000 | 1.400766000 | 1.103616000 |
| 8 | -0.000122000 | 2.426174000 | 1.716926000 |
| 6 | -0.000053000 | -1.280814000 | 1.372334000 |
| 8 | -0.000065000 | -2.108047000 | 2.190781000 |
| 1 | 0.000077000 | -0.222311000 | -1.907013000 |
| 6 | 3.111126000 | -1.618647000 | -1.118948000 |
| 1 | 2.650953000 | -1.773681000 | -2.093667000 |
| 1 | 4.195953000 | -1.589403000 | -1.232601000 |
| 1 | 2.843672000 | -2.456468000 | -0.475985000 |
| 6 | 3.200793000 | 1.212982000 | -1.503575000 |
| 1 | 2.747024000 | 1.125996000 | -2.489783000 |
| 1 | 2.979729000 | 2.205941000 | -1.112526000 |
| 1 | 4.282535000 | 1.099330000 | -1.591273000 |
| 6 | 3.489752000 | 0.128984000 | 1.125834000 |
| 1 | 4.557807000 | 0.109806000 | 0.903360000 |
| 1 | 3.238619000 | 1.072758000 | 1.608460000 |
| 1 | 3.249880000 | -0.676465000 | 1.818535000 |
| 6 | -3.489730000 | 0.128811000 | 1.125818000 |
| 1 | -3.249928000 | -0.676715000 | 1.818450000 |
| 1 | -3.238584000 | 1.072537000 | 1.608532000 |
| 1 | -4.557779000 | 0.109707000 | 0.903300000 |

| | | | |
|---|---|---|---|
| 6 | -3.200767000 | 1.213086000 | -1.503466000 |
| 1 | -4.282516000 | 1.099485000 | -1.591140000 |
| 1 | -2.979646000 | 2.206001000 | -1.112342000 |
| 1 | -2.747057000 | 1.126169000 | -2.489709000 |
| 6 | -3.111103000 | -1.618587000 | -1.119150000 |
| 1 | -4.195943000 | -1.589359000 | -1.232669000 |
| 1 | -2.651026000 | -1.773438000 | -2.093944000 |
| 1 | -2.843551000 | -2.456508000 | -0.476359000 |

**M3** complex for WH(NO)(CO)($PMe_3$)$_2$ with methanol
E (ZPE- corrected) = -1349.050665
G = -1349.107603

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.012962000 | -0.078178000 | -0.031553000 |
| 15 | 2.496251000 | -0.122589000 | -0.325828000 |
| 15 | -2.472995000 | -0.211589000 | -0.302545000 |
| 7 | 0.035601000 | -1.822882000 | 0.397731000 |
| 8 | 0.048038000 | -2.992277000 | 0.657995000 |
| 6 | 0.049652000 | 0.517749000 | 1.891922000 |
| 8 | 0.069054000 | 0.907690000 | 2.987461000 |
| 1 | -0.040486000 | -0.039295000 | -1.871878000 |
| 8 | 0.046978000 | 2.185260000 | -0.654622000 |
| 1 | -0.192721000 | 2.180601000 | -1.586326000 |
| 6 | -2.957140000 | -1.664324000 | -1.315360000 |
| 1 | -4.041348000 | -1.755569000 | -1.400229000 |
| 1 | -2.516256000 | -1.567342000 | -2.305972000 |
| 1 | -2.554053000 | -2.565846000 | -0.854922000 |
| 6 | -3.368658000 | 1.154554000 | -1.158915000 |
| 1 | -3.303279000 | 2.071173000 | -0.572921000 |
| 1 | -2.917719000 | 1.329191000 | -2.135519000 |
| 1 | -4.422664000 | 0.909480000 | -1.297905000 |
| 6 | -3.508656000 | -0.442037000 | 1.199170000 |
| 1 | -3.404654000 | 0.426568000 | 1.848374000 |
| 1 | -4.562217000 | -0.587244000 | 0.953330000 |
| 1 | -3.144786000 | -1.311641000 | 1.745288000 |
| 6 | 3.366597000 | 1.417170000 | -0.834990000 |
| 1 | 2.960505000 | 1.769586000 | -1.782246000 |
| 1 | 3.214935000 | 2.193417000 | -0.085985000 |
| 1 | 4.437027000 | 1.241879000 | -0.951407000 |
| 6 | 3.069493000 | -1.317572000 | -1.598202000 |
| 1 | 2.648832000 | -1.039085000 | -2.562978000 |
| 1 | 4.158580000 | -1.348675000 | -1.664635000 |
| 1 | 2.697150000 | -2.309501000 | -1.343915000 |
| 6 | 3.474518000 | -0.648318000 | 1.137937000 |
| 1 | 4.537973000 | -0.736875000 | 0.908489000 |
| 1 | 3.335416000 | 0.071694000 | 1.943299000 |
| 1 | 3.099928000 | -1.611966000 | 1.481695000 |
| 6 | -0.369632000 | 3.381772000 | 0.012090000 |
| 1 | -0.067331000 | 3.282825000 | 1.050292000 |
| 1 | 0.122426000 | 4.248515000 | -0.430184000 |
| 1 | -1.452079000 | 3.506774000 | -0.035946000 |

**MTS1** complex for WH(NO)(CO)($PMe_3$)$_2$ with methanol

E (ZPE- corrected) = -1349.040748
G = -1349.09658

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.031478000 | -0.040979000 | -0.104076000 |
| 15 | 2.553599000 | 0.050469000 | -0.148845000 |
| 15 | -2.499371000 | -0.061964000 | -0.162316000 |
| 7 | 0.030334000 | -1.801672000 | -0.488983000 |
| 8 | 0.031511000 | -2.954878000 | -0.799090000 |
| 6 | 0.019232000 | -0.447073000 | 1.844829000 |

| | | | |
|---|---|---|---|
| 8 | 0.007808000 | -0.677356000 | 2.981862000 |
| 1 | 0.047286000 | 0.799566000 | -1.890809000 |
| 8 | 0.245730000 | 2.195609000 | -0.178017000 |
| 1 | 0.131566000 | 1.599549000 | -1.286612000 |
| 6 | -3.148516000 | -1.723478000 | 0.260143000 |
| 1 | -2.857116000 | -1.972715000 | 1.279547000 |
| 1 | -4.235714000 | -1.753880000 | 0.177377000 |
| 1 | -2.711950000 | -2.467791000 | -0.404119000 |
| 6 | -3.335576000 | 0.276112000 | -1.767020000 |
| 1 | -4.415359000 | 0.132595000 | -1.699671000 |
| 1 | -3.129739000 | 1.299058000 | -2.080227000 |
| 1 | -2.931743000 | -0.393290000 | -2.525890000 |
| 6 | -3.452409000 | 1.009429000 | 0.991036000 |
| 1 | -3.127459000 | 0.814899000 | 2.012438000 |
| 1 | -3.272770000 | 2.059919000 | 0.769977000 |
| 1 | -4.522361000 | 0.810000000 | 0.913480000 |
| 6 | 3.362579000 | -1.475654000 | 0.461866000 |
| 1 | 4.448982000 | -1.407070000 | 0.391718000 |
| 1 | 3.078213000 | -1.642703000 | 1.499905000 |
| 1 | 3.016273000 | -2.327209000 | -0.122697000 |
| 6 | 3.357422000 | 0.292689000 | -1.784256000 |
| 1 | 3.035350000 | 1.244521000 | -2.205164000 |
| 1 | 4.445929000 | 0.283340000 | -1.706831000 |
| 1 | 3.039252000 | -0.499712000 | -2.460946000 |
| 6 | 3.324823000 | 1.370612000 | 0.863541000 |
| 1 | 4.410849000 | 1.369368000 | 0.760539000 |
| 1 | 2.926724000 | 2.333619000 | 0.548650000 |
| 1 | 3.063662000 | 1.221426000 | 1.910573000 |
| 6 | -0.676274000 | 3.234204000 | 0.051124000 |
| 1 | -1.013000000 | 3.233829000 | 1.092305000 |
| 1 | -0.208589000 | 4.201778000 | -0.154656000 |
| 1 | -1.561517000 | 3.149473000 | -0.592574000 |

**M4** complex for $W(OCH_3)(NO)(CO)(PMe_3)_2$

E (ZPE- corrected) = -1347.900988
G = -1347.956565

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.031323000 | -0.008328000 | -0.011430000 |
| 15 | -2.564084000 | 0.095827000 | -0.075257000 |
| 15 | 2.497673000 | 0.050321000 | -0.083910000 |
| 7 | 0.007504000 | -1.516983000 | -1.020330000 |
| 8 | 0.049002000 | -2.430534000 | -1.793953000 |
| 6 | 0.023759000 | -1.134832000 | 1.585978000 |
| 8 | 0.055779000 | -1.757160000 | 2.570082000 |
| 8 | -0.232689000 | 1.981639000 | 0.006262000 |
| 6 | 3.309261000 | 0.784862000 | -1.566169000 |
| 1 | 2.945951000 | 0.274418000 | -2.457954000 |
| 1 | 3.049178000 | 1.839347000 | -1.650398000 |
| 1 | 4.395349000 | 0.688802000 | -1.520503000 |
| 6 | 3.398055000 | 0.865810000 | 1.297471000 |
| 1 | 4.478400000 | 0.769389000 | 1.178600000 |
| 1 | 3.139505000 | 1.922781000 | 1.342400000 |
| 1 | 3.100602000 | 0.403336000 | 2.238006000 |
| 6 | 3.209229000 | -1.637930000 | -0.066645000 |
| 1 | 2.792258000 | -2.213599000 | -0.891957000 |
| 1 | 4.296487000 | -1.612871000 | -0.152882000 |
| 1 | 2.931552000 | -2.133016000 | 0.862628000 |
| 6 | -3.339871000 | 1.038776000 | 1.293221000 |
| 1 | -2.913392000 | 2.040968000 | 1.309184000 |
| 1 | -4.422534000 | 1.106390000 | 1.176644000 |
| 1 | -3.110879000 | 0.554829000 | 2.242049000 |
| 6 | -3.272931000 | 0.911534000 | -1.561739000 |
| 1 | -4.361414000 | 0.971597000 | -1.514414000 |

| | | | |
|---|---|---|---|
| 1 | -2.859188000 | 1.916331000 | -1.640504000 |
| 1 | -2.986131000 | 0.352573000 | -2.452220000 |
| 6 | -3.428230000 | -1.517125000 | -0.036737000 |
| 1 | -4.509428000 | -1.396926000 | -0.117578000 |
| 1 | -3.070224000 | -2.135187000 | -0.859386000 |
| 1 | -3.191090000 | -2.028956000 | 0.894968000 |
| 6 | 0.507830000 | 3.163518000 | 0.046905000 |
| 1 | 0.165971000 | 3.858700000 | -0.728335000 |
| 1 | 0.388561000 | 3.663771000 | 1.015332000 |
| 1 | 1.582685000 | 3.001027000 | -0.110858000 |

**M5** complex of $W(OCH_3)(NO)(CO)(PMe_3)_3$
E (ZPE- corrected) = -1808.98741
G = -1809.050934

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.060054000 | -0.255739000 | -0.101812000 |
| 15 | 2.460927000 | -0.670545000 | -0.017004000 |
| 15 | 0.280019000 | 2.331339000 | 0.124755000 |
| 15 | -2.604047000 | -0.275892000 | 0.044317000 |
| 7 | -0.058033000 | -0.100926000 | -1.918572000 |
| 8 | -0.042715000 | 0.004805000 | -3.116199000 |
| 6 | -0.265020000 | -2.229618000 | -0.327483000 |
| 8 | -0.387894000 | -3.363505000 | -0.540407000 |
| 8 | -0.079750000 | -0.210109000 | 1.979517000 |
| 6 | -3.667412000 | 1.159142000 | 0.512683000 |
| 1 | -3.594690000 | 1.940651000 | -0.241106000 |
| 1 | -4.712005000 | 0.855970000 | 0.601341000 |
| 1 | -3.337021000 | 1.563185000 | 1.469206000 |
| 6 | -3.223906000 | -1.526755000 | 1.239450000 |
| 1 | -4.314334000 | -1.562594000 | 1.244562000 |
| 1 | -2.835365000 | -2.509181000 | 0.977321000 |
| 1 | -2.867526000 | -1.273597000 | 2.236695000 |
| 6 | -3.385283000 | -0.797996000 | -1.531009000 |
| 1 | -2.987924000 | -1.768427000 | -1.823926000 |
| 1 | -4.470053000 | -0.864873000 | -1.437440000 |
| 1 | -3.131179000 | -0.086577000 | -2.315790000 |
| 6 | 2.942315000 | -2.398136000 | 0.392143000 |
| 1 | 2.559704000 | -2.657179000 | 1.378544000 |
| 1 | 2.499109000 | -3.081512000 | -0.330068000 |
| 1 | 4.026571000 | -2.520965000 | 0.385844000 |
| 6 | 3.522558000 | 0.245785000 | 1.180647000 |
| 1 | 3.511591000 | 1.312231000 | 0.962323000 |
| 1 | 3.125407000 | 0.102610000 | 2.185123000 |
| 1 | 4.554303000 | -0.107814000 | 1.150990000 |
| 6 | 3.334494000 | -0.419108000 | -1.611764000 |
| 1 | 4.378292000 | -0.729143000 | -1.545865000 |
| 1 | 2.832669000 | -0.997635000 | -2.386114000 |
| 1 | 3.290518000 | 0.628304000 | -1.904370000 |
| 6 | -1.084277000 | 3.480509000 | -0.339601000 |
| 1 | -1.427275000 | 3.250898000 | -1.348059000 |
| 1 | -1.920128000 | 3.362433000 | 0.345702000 |
| 1 | -0.747743000 | 4.518006000 | -0.307659000 |
| 6 | 0.702636000 | 2.932653000 | 1.806192000 |
| 1 | 0.789928000 | 4.019520000 | 1.837949000 |
| 1 | -0.070456000 | 2.598651000 | 2.496035000 |
| 1 | 1.638238000 | 2.482672000 | 2.132018000 |
| 6 | 1.618059000 | 3.036828000 | -0.926460000 |
| 1 | 2.580853000 | 2.606138000 | -0.658903000 |
| 1 | 1.414936000 | 2.788918000 | -1.968276000 |
| 1 | 1.677502000 | 4.121301000 | -0.823376000 |
| 6 | 0.138811000 | -1.181183000 | 2.947413000 |
| 1 | -0.315689000 | -2.153438000 | 2.698743000 |
| 1 | 1.211880000 | -1.374304000 | 3.120002000 |
| 1 | -0.278378000 | -0.868851000 | 3.915081000 |

**M3** complex of $WH(NO)(CO)(PMe_3)_3$
E (ZPE- corrected) = -1309.766603
G = -1309.821434

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.003161000 | -0.050342000 | -0.039246000 |
| 15 | -2.495816000 | -0.009171000 | -0.293422000 |
| 15 | 2.482192000 | -0.020248000 | -0.292374000 |
| 7 | 0.030619000 | 1.727207000 | 0.213307000 |
| 8 | 0.061275000 | 2.915889000 | 0.353344000 |
| 6 | -0.013137000 | -0.466162000 | 1.931666000 |
| 8 | -0.017664000 | -0.757320000 | 3.055934000 |
| 1 | -0.006953000 | -0.300589000 | -1.869801000 |
| 8 | -0.081864000 | -2.401205000 | -0.460664000 |
| 1 | 0.622296000 | -2.945817000 | -0.096680000 |
| 1 | 0.088951000 | -2.288574000 | -1.406657000 |
| 6 | 3.064789000 | 1.046290000 | -1.669700000 |
| 1 | 4.154178000 | 1.079177000 | -1.726374000 |
| 1 | 2.656489000 | 0.672914000 | -2.607252000 |
| 1 | 2.683023000 | 2.055311000 | -1.516630000 |
| 6 | 3.387330000 | -1.592446000 | -0.632979000 |
| 1 | 3.248385000 | -2.290656000 | 0.193331000 |
| 1 | 3.011233000 | -2.048945000 | -1.548843000 |
| 1 | 4.457000000 | -1.414426000 | -0.752599000 |
| 6 | 3.433932000 | 0.654327000 | 1.126125000 |
| 1 | 3.287588000 | 0.018029000 | 1.997897000 |
| 1 | 4.499991000 | 0.729934000 | 0.904728000 |
| 1 | 3.046315000 | 1.643963000 | 1.365866000 |
| 6 | -3.353851000 | -1.568246000 | -0.758934000 |
| 1 | -2.968073000 | -1.924654000 | -1.713251000 |
| 1 | -3.166812000 | -2.334066000 | -0.007438000 |
| 1 | -4.429664000 | -1.411109000 | -0.848187000 |
| 6 | -3.077077000 | 1.152041000 | -1.591795000 |
| 1 | -2.654494000 | 0.854647000 | -2.550052000 |
| 1 | -4.166299000 | 1.170777000 | -1.658648000 |
| 1 | -2.714940000 | 2.153363000 | -1.360499000 |
| 6 | -3.469011000 | 0.543864000 | 1.163223000 |
| 1 | -4.535186000 | 0.610995000 | 0.939373000 |
| 1 | -3.314476000 | -0.152613000 | 1.986272000 |
| 1 | -3.106419000 | 1.521595000 | 1.478861000 |

**MTS1** complex of $WH(NO)(CO)(PMe_3)_3$
E (ZPE- corrected) = -1309.759125
G = -1309.812625

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | -0.000604000 | -0.064092000 | -0.084450000 |
| 15 | -2.519891000 | -0.138047000 | -0.170667000 |
| 15 | 2.511636000 | -0.175195000 | -0.149771000 |
| 7 | 0.062839000 | 1.677625000 | -0.552618000 |
| 8 | 0.113025000 | 2.815408000 | -0.911021000 |
| 6 | -0.032444000 | 0.427175000 | 1.845629000 |
| 8 | -0.049557000 | 0.698715000 | 2.973075000 |
| 1 | 0.023266000 | -1.024355000 | -1.805597000 |
| 8 | -0.178018000 | -2.310655000 | 0.001800000 |
| 1 | 0.596625000 | -2.815411000 | 0.260724000 |
| 1 | -0.027390000 | -1.786246000 | -1.145839000 |
| 6 | 3.275411000 | 0.067378000 | -1.804462000 |
| 1 | 4.365416000 | 0.050624000 | -1.753845000 |
| 1 | 2.932631000 | -0.714020000 | -2.481475000 |
| 1 | 2.952263000 | 1.026913000 | -2.207367000 |
| 6 | 3.355887000 | 1.112442000 | 0.845742000 |
| 1 | 3.105628000 | 0.980628000 | 1.897352000 |
| 1 | 4.439272000 | 1.071291000 | 0.722081000 |
| 1 | 2.994704000 | 2.091920000 | 0.534014000 |
| 6 | 3.331897000 | -1.719370000 | 0.424444000 |

| | | | |
|---|---|---|---|
| 1 | 3.036863000 | -1.932199000 | 1.451673000 |
| 1 | 3.030562000 | -2.557261000 | -0.204850000 |
| 1 | 4.418024000 | -1.629838000 | 0.381119000 |
| 6 | -3.299504000 | -0.456737000 | -1.804901000 |
| 1 | -2.980324000 | -1.431693000 | -2.171560000 |
| 1 | -4.388935000 | -0.433571000 | -1.745079000 |
| 1 | -2.963439000 | 0.297134000 | -2.516188000 |
| 6 | -3.308248000 | -1.407364000 | 0.892075000 |
| 1 | -4.391782000 | -1.417140000 | 0.765784000 |
| 1 | -2.899130000 | -2.383865000 | 0.637923000 |
| 1 | -3.070317000 | -1.202460000 | 1.935205000 |
| 6 | -3.334191000 | 1.418776000 | 0.349245000 |
| 1 | -4.419864000 | 1.346780000 | 0.270505000 |
| 1 | -3.060981000 | 1.642351000 | 1.379513000 |
| 1 | -2.980879000 | 2.236959000 | -0.277324000 |

**M4** complex of $WH(NO)(CO)(PMe_3)_3$
E (ZPE- corrected) = -1308.618953
G = -1308.673233

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.004984000 | -0.071493000 | -0.007365000 |
| 15 | 2.531985000 | -0.223020000 | -0.058195000 |
| 15 | -2.501514000 | -0.271522000 | -0.058689000 |
| 7 | -0.046360000 | 1.371452000 | -1.108348000 |
| 8 | -0.090907000 | 2.225425000 | -1.945856000 |
| 6 | -0.048204000 | 1.149071000 | 1.520259000 |
| 8 | -0.081048000 | 1.825282000 | 2.467867000 |
| 8 | 0.187358000 | -2.079004000 | 0.119896000 |
| 1 | -0.542678000 | -2.694279000 | 0.198487000 |
| 6 | -3.226237000 | -1.163193000 | -1.498270000 |
| 1 | -2.941486000 | -0.648872000 | -2.415872000 |
| 1 | -2.825899000 | -2.176124000 | -1.543657000 |
| 1 | -4.314745000 | -1.213410000 | -1.441207000 |
| 6 | -3.290364000 | -1.136971000 | 1.359522000 |
| 1 | -4.373961000 | -1.193544000 | 1.245380000 |
| 1 | -2.891647000 | -2.148049000 | 1.444921000 |
| 1 | -3.053882000 | -0.604655000 | 2.280045000 |
| 6 | -3.386864000 | 1.330051000 | -0.108436000 |
| 1 | -3.027994000 | 1.908077000 | -0.959212000 |
| 1 | -4.465293000 | 1.188726000 | -0.193179000 |
| 1 | -3.165652000 | 1.892701000 | 0.797323000 |
| 6 | 3.274739000 | -1.090891000 | 1.375907000 |
| 1 | 2.823444000 | -2.079454000 | 1.451833000 |
| 1 | 4.356350000 | -1.190355000 | 1.273030000 |
| 1 | 3.049922000 | -0.540392000 | 2.288710000 |
| 6 | 3.222566000 | -1.157519000 | -1.480909000 |
| 1 | 4.308715000 | -1.243666000 | -1.422869000 |
| 1 | 2.780260000 | -2.153071000 | -1.490397000 |
| 1 | 2.954698000 | -0.654527000 | -2.409852000 |
| 6 | 3.435542000 | 1.367295000 | -0.127567000 |
| 1 | 4.513737000 | 1.214674000 | -0.193438000 |
| 1 | 3.096528000 | 1.932765000 | -0.994851000 |
| 1 | 3.207938000 | 1.951221000 | 0.763210000 |

**M5** complex of $WH(NO)(CO)(PMe_3)_3$
E (ZPE- corrected) = -1769.706346
G = -1769.767617

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.002717000 | -0.349595000 | 0.049091000 |
| 15 | -2.519465000 | -0.480112000 | -0.232336000 |
| 15 | -0.008342000 | 2.258988000 | -0.019388000 |
| 15 | 2.527126000 | -0.469512000 | -0.234653000 |
| 7 | 0.004572000 | -0.227053000 | 1.868550000 |
| 8 | 0.004005000 | -0.116174000 | 3.065070000 |

| | | | |
|---|---|---|---|
| 6 | 0.003082000 | -2.341952000 | 0.214448000 |
| 8 | 0.002392000 | -3.489644000 | 0.380633000 |
| 6 | -3.558956000 | -0.222130000 | 1.258133000 |
| 1 | -4.615467000 | -0.389362000 | 1.043855000 |
| 1 | -3.236353000 | -0.909547000 | 2.039105000 |
| 1 | -3.425795000 | 0.791044000 | 1.633378000 |
| 6 | -3.117893000 | -2.117163000 | -0.820250000 |
| 1 | -2.637548000 | -2.352766000 | -1.769546000 |
| 1 | -2.843120000 | -2.888945000 | -0.103167000 |
| 1 | -4.200236000 | -2.121549000 | -0.958969000 |
| 6 | -3.298637000 | 0.612449000 | -1.492192000 |
| 1 | -2.731872000 | 0.512233000 | -2.417262000 |
| 1 | -4.341088000 | 0.343410000 | -1.668083000 |
| 1 | -3.255075000 | 1.653511000 | -1.176965000 |
| 6 | 1.414476000 | 3.119790000 | 0.776116000 |
| 1 | 1.514664000 | 2.761443000 | 1.800314000 |
| 1 | 2.338788000 | 2.902823000 | 0.245070000 |
| 1 | 1.265697000 | 4.200671000 | 0.790673000 |
| 6 | -0.088400000 | 3.066587000 | -1.666026000 |
| 1 | 0.743089000 | 2.717426000 | -2.275613000 |
| 1 | -1.003615000 | 2.762793000 | -2.171072000 |
| 1 | -0.057866000 | 4.154166000 | -1.587015000 |
| 6 | -1.374843000 | 3.080194000 | 0.905048000 |
| 1 | -2.335569000 | 2.857864000 | 0.445489000 |
| 1 | -1.386828000 | 2.696258000 | 1.925026000 |
| 1 | -1.243559000 | 4.162969000 | 0.932935000 |
| 6 | 3.280266000 | 0.561675000 | -1.560328000 |
| 1 | 3.226621000 | 1.618425000 | -1.304268000 |
| 1 | 4.324200000 | 0.295253000 | -1.731224000 |
| 1 | 2.705473000 | 0.404373000 | -2.472392000 |
| 6 | 3.146807000 | -2.128171000 | -0.732528000 |
| 1 | 4.228618000 | -2.125516000 | -0.875179000 |
| 1 | 2.884845000 | -2.862800000 | 0.027126000 |
| 1 | 2.666237000 | -2.422906000 | -1.665017000 |
| 6 | 3.570842000 | -0.114926000 | 1.233299000 |
| 1 | 3.429340000 | 0.917016000 | 1.548753000 |
| 1 | 3.257461000 | -0.758739000 | 2.054214000 |
| 1 | 4.628206000 | -0.284094000 | 1.024951000 |
| 8 | -0.004027000 | -0.249916000 | -2.057223000 |
| 1 | -0.001555000 | -1.068756000 | -2.554195000 |

**M1…2$H_2O$** complex of $Mo_{tris}$
E (ZPE- corrected) = -1493.529199
G = -1494.701003

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.541661000 | 0.047961000 | 0.018249000 |
| 15 | 1.103429000 | 1.611481000 | 1.046539000 |
| 15 | -1.831046000 | -1.440350000 | -1.467678000 |
| 7 | -1.666991000 | -0.054986000 | 1.448610000 |
| 8 | -2.403294000 | -0.139996000 | 2.362949000 |
| 6 | -1.482496000 | 1.629303000 | -0.790855000 |
| 8 | -2.013475000 | 2.533869000 | -1.259081000 |
| 1 | 2.428652000 | 1.210263000 | 1.316710000 |
| 1 | 0.798156000 | 2.168802000 | 2.305267000 |
| 1 | 1.407454000 | 2.814591000 | 0.378736000 |
| 1 | -1.362371000 | -2.730875000 | -1.812572000 |
| 1 | -3.139787000 | -1.827913000 | -1.108210000 |
| 1 | -2.122539000 | -1.018971000 | -2.780889000 |
| 1 | 0.573983000 | 0.067064000 | -1.455435000 |
| 8 | 3.040128000 | 0.593881000 | -2.007961000 |
| 1 | 2.088360000 | 0.421823000 | -1.843550000 |
| 1 | 3.202552000 | 0.311301000 | -2.911355000 |
| 15 | 0.932844000 | -1.906761000 | 0.691411000 |
| 1 | 0.717698000 | -2.549906000 | 1.929170000 |
| 1 | 2.328018000 | -1.735149000 | 0.794564000 |

| | | | |
|---|---|---|---|
| 1 | 0.945312000 | -3.072873000 | -0.106401000 |
| 8 | 4.277795000 | -0.395910000 | 0.308687000 |
| 1 | 3.972597000 | -0.059282000 | -0.554282000 |
| 1 | 5.187965000 | -0.104464000 | 0.395842000 |

**M2H$_2$OTS2** complex of Mo$_{tris}$
E (ZPE- corrected) = -1494.605838
G = -1494.655652

| At. No. | X | Y | Z |
|---|---|---|---|
| 42 | -0.385885000 | 0.034486000 | -0.042861000 |
| 15 | 1.344636000 | 1.531133000 | 1.027419000 |
| 15 | -2.075289000 | -1.453834000 | -1.156280000 |
| 7 | -1.398065000 | 0.012537000 | 1.416112000 |
| 8 | -2.092984000 | -0.034144000 | 2.370697000 |
| 6 | -1.327000000 | 1.674725000 | -0.726261000 |
| 8 | -1.860262000 | 2.623373000 | -1.087966000 |
| 1 | 2.679889000 | 1.129908000 | 1.188648000 |
| 1 | 1.096780000 | 1.893592000 | 2.378871000 |
| 1 | 1.540003000 | 2.830150000 | 0.534653000 |
| 1 | -1.878444000 | -2.847062000 | -1.308247000 |
| 1 | -3.339039000 | -1.521054000 | -0.535636000 |
| 1 | -2.518164000 | -1.209894000 | -2.473483000 |
| 1 | 0.252738000 | -0.652225000 | -2.039501000 |
| 8 | 1.891373000 | 0.898210000 | -1.365766000 |
| 1 | 0.874552000 | -0.111159000 | -1.931947000 |
| 1 | 1.908922000 | 1.671805000 | -1.938399000 |
| 15 | 1.085800000 | -1.947474000 | 0.664899000 |
| 1 | 1.264112000 | -2.181450000 | 2.042406000 |
| 1 | 2.433467000 | -1.908566000 | 0.251200000 |
| 1 | 0.768467000 | -3.272476000 | 0.293736000 |
| 8 | 4.001466000 | -0.582866000 | -0.657427000 |
| 1 | 3.316143000 | 0.026075000 | -1.033770000 |
| 1 | 4.712255000 | -0.616133000 | -1.300478000 |

**M1…2H$_2$O** complex of W$_{tris}$
E (ZPE- corrected) = -1493.529199
G = -1493.582779

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.442552000 | -0.041935000 | 0.002297000 |
| 15 | -1.146937000 | -1.816190000 | -0.738192000 |
| 15 | 1.696277000 | 1.731311000 | 1.188577000 |
| 7 | 1.573368000 | -0.163700000 | -1.443184000 |
| 8 | 2.298488000 | -0.218189000 | -2.374841000 |
| 1 | -1.442619000 | -2.869973000 | 0.150773000 |
| 1 | -0.784966000 | -2.602761000 | -1.850527000 |
| 1 | -2.472837000 | -1.516585000 | -1.116826000 |
| 1 | 1.970290000 | 1.570921000 | 2.562046000 |
| 1 | 3.005081000 | 2.050959000 | 0.770508000 |
| 1 | 1.209999000 | 3.058727000 | 1.271309000 |
| 1 | -0.702530000 | 0.178256000 | 1.451058000 |
| 8 | -3.192420000 | 0.146396000 | 2.134855000 |
| 1 | -2.235483000 | 0.163284000 | 1.924233000 |
| 1 | -3.292807000 | -0.518303000 | 2.821029000 |
| 6 | 1.445222000 | -1.433224000 | 1.065582000 |
| 8 | 2.009630000 | -2.229584000 | 1.676751000 |
| 15 | -1.078351000 | 1.710728000 | -1.035448000 |
| 1 | -0.856292000 | 2.114083000 | -2.368958000 |
| 1 | -2.464634000 | 1.464543000 | -1.116329000 |
| 1 | -1.145049000 | 3.002621000 | -0.466729000 |
| 8 | -4.357862000 | 0.046452000 | -0.414139000 |
| 1 | -4.078805000 | 0.061327000 | 0.520537000 |
| 1 | -5.270651000 | 0.343012000 | -0.418334000 |

**M2H$_2$OTS3** complex of W$_{tris}$

E (ZPE- corrected) = -1493.475867
G = -1493.52746

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.268267000 | 0.034192000 | 0.028877000 |
| 15 | -1.303844000 | 1.810197000 | 0.775471000 |
| 15 | 1.914125000 | -1.590234000 | -0.827103000 |
| 7 | 1.216294000 | 0.204599000 | 1.533347000 |
| 8 | 1.879373000 | 0.358409000 | 2.512633000 |
| 1 | -2.062215000 | 2.539573000 | -0.161612000 |
| 1 | -0.701921000 | 2.899502000 | 1.437319000 |
| 1 | -2.344913000 | 1.570698000 | 1.699811000 |
| 1 | 1.929246000 | -1.944700000 | -2.196427000 |
| 1 | 3.276062000 | -1.235713000 | -0.722211000 |
| 1 | 2.046489000 | -2.909500000 | -0.326159000 |
| 1 | 0.311207000 | 1.117470000 | -2.119840000 |
| 8 | -1.458355000 | -0.519518000 | -2.110428000 |
| 1 | -0.963490000 | 0.185300000 | -2.578327000 |
| 1 | -1.311166000 | -1.329538000 | -2.612022000 |
| 6 | 1.126222000 | 1.429517000 | -1.214362000 |
| 8 | 1.897487000 | 2.291066000 | -1.523556000 |
| 15 | -1.284863000 | -1.779559000 | 0.970681000 |
| 1 | -2.224882000 | -1.456173000 | 1.975396000 |
| 1 | -2.166320000 | -2.561273000 | 0.190770000 |
| 1 | -0.681942000 | -2.858138000 | 1.657270000 |
| 8 | -3.844388000 | -0.027766000 | -0.550784000 |
| 1 | -3.218810000 | -0.168647000 | -1.274898000 |
| 1 | -4.684681000 | 0.188018000 | -0.961878000 |

**M2…$H_2O$** complex of $W_{tris}$
E (ZPE- corrected) =
G =

| At. No. | X | Y | Z |
|---|---|---|---|
| 74 | 0.201009000 | -0.014886000 | 0.025890000 |
| 15 | -1.334698000 | 1.725882000 | 0.901475000 |
| 15 | 1.896302000 | -1.493686000 | -0.966571000 |
| 7 | 1.204912000 | 0.115811000 | 1.509220000 |
| 8 | 1.884050000 | 0.222263000 | 2.480467000 |
| 1 | -2.133064000 | 2.489022000 | 0.021545000 |
| 1 | -0.703420000 | 2.795872000 | 1.567523000 |
| 1 | -2.342682000 | 1.474872000 | 1.862521000 |
| 1 | 1.856813000 | -1.799283000 | -2.350777000 |
| 1 | 3.235391000 | -1.047814000 | -0.925957000 |
| 1 | 2.147966000 | -2.819437000 | -0.531937000 |
| 1 | 0.544246000 | 1.647981000 | -2.210647000 |
| 8 | -1.068280000 | -0.049355000 | -1.979082000 |
| 1 | -0.597085000 | 0.677789000 | -2.464162000 |
| 1 | -0.977488000 | -0.848085000 | -2.510706000 |
| 6 | 1.105324000 | 1.560000000 | -1.138758000 |
| 8 | 2.000195000 | 2.359658000 | -1.023322000 |
| 15 | -1.266323000 | -1.877148000 | 0.865987000 |
| 1 | -2.161209000 | -1.681196000 | 1.945210000 |
| 1 | -2.204887000 | -2.497736000 | 0.010076000 |
| 1 | -0.688375000 | -3.069653000 | 1.361680000 |
| 8 | -3.793015000 | -0.059650000 | -0.828080000 |
| 1 | -3.014760000 | 0.094126000 | -1.377784000 |
| 1 | -4.515228000 | 0.405357000 | -1.257630000 |

**Methanol**
E (ZPE- corrected) = -115.727521
G = -115.750308

| At. No. | X | Y | Z |
|---|---|---|---|
| 8 | -0.748149000 | 0.121890000 | 0.000021000 |
| 1 | -1.147679000 | -0.751010000 | 0.000141000 |

| | | | |
|---|---|---|---|
| 6 | 0.665401000 | -0.020246000 | 0.000015000 |
| 1 | 1.083381000 | 0.984704000 | -0.006901000 |
| 1 | 1.029115000 | -0.537820000 | 0.893651000 |
| 1 | 1.027969000 | -0.549518000 | -0.887150000 |

**$P(CH_3)_3$**
E (ZPE- corrected) = -461.07206
G = -461.10133

| At. No. | X | Y | Z |
|---|---|---|---|
| 15 | 0.002402000 | -0.000676000 | -0.596183000 |
| 6 | 1.625096000 | -0.189039000 | 0.277682000 |
| 1 | 1.520497000 | -0.145097000 | 1.364319000 |
| 1 | 2.074503000 | -1.144536000 | 0.005226000 |
| 1 | 2.305713000 | 0.599779000 | -0.043412000 |
| 6 | -0.649036000 | 1.498612000 | 0.275788000 |
| 1 | -0.600964000 | 1.404227000 | 1.363337000 |
| 1 | -0.075025000 | 2.374649000 | -0.026968000 |
| 1 | -1.685975000 | 1.664480000 | -0.018134000 |
| 6 | -0.978153000 | -1.308798000 | 0.276291000 |
| 1 | -0.651696000 | -2.294145000 | -0.056611000 |
| 1 | -0.879324000 | -1.251064000 | 1.362862000 |
| 1 | -2.031205000 | -1.202805000 | 0.013559000 |

**$PH_3$**
E (ZPE- corrected) = -343.15357
G = -343.17460

| At. No. | X | Y | Z |
|---|---|---|---|
| 15 | -0.000020000 | 0.000005000 | -0.128223000 |
| 1 | 0.644265000 | -1.001918000 | 0.641023000 |
| 1 | -1.189718000 | -0.056898000 | 0.641241000 |
| 1 | 0.545746000 | 1.058748000 | 0.641084000 |

**$H_2O$**
E (ZPE- corrected) =-76.44536
G = -76.46300

| At. No. | X | Y | Z |
|---|---|---|---|
| 8 | 0.000000000 | 0.000000000 | 0.117110000 |
| 1 | 0.000000000 | 0.761700000 | -0.468439000 |
| 1 | 0.000000000 | -0.761700000 | -0.468439000 |

**$H_2$**
E (ZPE- corrected) = -1.16993
G = -1.18142

| At. No. | X | Y | Z |
|---|---|---|---|
| 1 | 0.000000000 | 0.000000000 | 0.371369000 |
| 1 | 0.000000000 | 0.000000000 | -0.371369000 |