Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Adaptive Aromaticity in 16-valence-electron Metallazapentalenes

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1. 3D structures of hetero-metallapentalenes.

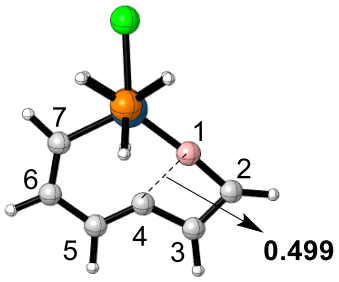


Fig. S1. Optimized structures of osmaborapentalene. Weak interaction between C4 and boron atom (WBI of B-C4 is 0.499).

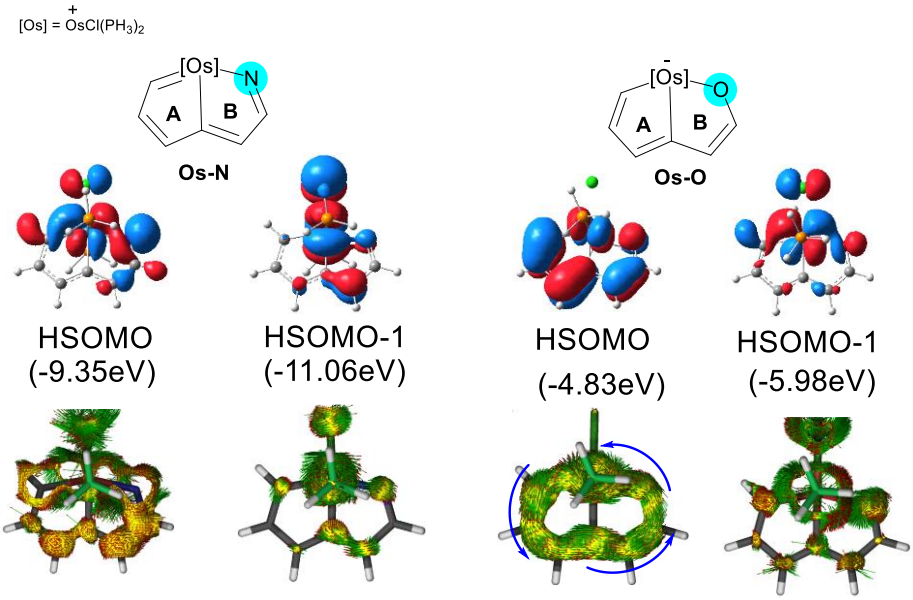


Fig. S2. Biorthogonalized SOMOs and the ACID plots of SOMOs of **Os-N** and **Os-O** in the T_1 state. Isovalues for MO and ACID plots are 0.030 and 0.010 a.u., respectively. (For high-resolution ACID plots, see Fig. S17-S20)

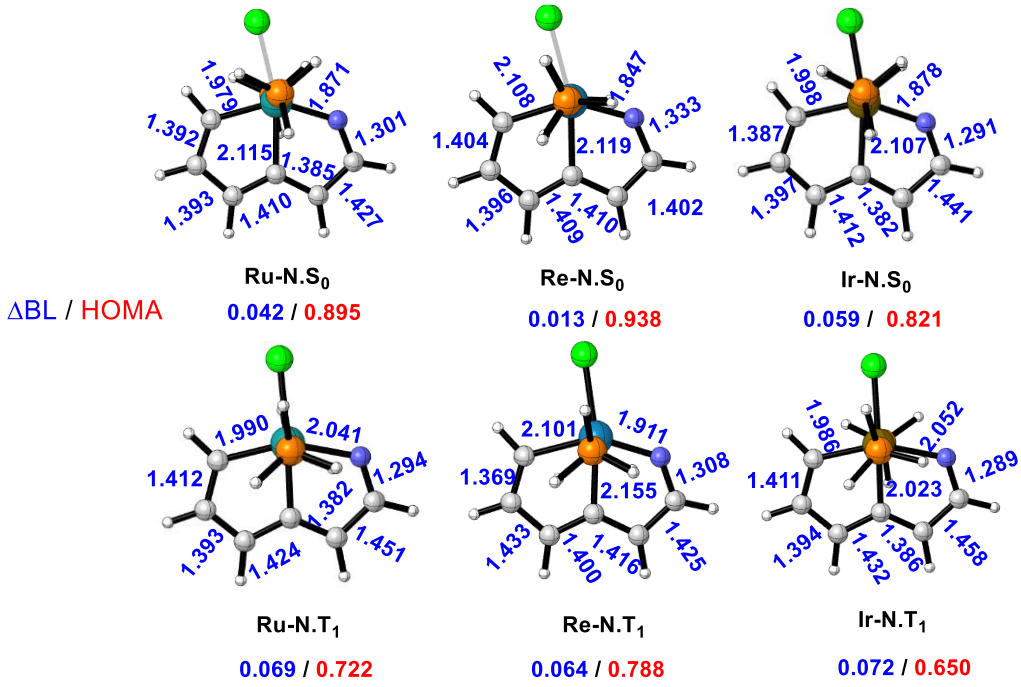


Fig. S3. Selected bond lengths (Å, blue) and HOMA values (red) in metallazapentalenes, the NICS(1)$_{zz}$ values of rings A and B are separated by the slash "/".

2. Functional comparison

1) BLAs

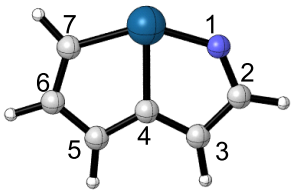


Table S1. BLAs of osmazapentalenes in the S_0 state with B3LYP, ωB97X, B3PW91, PBE0, and TPSS functionals. Bond length given in Å.

Bonds of **Os-N.S_0**	B3LYP	ωB97X	B3PW91	PBE0	TPSS
Os-N	1.850	1.834	1.839	1.833	1.854
N-C2	1.312	1.303	1.31	1.308	1.324
C2-C3	1.418	1.421	1.414	1.413	1.418
C3-C4	1.395	1.383	1.394	1.392	1.406
C4-C5	1.409	1.413	1.408	1.407	1.414
C5-C6	1.393	1.384	1.391	1.389	1.399
C6-C7	1.398	1.397	1.396	1.395	1.404
Os-C7	1.991	1.971	1.980	1.975	1.997
Os-C4	2.108	2.081	2.089	2.081	2.101
BLAs	0.025	0.038	0.023	0.024	0.019
RD %[a]	0	0.7%	0.3%	0.5%	0.4%

[a] Relative deviation (RD) = Average $\Sigma[(|BL_{B3LYP} - BL_{other\ functionals}|)/BL_{other\ functionals}]$

Table S2. BLAs of osmazapentalenes in the T_1 state with B3LYP, ωB97X, B3PW91, PBE0, and TPSS functionals. Bond length given in Å.

Bonds of **Os-N.T_1**	B3LYP	ωB97X	B3PW91	PBE0	TPSS
Os-N	1.997	1.992	1.978	1.973	1.979
N-C2	1.304	1.294	1.304	1.302	1.317
C2-C3	1.444	1.451	1.438	1.437	1.438
C3-C4	1.39	1.377	1.39	1.388	1.406
C4-C5	1.424	1.43	1.422	1.421	1.426
C5-C6	1.394	1.383	1.392	1.39	1.404
C6-C7	1.418	1.418	1.416	1.415	1.416
Os-C7	2.005	1.988	1.994	1.988	2.016
Os-C4	2.061	2.048	2.049	2.046	2.061
BLAs	0.054	0.074	0.048	0.049	0.034
RD %[a]	0	0.6%	0.3%	0.5%	0.5%

[a] Relative deviation (RD) = Average $\Sigma[(|BL_{B3LYP} - BL_{other\ functionals}|)/BL_{other\ functionals}]$

Table S3. BLAs of ruthenazapentalenes in the S_0 state with B3LYP, ωB97X, B3PW91, PBE0, and TPSS functionals. Bond length given in Å.

Bonds of **Ru-N.S_0**	B3LYP	ωB97X	B3PW91	PBE0	TPSS
Ru-N	1.871	1.857	1.856	1.85	1.872
N-C2	1.301	1.291	1.299	1.297	1.313
C2-C3	1.427	1.433	1.422	1.422	1.425
C3-C4	1.385	1.372	1.385	1.383	1.398
C4-C5	1.41	1.416	1.408	1.407	1.413
C5-C6	1.393	1.383	1.39	1.389	1.4
C6-C7	1.392	1.392	1.391	1.39	1.397
Ru-C7	1.979	1.957	1.966	1.961	1.988
Ru-C4	2.115	2.083	2.093	2.084	2.108
BLAs	0.042	0.061	0.037	0.039	0.028
RD %[a]	0	0.7%	0.4%	0.5%	0.4%

[a] Relative deviation (RD) = Average $\Sigma[(|BL_{B3LYP} - BL_{other\ functionals}|)/BL_{other\ functionals}]$

Table S4. BLAs of ruthenazapentalenes in the T_1 state with B3LYP, ωB97X, B3PW91, PBE0, and TPSS functionals. Bond length given in Å.

Bonds of **Ru-N.T_1**	B3LYP	ωB97X	B3PW91	PBE0	TPSS
Ru-N	2.041	2.051	2.014	2.01	2.017
N-C2	1.294	1.284	1.294	1.292	1.309
C2-C3	1.451	1.459	1.444	1.444	1.445
C3-C4	1.382	1.369	1.382	1.38	1.396
C4-C5	1.424	1.433	1.421	1.421	1.425
C5-C6	1.393	1.381	1.391	1.389	1.401
C6-C7	1.412	1.415	1.411	1.41	1.417
Ru-C7	1.99	1.963	1.977	1.97	1.999
Ru-C4	2.066	2.049	2.053	2.049	2.065
BLAs	0.069	0.09	0.062	0.064	0.049
RD %[a]	0	0.7%	0.4%	0.5%	0.6%

[a] Relative deviation (RD) = Average $\Sigma[(|BL_{B3LYP} - BL_{other\ functional}|)/BL_{other\ functional}]$

2) NICS(1)$_{zz}$ comparison

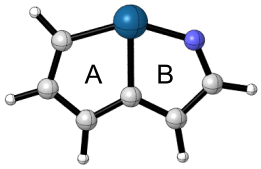


Table S5. NICS(1)$_{zz}$ values (in ppm) for rings A and B in metallazapentalenes with B3LYP, ωB97X, B3PW91, PBE0, and TPSS functionals.

Functional	B3LYP	ωB97X	B3PW91	PBE0	TPSS
Os-N.S_0	-23.3/-25.1	-23.5/-25.8	-23.8/-25.3	-24.3/-25.9	-22.9/-24.3
Os-N.T_1	-22.1/-21.5	-20.8/-20.6	-23.0/-22.9	-23.6/-23.8	-20.0/-19.1
Ru-N.S_0	-19.6/-20.2	-18.8/-19.1	-20.0/-20.7	-20.3/-20.9	-19.4/-20.3
Ru-N.T_1	-19.0/-17.9	-16.6/-15.5	-20.2/-19.6	-20.7/-20.2	-20.5/-20.3

3. ΔE_{ST}[a] values (kcal mol^{-1}) of metallazapentalenes.

Table S6. ΔE_{ST} values (kcal mol^{-1}) of metallazapentalenes.

ΔE_{ST} (kcal/mol)						
Os-N	**Ru-N**	**Re-N**	**Ir-N**	**Os-N.$SnCl_3$**	**Os-N.BMe_2**	**Os-N.H**
35.9	29.9	31.4	26.9	28.3	27.4	30.9
Os-N.PMe_3	**Os-N.H_2O**	**Os-N.NH_3**	**Os-N.NH_2**	**Os-N.I**	**Os-N.OH**	**Os-N.Br**
35.0	36.3	38.4	30.9	30.8	36.0	34.2
Os-N.F	**Os-N.CO**	**Os-N.PF_3**	**Os-N.iso1**	**Os-N.iso2**	**Os-O**	
39.6	35.0	36.5	29.4	27.6	1.1	

[a] $\Delta E_{ST} = E_{T1} - E_{S0}$

4. Signed modulus density plots of GIMIC for metazallapentalenes.

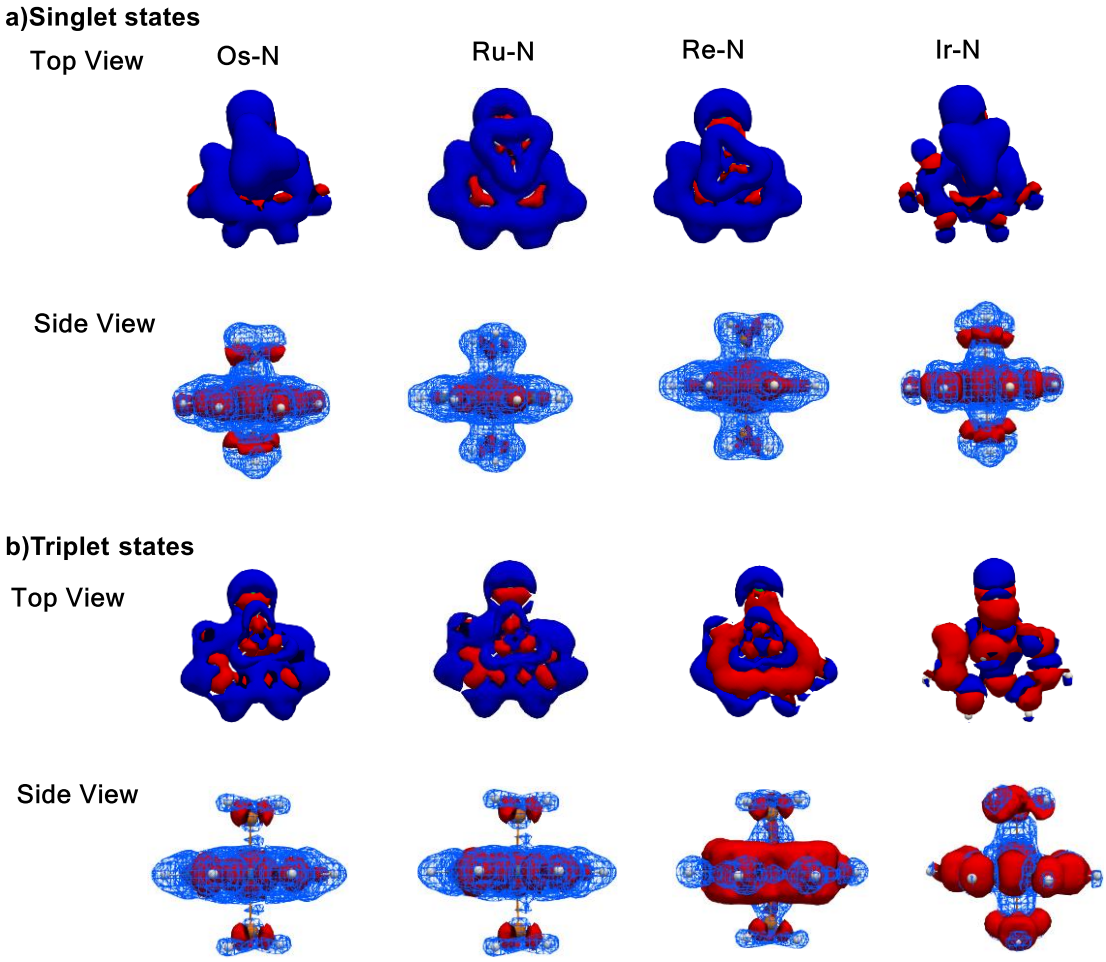


Fig. S4. Signed modulus density plots of GIMIC (isovalue: 0.015) for metazallapentalenes. Blue-solid and blue-wireframe density surfaces representing the same diatropic contributions are presented in top and side views, respectively. Red density surfaces correspond to paratropic contributions.

5 EDDB analysis of metallazapentalenes.

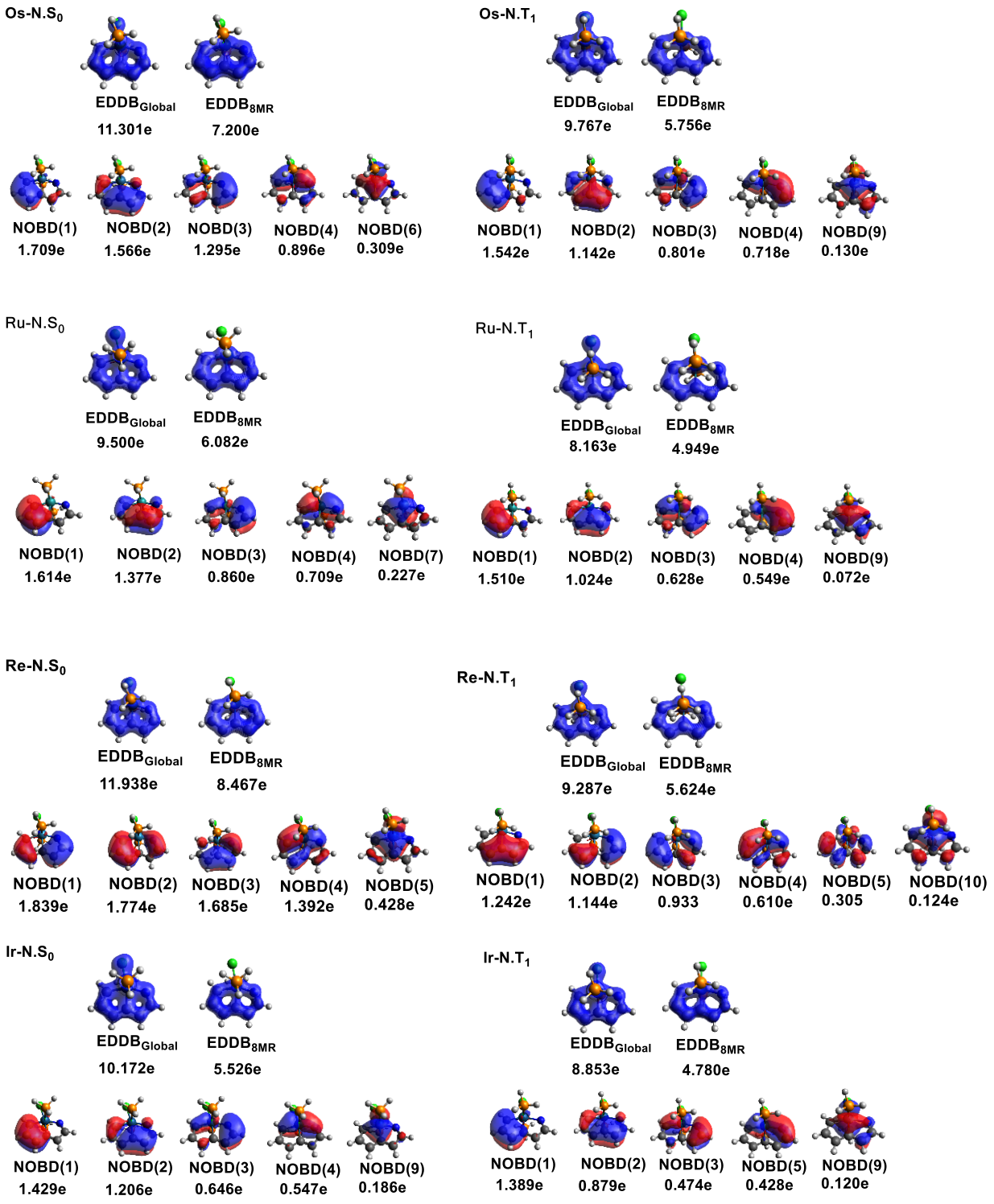


Fig. S5. π-EDDB analysis of metallazapentalenes . (Isovalue: 0.01 a.u.)

6. Spin density of osmazapentalenes with different ligands.

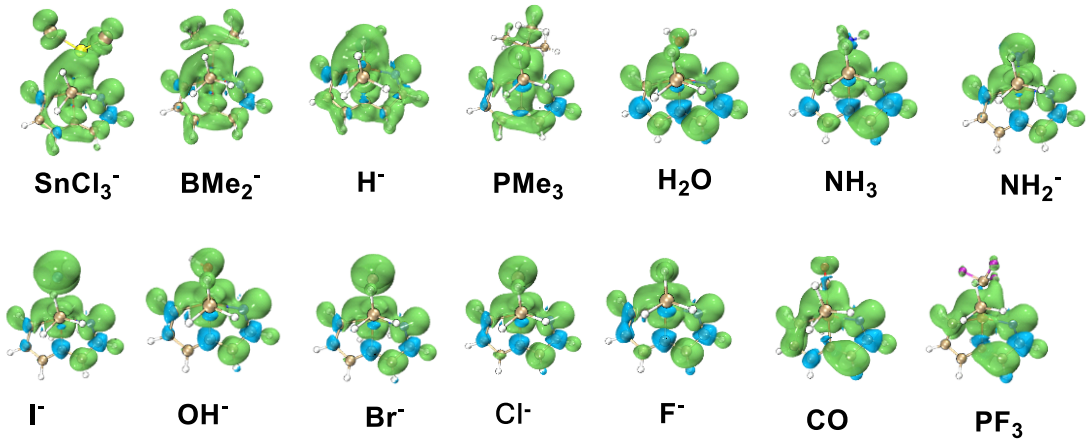


Fig. S6. Spin density analysis (isovalue 0.001 a.u.) for osmazapentalenes with different ligands.

7. The aromaticity of osmazapentalenes with the nitrogen atom at the meta and para positions.

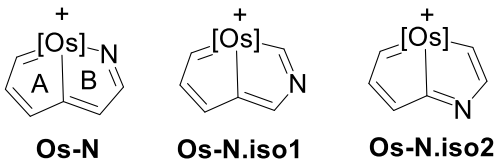
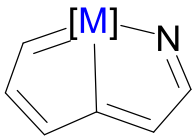


Table S7. NICS(1)$_{zz}$ values (ppm) for rings A / B and relative electronic energy values (ΔE , kcal/mol) in metallazapentalenes for the S_0 and T_1 states. [Os] = $OsCl(PH_3)_2$

Compounds		**Os-N**	**Os-N.iso1**	**Os-N.iso2**
NICS(1)$_{zz}$	S_0	-23.3/-25.1	-21.0/-23.1	-20.7/-27.7
	T_1	-22.1/-21.5	-16.5/-20.3	-22.1/-23.9
ΔE	S_0	0	15.4	20.3
	T_1	35.9	44.8	47.9

8. Aromaticity comparison of simplified and experimental models of metallazapentalenes on the different level theory.



M = Os^{+}, Ru^{+}, Re, Ir^{2+}

Table S8. The NICS(1)$_{zz}$ values (ppm) for rings A and B in metallazapentalenes. Level of theory: (U)B3LYP/def2-TZVP.

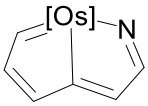
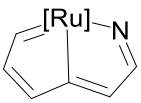
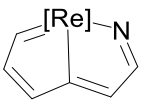
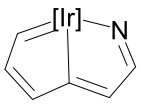
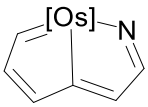
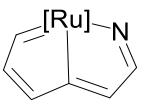
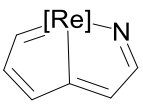
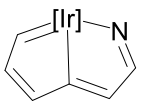
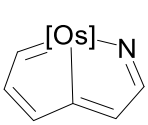
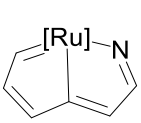
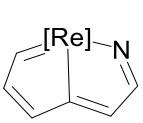
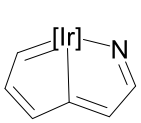
S_0				
[M] = $MCl(PH_3)_2$	-23.3/-25.1	-19.6/-20.2	-24.3/-25.5	-17.8/-17.2
[M] = $MCl(PMe_3)_2$	-22.3/-27.2	-19.6/-23.0	-20.9/-26.1	-17.2/-19.9
[M] = $MCl(PPh_3)_2$	-25.3/-27.6	-22.6/-24.1	-23.1/-26.1	-19.7/-20.5
T_1				
[M] = $MCl(PH_3)_2$	-22.1/-21.5	-19.0/-17.9	-1.0/5.4	-11.6/-12.2
[M] = $MCl(PMe_3)_2$	-22.6/-22.0	-18.7/-18.2	-4.9/2.1	-13.8/-16.2
[M] = $MCl(PPh_3)_2$	-27.4/-22.0	-23.8/-17.9	-18.4/-10.8	-18.4/-23.0

Table S9. The NICS(1)*zz* values (ppm) for rings A and B in metallazapentalenes. Level of theory: (U)B3LYP/6-31+G(d)~LanL2DZ.

S_0				
[M] = $MCl(PH_3)_2$	-23.1/-24.7	-18.7/-19.1	-23.7/-25.4	-16.9/-16.4
[M] = $MCl(PMe_3)_2$	-21.8/-27.0	-18.5/-22.0	-20.6/-26.3	-16.2/-19.1
[M] = $MCl(PPh_3)_2$	-25.0/-27.5	-21.8/-23.3	-22.9/-26.5	-18.9/-19.8

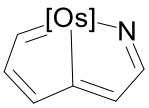
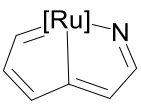
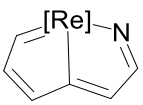
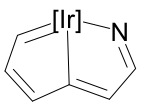
T_1				
[M] = $MCl(PH_3)_2$	-20.9/-20.5	-17.8/-17.0	-1.0/5.1	-10.6/-11.2
[M] = $MCl(PMe_3)_2$	-21.3/-20.9	-17.0/-16.9	-4.5/2.4	-12.7/-15.6
[M] = $MCl(PPh_3)_2$	-26.5/-20.9	-22.3/-16.7	-21.4/-14.9	-18.0/-22.6

Table S10. The NICS(1)*zz* values (ppm) for rings A and B in hetero-metallapentalenes. [M] = $MCl(PH_3)_2$. Level of theory: (U)B3LYP/6-31+G(d)~LanL2DZ.

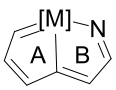
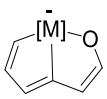
$NICS(1)_{zz}$				
	S_0	T_1	S_0	T_1
Ru^+	-18.7/-19.1	-17.8/-17.0	-1.1/-12.2	0.1/-4.5
Os^+	-23.1/-24.7	-20.9/-20.5	-1.8/-14.4	1.9/-5.2
Re	-23.7/-25.4	-1.0/5.1	-5.2/-11.1	7.0/-4.0
Ir^{2+}	-16.9/-16.4	-10.6/-11.2	-0.1/-11.3	0.4/-2.7

Table S11 EDDB analysis for metallazapentalenes (unit: e). Level of theory: (U)B3LYP/6-31+G(d)~LanL2DZ.

Species	$EDDB_{Global}$	$EDDB_{8MR}$	π-$EDDB_{8MR}$	π-$EDDB_{8MR}(\alpha)$	π-$EDDB_{8MR}(\beta)$
Os-N.S_0	10.182	7.023	5.743	/	/
Os-N.T_1	8.510	5.553	4.337	2.150	2.187
Ru-N.S_0	9.513	6.053	4.684	/	/
Ru-N.T_1	8.155	4.983	3.373	1.760	1.977
Re-N.S_0	11.401	8.421	7.114	/	/
Re-N.T_1	8.557	5.526	4.304	1.850	2.454
Ir-N.S_0	9.012	5.276	3.932	/	/
Ir-N.T_1	7.975	4.427	3.104	1.555	1.585

9. ACID plots of hetero-metallapentalenes

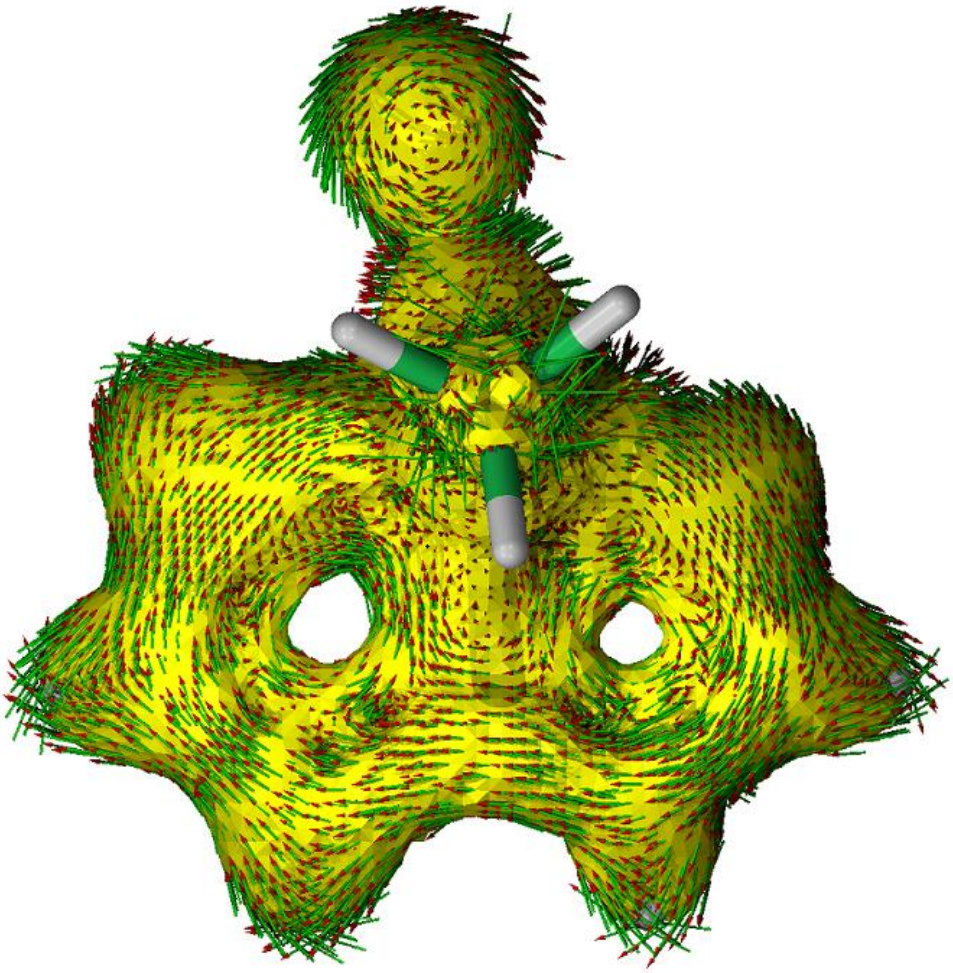


Fig. S7. ACID plot of **Os-N.S$_0$**. Isovalue for ACID is 0.030 a.u.

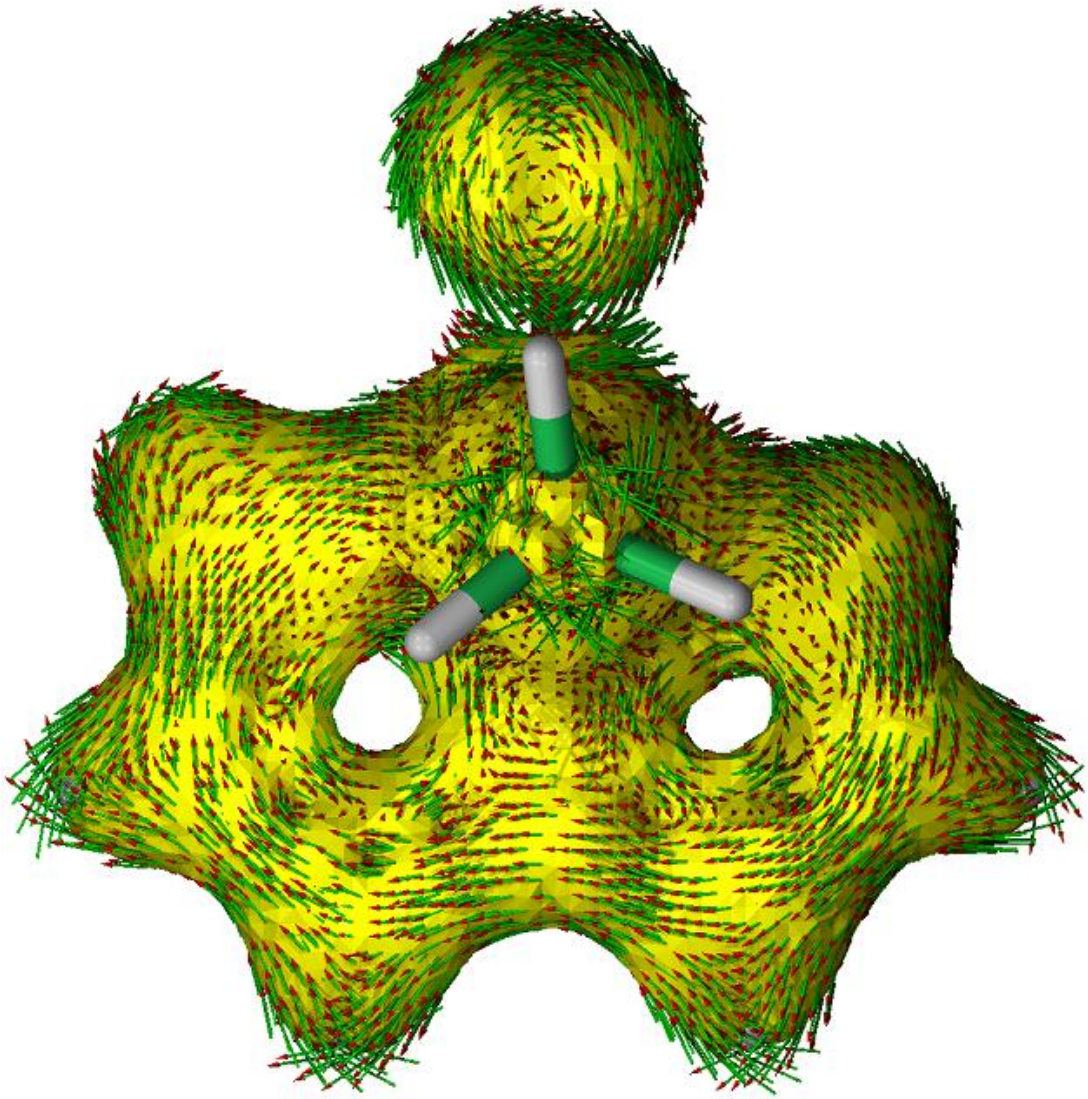


Fig. S8. ACID plot of **Os-N.T$_1$**. Isovalue for ACID is 0.030 a.u.

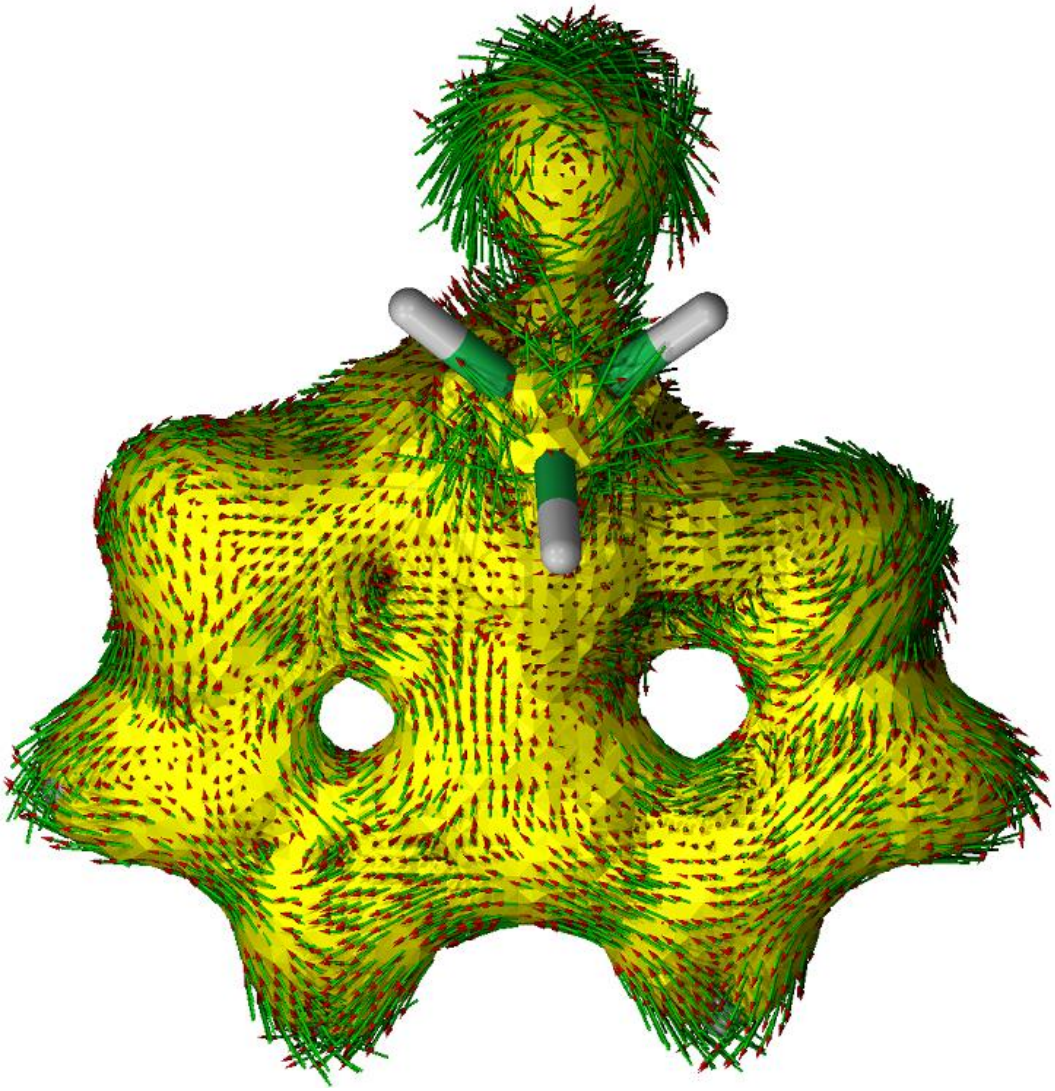


Fig. S9. ACID plot of **Os-O.S$_0$**. Isovalue for ACID is 0.030 a.u.

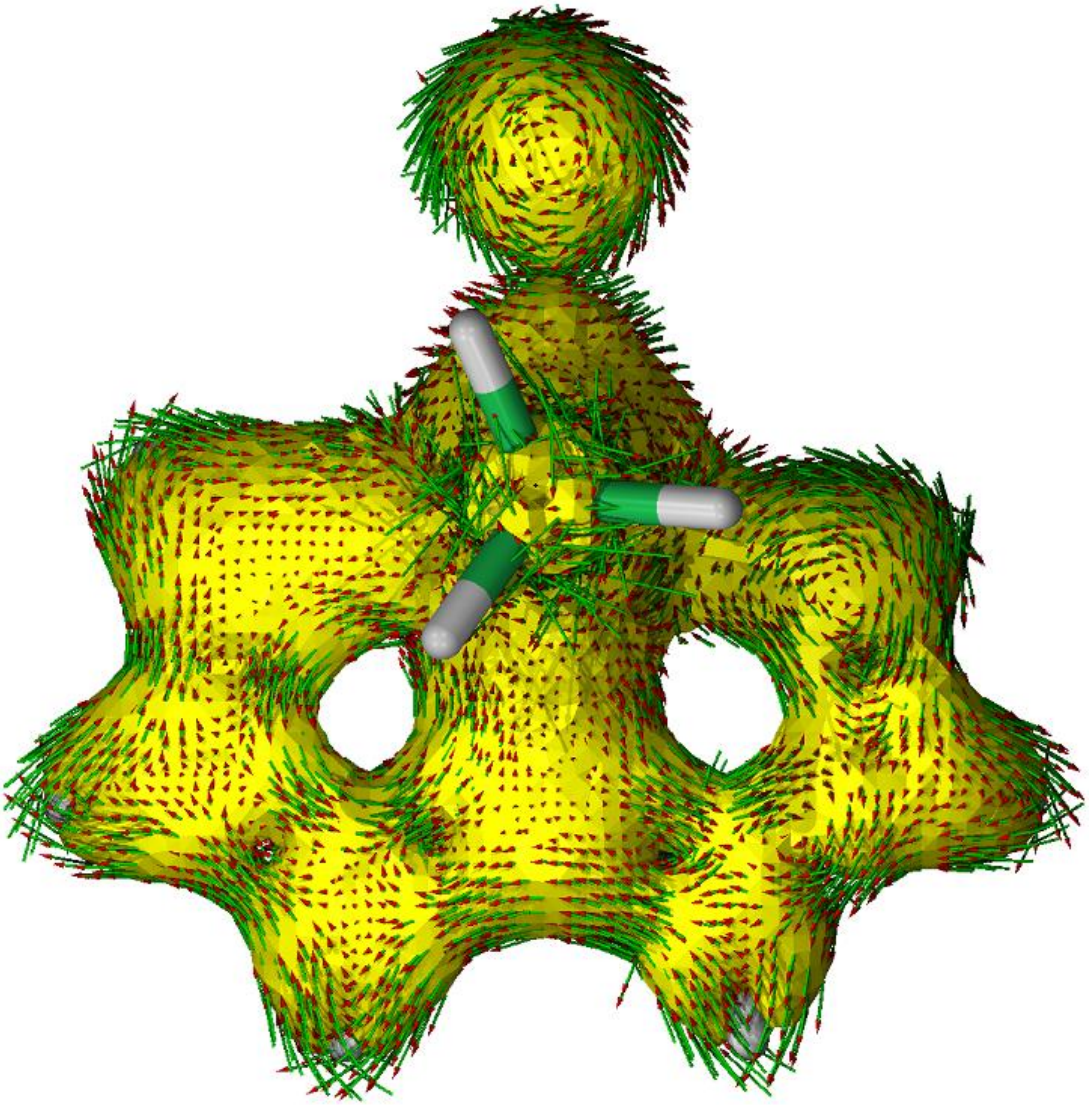


Fig. S10. ACID plot of **Os-O.T$_1$**. Isovalue for ACID is 0.030 a.u.

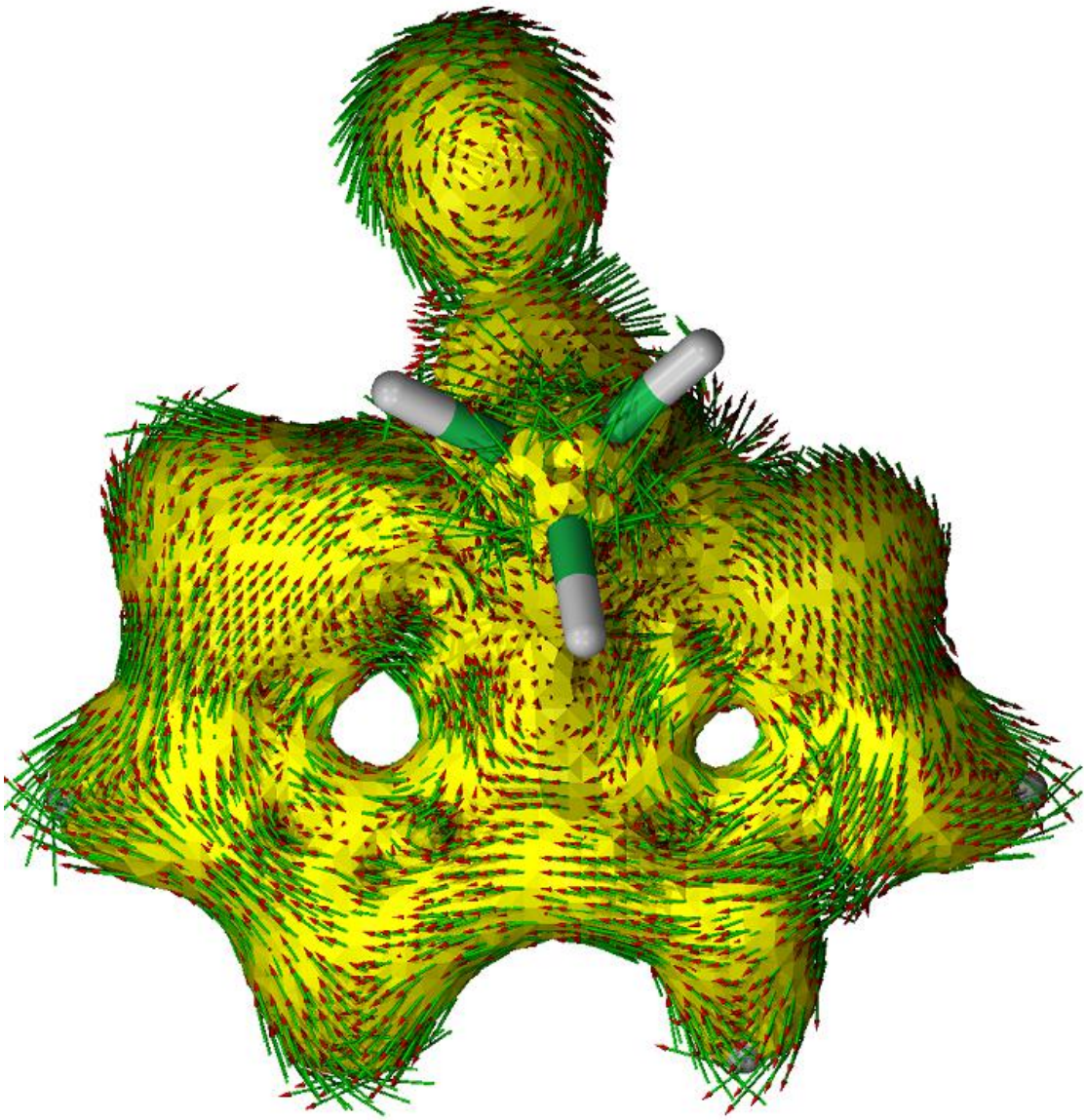


Fig. S11. ACID plot of **Ru-N.S$_0$**. Isovalue for ACID is 0.030 a.u.

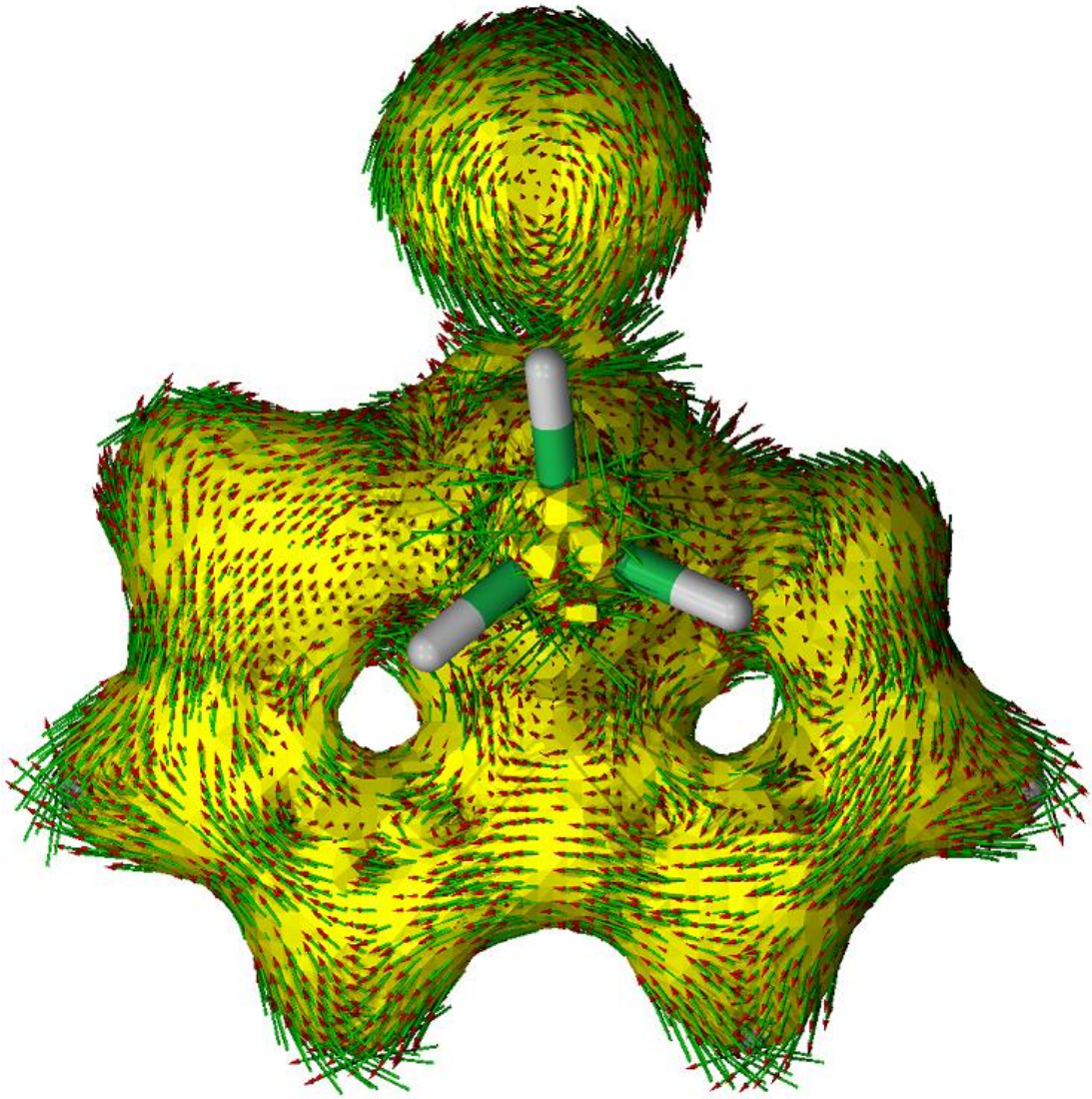


Fig. S12. ACID plot of **Ru-N.T$_1$**. Isovalue for ACID is 0.030 a.u.

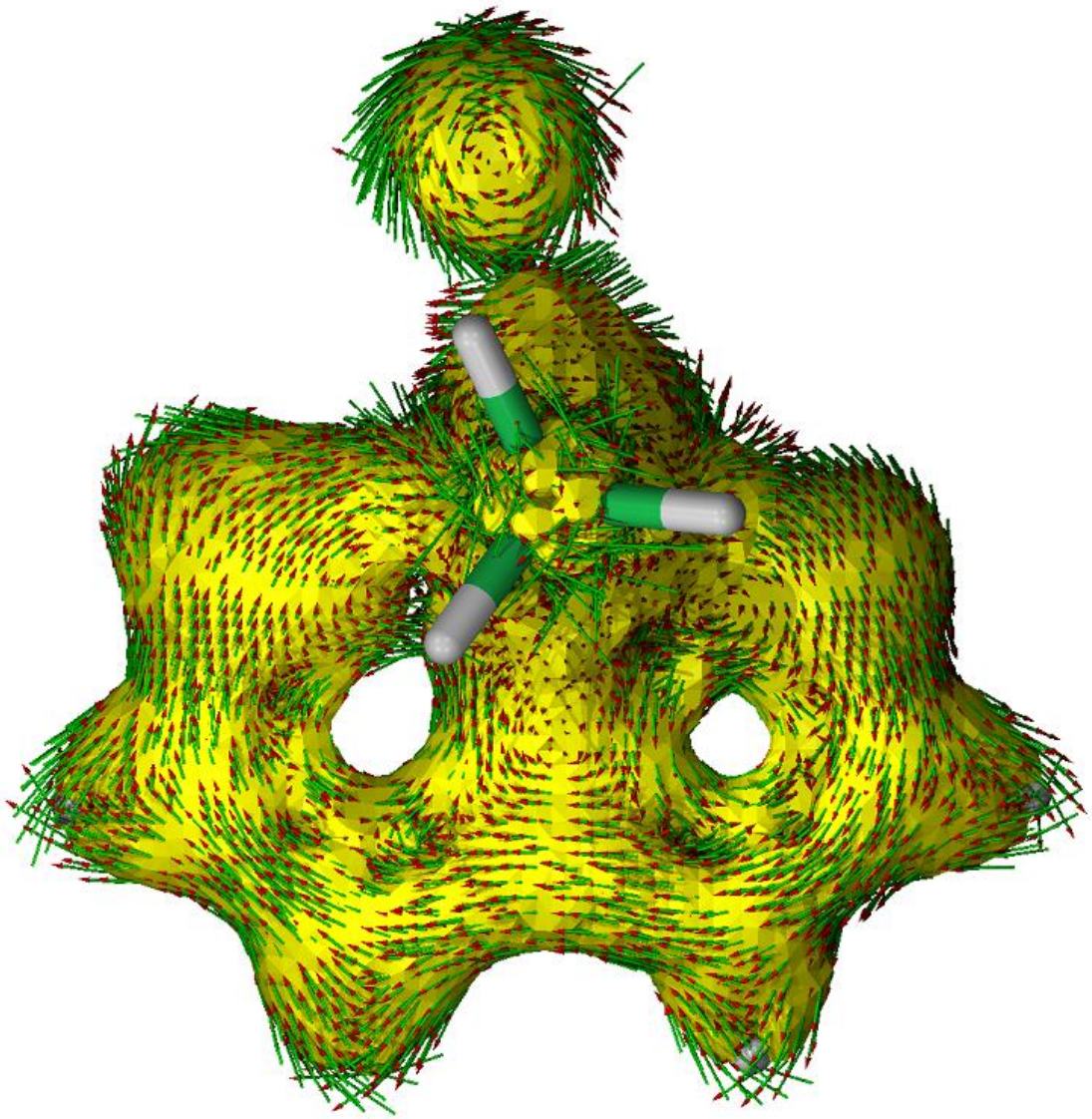


Fig. S13. ACID plot of **Re-N.S$_0$**. Isovalue for ACID is 0.030 a.u.

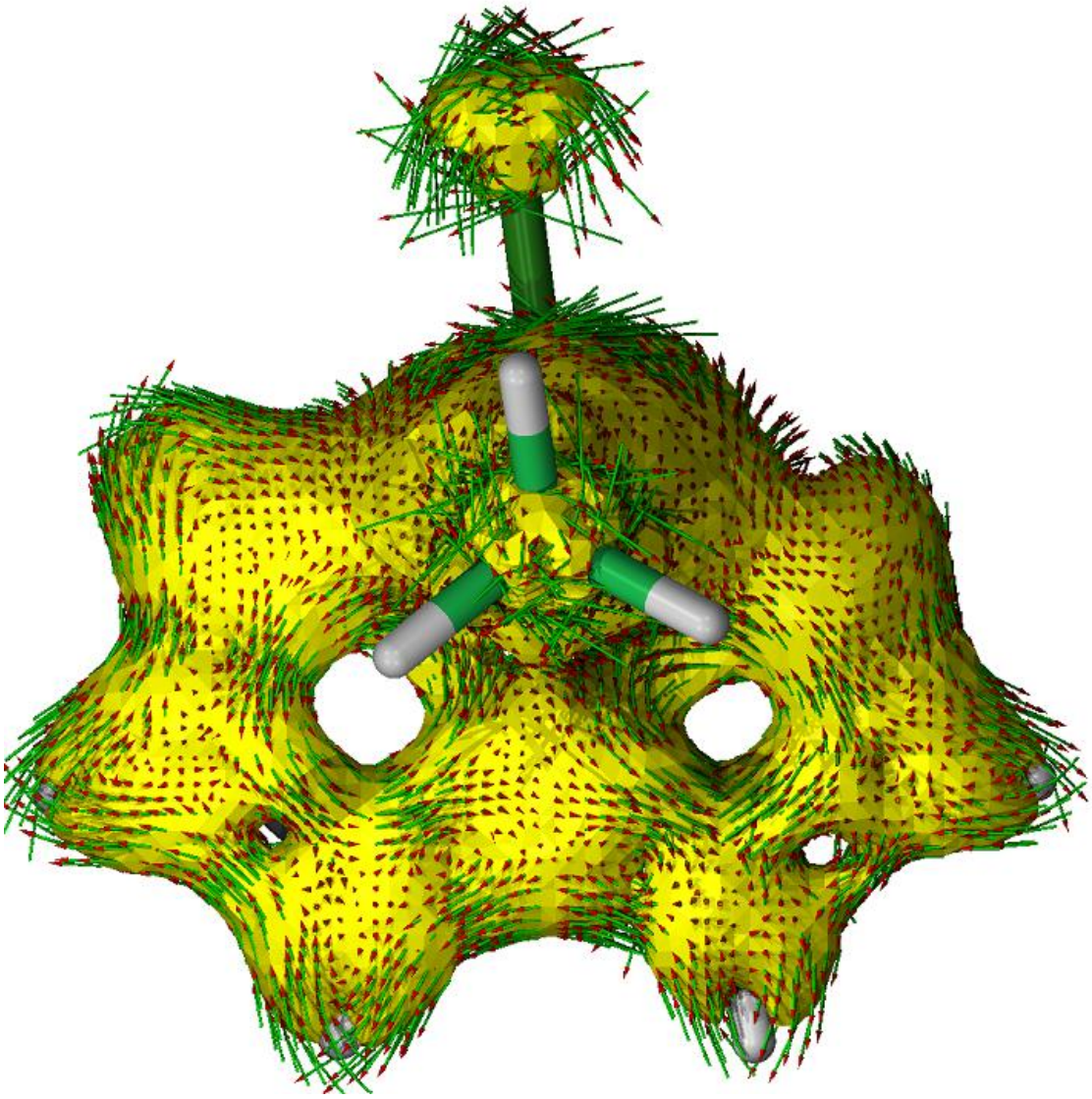


Fig. S14. ACID plot of **Re-N.T$_1$**. Isovalue for ACID is 0.030 a.u.

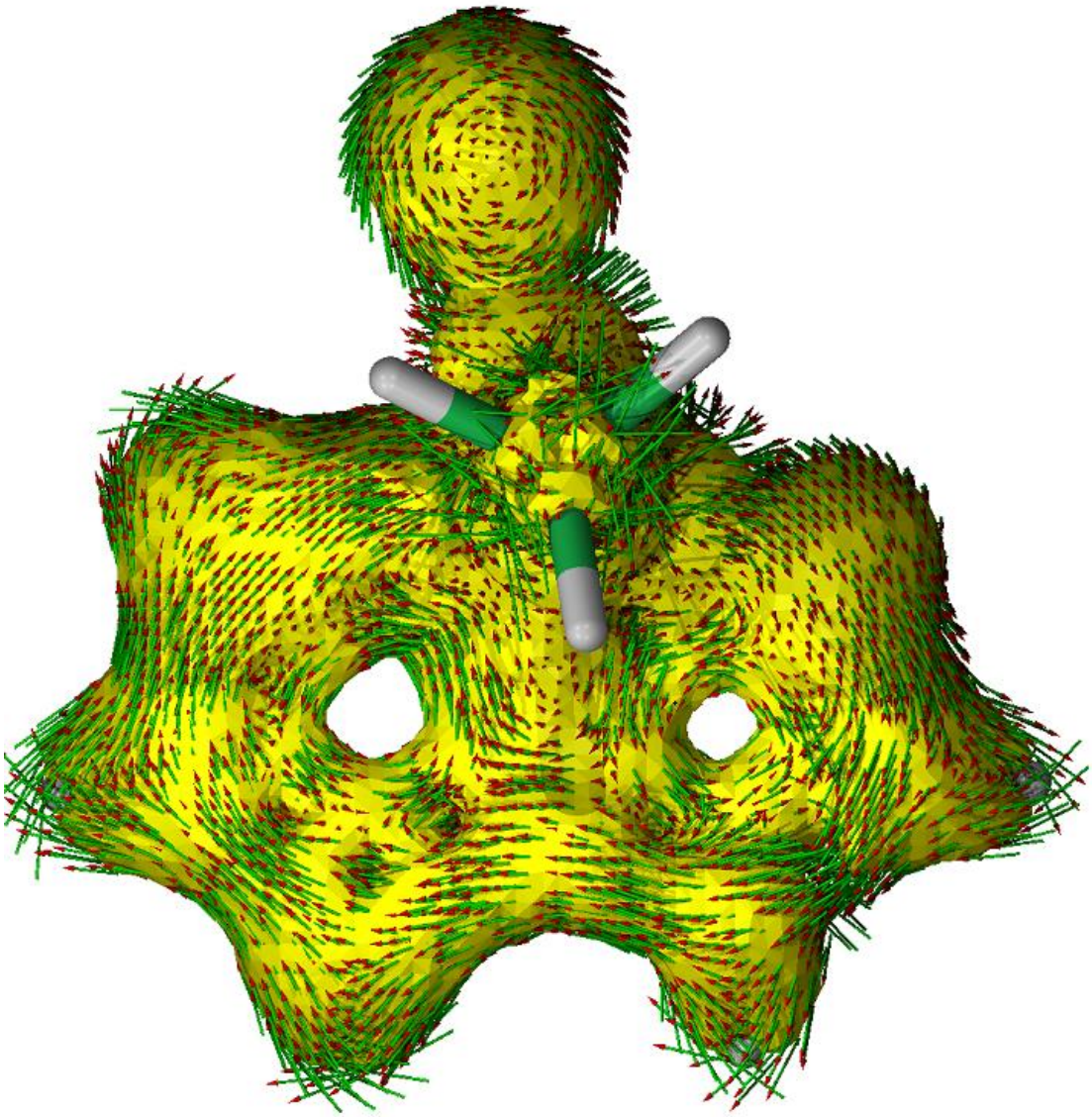


Fig. S15. ACID plot of **Ir-N.S$_0$**. Isovalue for ACID is 0.030 a.u.

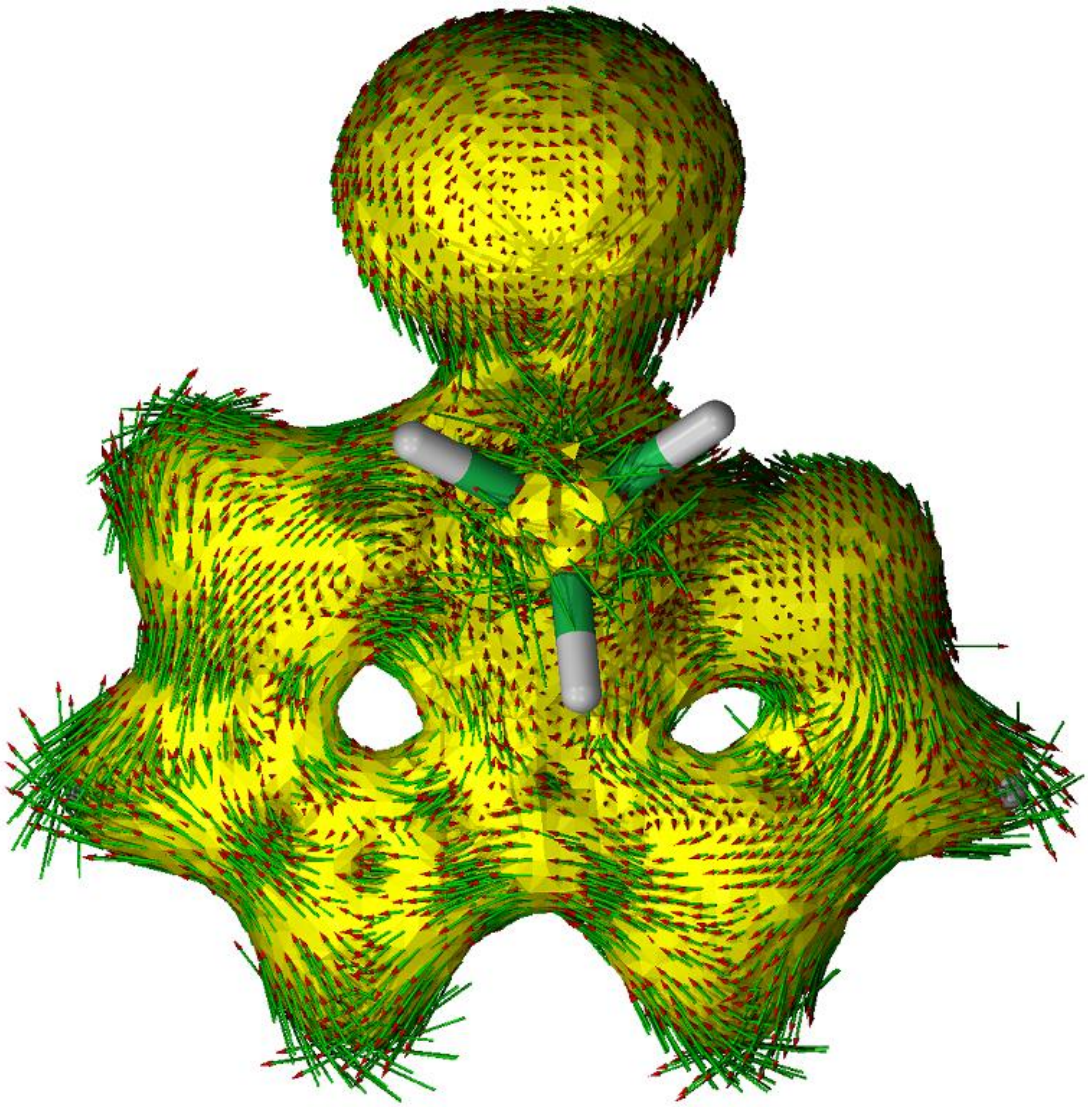


Fig. S16. ACID plot of **Ir-N.T$_1$**. Isovalue for ACID is 0.030 a.u.

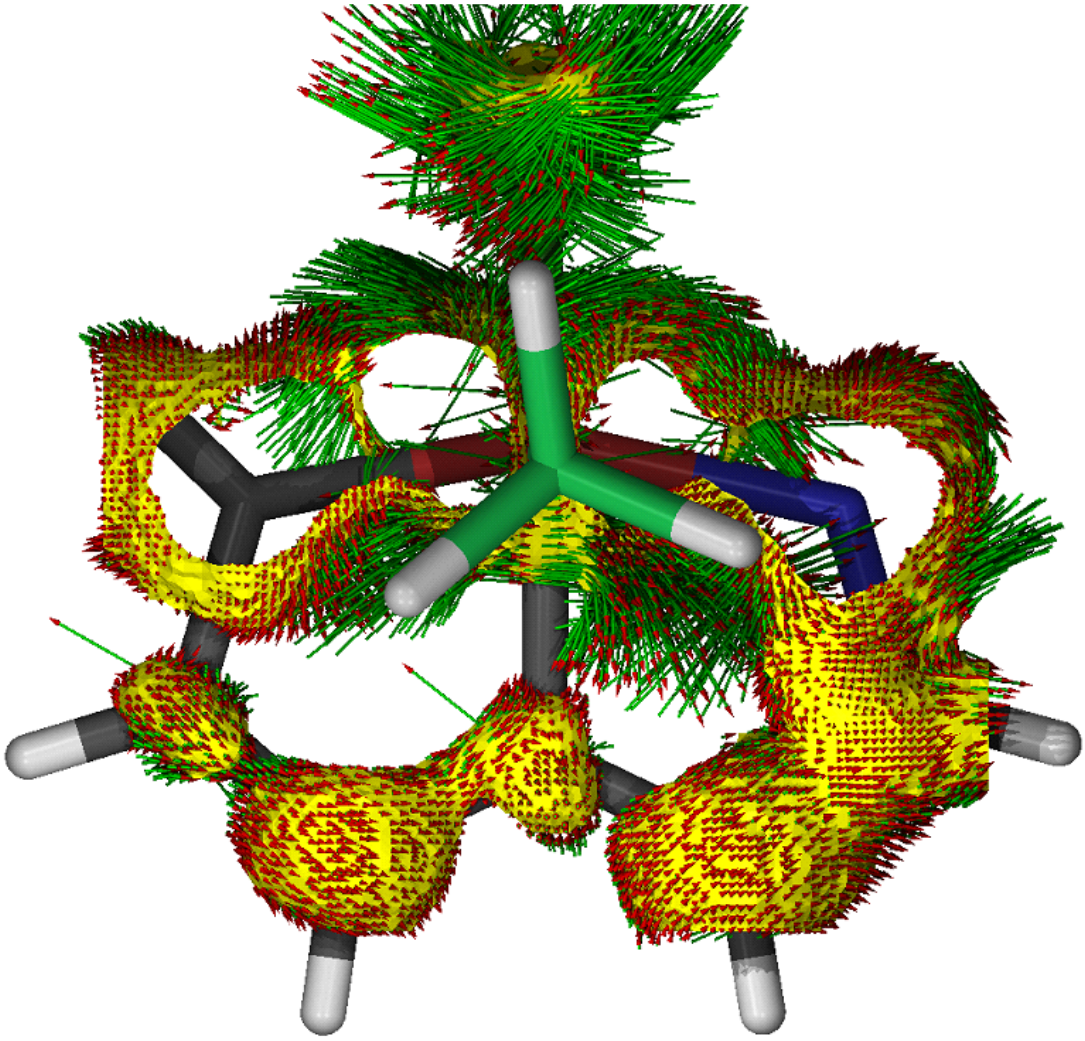


Fig. S17. ACID plot of HSOMO of **Os-N.T$_1$**. Isovalue for ACID is 0.010 a.u.

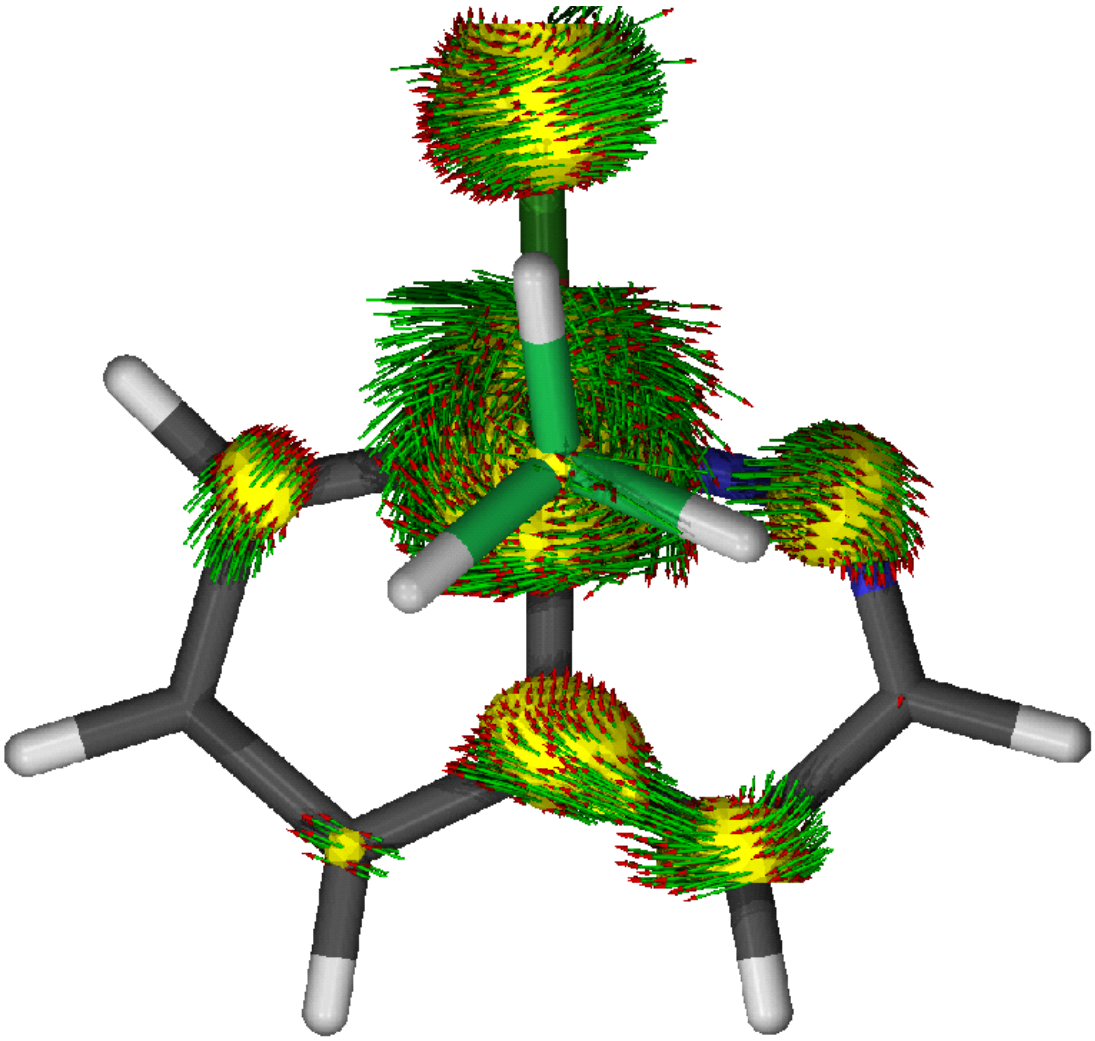


Fig. S18. ACID plot of HSOMO-1 of **Os-N.T$_1$**. Isovalue for ACID is 0.010 a.u.

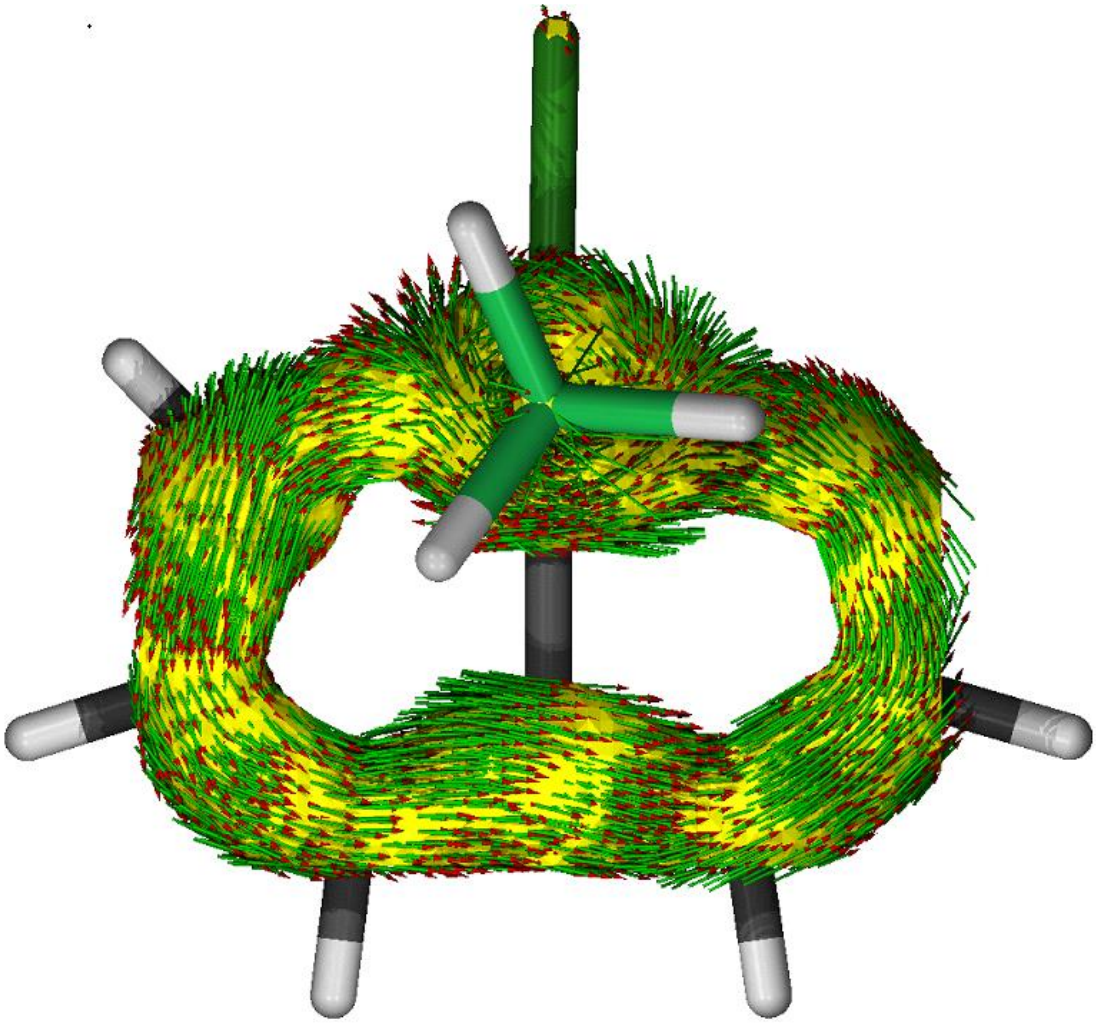


Fig. S19. ACID plot of HSOMO of **Os-O.T$_1$**. Isovalue for ACID is 0.010 a.u.

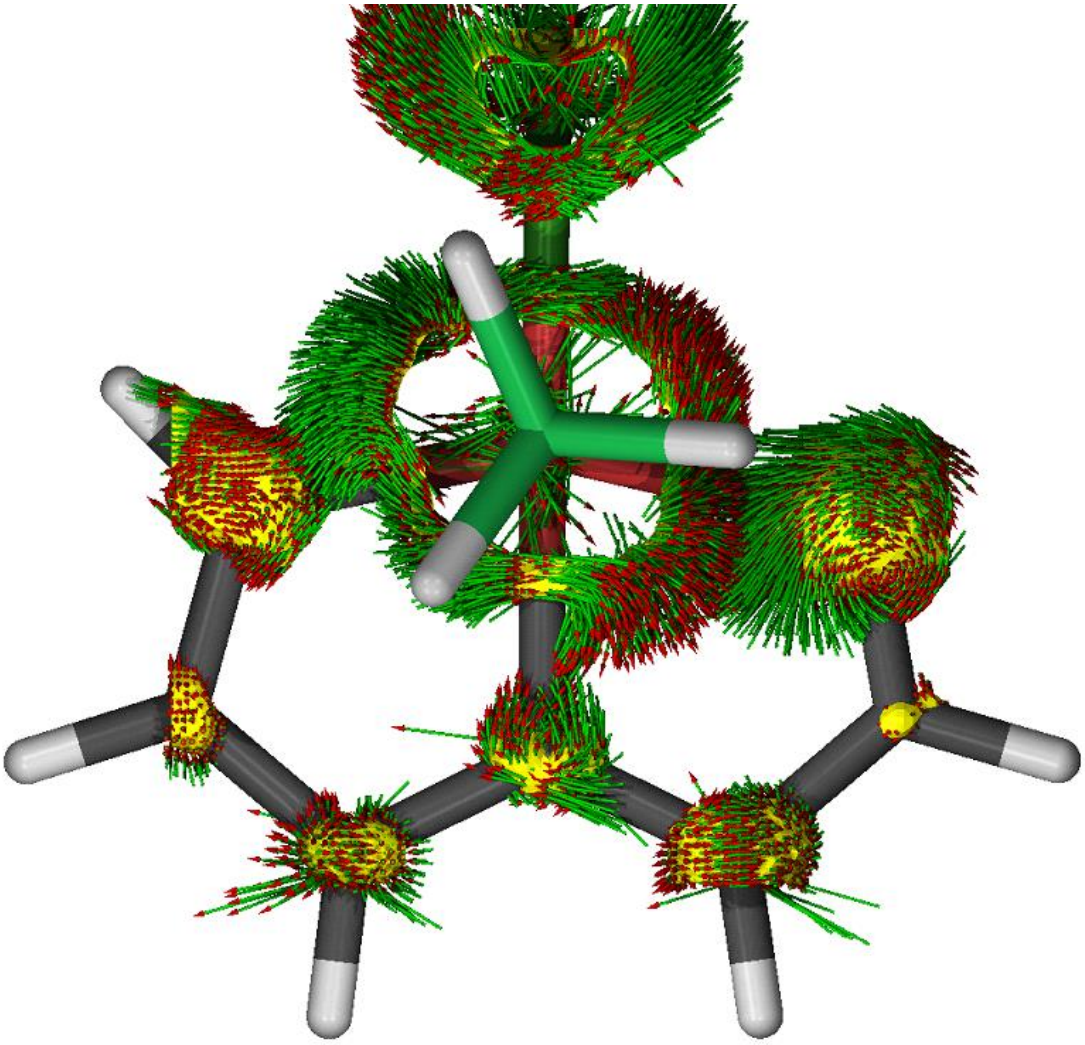


Fig. S20. ACID plot of HSOMO-1 of **Os-N.T$_1$**. Isovalue for ACID is 0.010 a.u.

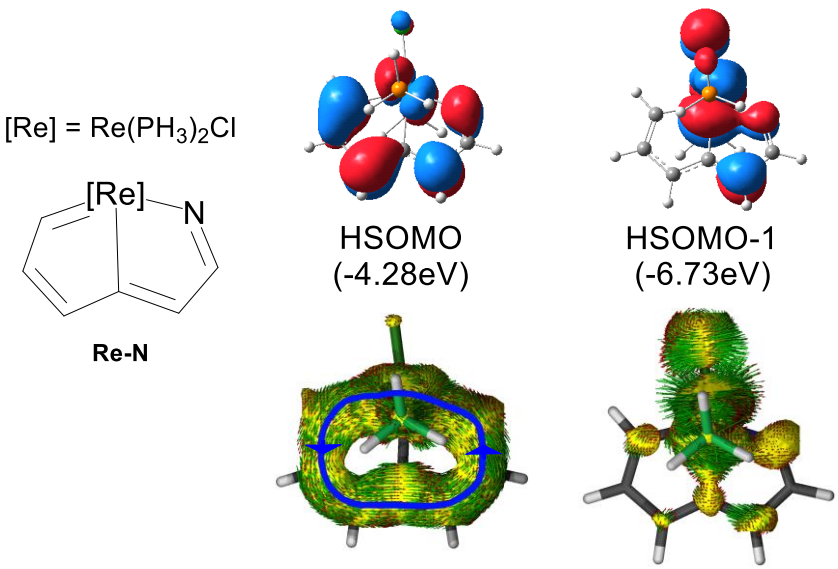


Fig. S21. Biorthogonalized SOMOs and the ACID plots of SOMOs of **Re-N** in the T_1 state. Isovalues for MO and ACID plots are 0.030 and 0.010 a.u., respectively. (The high-resolution ACID plots are provided in the Fig. S22-S23)

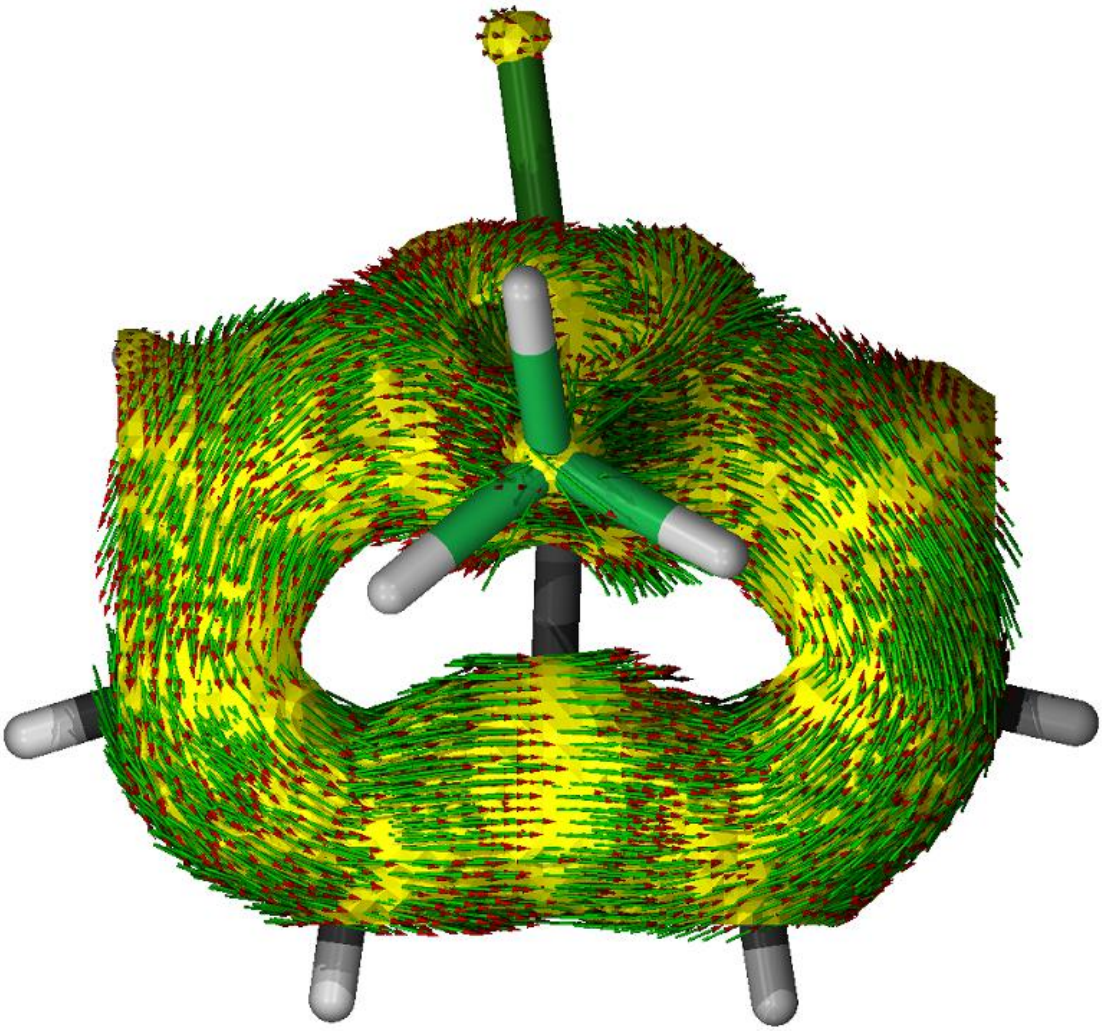


Fig. S22. ACID plot of HSOMO of **Re-N.T$_1$**. Isovalue for ACID is 0.010 a.u.

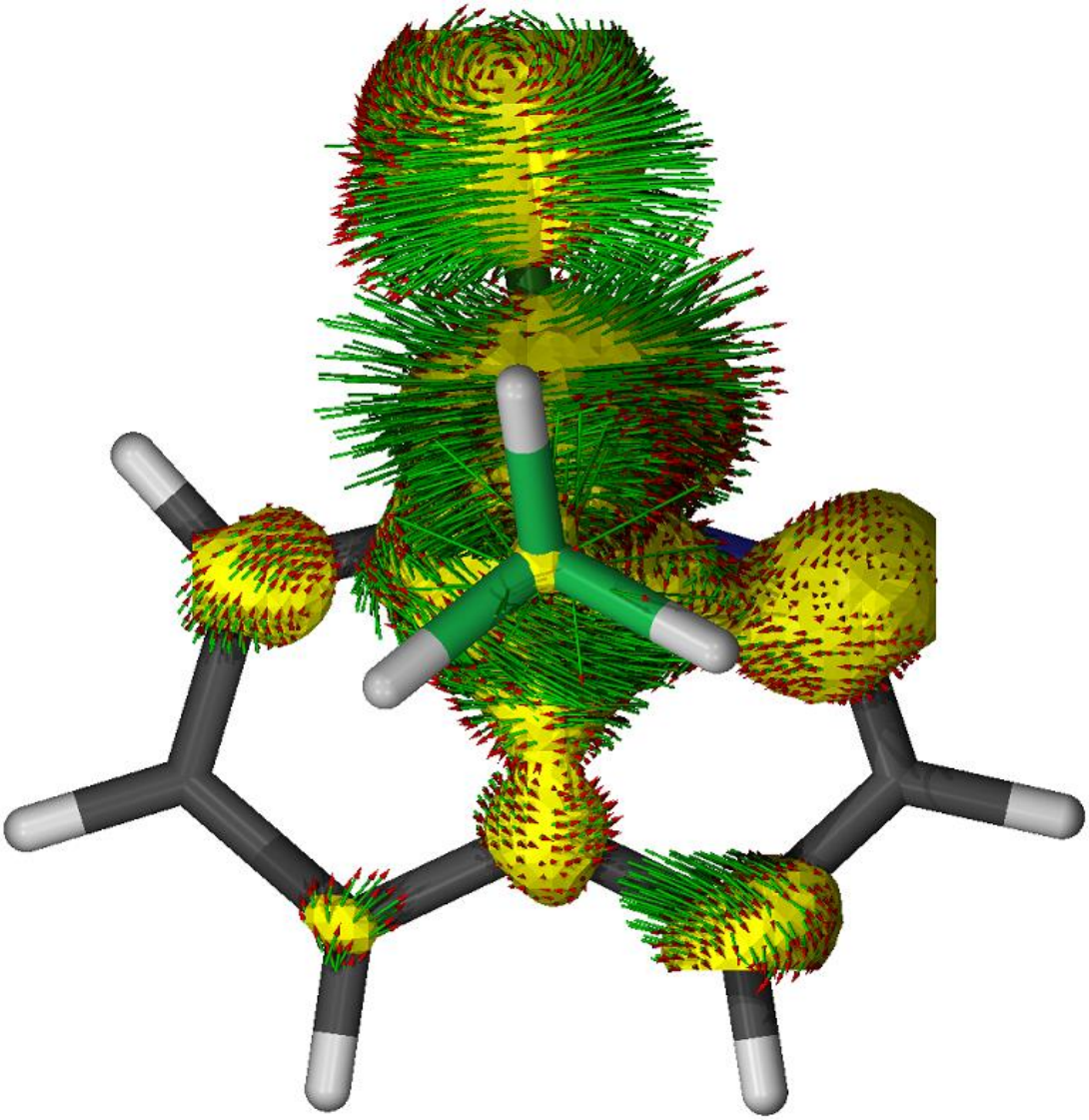


Fig. S23. ACID plot of HSOMO-1 of **Re-N.T$_1$**. Isovalue for ACID is 0.010 a.u.

Cartesian coordinates

Os-B.S_0

Energy = -378.905633 a.u.

1 1

C 1.487274000 0.000618000 2.351992000
C 2.162546000 -0.000499000 0.035874000
C 2.252918000 -0.001514000 -2.268607000
C 3.033577000 -0.001039000 -1.134416000
H 4.124928000 -0.001097000 -1.053661000
C 0.217791000 0.000814000 1.888720000
C 2.512374000 -0.000128000 1.345462000
H 3.568058000 -0.000256000 1.614465000
Os -0.328536000 0.000074000 -0.047776000
P -0.463701000 2.413783000 -0.005732000
H -0.947026000 3.061360000 -1.173328000
H 0.719011000 3.154497000 0.255857000
H -1.342245000 2.947280000 0.973623000
P -0.465323000 -2.413555000 -0.004317000
H 0.716829000 -3.155122000 0.257414000
H -0.948774000 -3.060408000 -1.172261000
H -1.344576000 -2.946554000 0.974649000
H -0.664534000 0.001497000 2.538118000
H 1.722745000 0.000965000 3.413475000
H 2.526646000 -0.002022000 -3.312312000
B 1.081997000 -0.000949000 -1.354051000
Cl -2.625639000 0.000355000 -0.357540000

Os-C.S_0

Energy = -392.776023 a.u.

1 1

Os 0.000000000 0.000000000 0.258764000
P 0.000000000 2.423902000 0.331151000
C 1.873837000 -0.047058000 -0.364458000
C 2.318347000 -0.075226000 -1.665864000
C 1.231061000 -0.043792000 -2.556638000
H 1.331603000 -0.052461000 -3.640646000
C 0.000000000 0.000000000 -1.897317000
C -1.231061000 0.043792000 -2.556638000
H -1.331603000 0.052461000 -3.640646000
Cl 0.000000000 0.000000000 2.635634000
H 1.234189000 3.057718000 0.633412000
H -0.385294000 3.123313000 -0.843076000
H -0.848886000 3.015391000 1.302444000
C -1.873837000 0.047058000 -0.364458000
C -2.318347000 0.075226000 -1.665864000
H -2.532940000 0.041596000 0.514200000
P 0.000000000 -2.423902000 0.331151000
H 0.848886000 -3.015391000 1.302444000
H -1.234189000 -3.057718000 0.633412000
H 0.385294000 -3.123313000 -0.843076000
H 3.364550000 -0.109882000 -1.955796000
H -3.364550000 0.109882000 -1.955796000
H 2.532940000 -0.041596000 0.514200000

Os-C.T_1

Energy = -392.739798 a.u.

1 3

Os 0.000000000 0.000000000 0.299388000
P -2.417624000 0.000000000 0.049466000
C 0.000000000 2.006513000 -0.162772000
C 0.000000000 2.359027000 -1.511611000
C 0.000000000 1.262517000 -2.394509000
H 0.000000000 1.380060000 -3.478250000
C 0.000000000 0.000000000 -1.767630000
C 0.000000000 -1.262517000 -2.394509000
H 0.000000000 -1.380060000 -3.478250000
Cl 0.000000000 0.000000000 2.635175000
H -3.179317000 0.000000000 1.246942000
H -2.975806000 1.101362000 -0.649987000
H -2.975806000 -1.101362000 -0.649987000
C 0.000000000 -2.006513000 -0.162772000
C 0.000000000 -2.359027000 -1.511611000
H 0.000000000 -2.794079000 0.596756000
P 2.417624000 0.000000000 0.049466000
H 2.975806000 1.101362000 -0.649987000
H 3.179317000 0.000000000 1.246942000
H 2.975806000 -1.101362000 -0.649987000
H 0.000000000 3.387242000 -1.866972000
H 0.000000000 -3.387242000 -1.866972000
H 0.000000000 2.794079000 0.596756000

Os-N.S_0

Energy = -408.841951 a.u.

1 1

C 1.25037800 0.04108100 2.50268700
C 1.85100400 -0.20674200 0.26249400
C 1.85218400 -0.40442400 -2.03225800
C 2.65290200 -0.40384000 -0.86140000

H 3.73216200 -0.54092400 -0.85372000
C 0.00542000 0.13859700 1.87396200
C 2.29356900 -0.15243700 1.59960100
H 3.33798700 -0.25339200 1.88955800
Os -0.21246200 0.02088100 -0.10155300
P -0.73151600 -2.35966000 0.01688900
H -1.55025500 -2.76292800 1.10060600
H -1.46413000 -2.85154400 -1.09318300
H 0.33001700 -3.30129500 0.09345000
P 0.01667100 2.43543000 -0.25480100
H -1.15962200 3.17041500 0.03995500
H 0.97616100 3.06442900 0.58240700
H 0.37703900 2.95497100 -1.52644100
H -0.89907200 0.29017800 2.46720600
H 1.38386800 0.10755500 3.57913000
H 2.18911900 -0.53400400 -3.05905100
N 0.58316000 -0.21869400 -1.75501200
Cl -2.58225700 0.31708600 0.01655200

Os-N.T_1

Energy = -408.785437 a.u.

1 3

C 2.43667000 -1.33751700 0.00000000
C 0.11574400 -1.78772800 0.00000000
C -2.22389200 -1.55305300 0.00000000
C -1.10097000 -2.46035900 0.00000000
H -1.21776900 -3.54403400 0.00000000
C 1.96449400 -0.00073100 0.00000000
C 1.44018400 -2.31202900 0.00000000
H 1.65842200 -3.37952800 0.00000000
Os -0.02251200 0.26821500 0.00000000
P -0.07063000 0.09941300 2.43864500
H 0.02151000 1.32023400 3.15376600
H -1.24403900 -0.48136300 2.98582900
H 0.95138600 -0.67614200 3.04468600
P -0.07063000 0.09941300 -2.43864500
H 0.02151000 1.32023400 -3.15376600
H 0.95138600 -0.67614200 -3.04468600
H -1.24403900 -0.48136300 -2.98582900
H 2.70740600 0.80330400 0.00000000
H 3.49441900 -1.59181200 0.00000000
H -3.26005000 -1.89986200 0.00000000
N -1.94328600 -0.27964000 0.00000000
Cl -0.07063000 2.62268800 0.00000000

Os-O.S_0

Energy = -429.543874 a.u.

0 1

C 1.77619200 -0.12114200 2.20396200
C 1.73705400 -0.58829600 -0.09262600
C 1.13310900 -1.02816000 -2.30703500
C 2.17824700 -0.95633400 -1.37474700
H 3.19394500 -1.25693600 -1.62558200
C 0.35829100 -0.02938800 1.93129800
C 2.53107000 -0.48615000 1.11092100
H 3.60592800 -0.66219200 1.14640100
Os -0.16462300 0.04036900 0.07424900
P -1.53027500 -1.86527900 0.44334200
H -2.32867000 -1.86688000 1.62144400
H -2.52808200 -2.10995900 -0.53655800
H -0.98374700 -3.18080800 0.55393700
P 0.76141800 2.19973700 -0.32253900
H -0.05391400 3.32143900 -0.01604300
H 1.96796100 2.55375300 0.34810100
H 1.13299900 2.53293900 -1.65822600
H -0.29272200 -0.28217900 2.78116100
H 2.19417800 -0.02161400 3.20590100
H 1.26512200 -1.43054000 -3.31706300
Cl -2.40823500 1.11742700 -0.17472000
O -0.05907500 -0.67766700 -1.97735900

Os-O.T_1

Energy = -429.540611 a.u.

0 3

C 2.78888200 -0.40300400 0.00000000
C 0.78413500 -1.65149600 0.00000000
C -1.44825700 -2.37919500 0.00000000
C -0.10921800 -2.75327800 0.00000000
H 0.20040900 -3.79659900 0.00000000
C 1.89203700 0.66270000 0.00000000
C 2.19357000 -1.68825200 0.00000000
H 2.76946200 -2.61331700 0.00000000
Os -0.07417400 0.20212300 0.00000000
P -0.10921800 0.27465500 2.37300700
H -0.13490200 1.55500100 2.99051400
H -1.21104300 -0.33363900 3.04164900
H 0.95862900 -0.32871900 3.09785100
P -0.10921800 0.27465500 -2.37300700

H	-0.13490200	1.55500100	-2.99051400
H	0.95862900	-0.32871900	-3.09785100
H	-1.21104300	-0.33363900	-3.04164900
H	2.26670800	1.68987900	0.00000000
H	3.86968700	-0.26409800	0.00000000
H	-2.27334200	-3.09785600	0.00000000
Cl	-1.14822100	2.41042400	0.00000000
O	-1.77895400	-1.12579200	0.00000000

Re-N.S_0

Energy = -397.122027 a.u.

0 1

C	2.53043800	-1.16971000	0.00000000
C	0.29952800	-1.84183800	0.00000000
C	-1.99939200	-1.94853400	0.00000000
C	-0.81761000	-2.70275900	0.00000000
H	-0.77992000	-3.79190700	0.00000000
C	1.87643800	0.07240800	0.00000000
C	1.64735100	-2.25082700	0.00000000
H	1.96678200	-3.29341000	0.00000000
P	-0.05910600	0.28100300	2.43103500
H	0.28868200	1.50106000	3.07826200
H	-1.23891500	-0.03712500	3.16647500
H	0.84871100	-0.59662700	3.09257900
P	-0.05910600	0.28100300	-2.43103500
H	0.28868200	1.50106000	-3.07826200
H	0.84871100	-0.59662700	-3.09257900
H	-1.23891500	-0.03712500	-3.16647500
H	2.47626600	0.98763400	0.00000000
H	3.61377600	-1.28370100	0.00000000
H	-3.01713700	-2.33783400	0.00000000
N	-1.76576600	-0.63651200	0.00000000
Cl	-0.05910600	2.68557100	0.00000000
Re	-0.13518500	0.23203900	0.00000000

Re-N.T_1

Energy = -397.068512 a.u.

0 3

P	-0.01506200	0.00636200	2.40742100
C	1.36185100	2.37926200	0.00000000
C	-0.01506200	2.74707100	0.00000000
H	-0.36565500	3.77861400	0.00000000
C	-0.84960700	1.60253800	0.00000000
C	-2.24794200	1.54363900	0.00000000
H	-2.88674800	2.42701100	0.00000000
Cl	1.05151100	-2.48863400	0.00000000
H	0.35150800	-1.05311600	3.28761000
H	0.69935000	1.07589800	3.02051600
H	-1.32781100	0.27285100	2.87999400
C	-1.81062600	-0.77232400	0.00000000
C	-2.76655000	0.20796600	0.00000000
H	-2.08118100	-1.83099500	0.00000000
P	-0.01506200	0.00636200	-2.40742100
H	0.69935000	1.07589800	-3.02051600
H	0.35150800	-1.05311600	-3.28761000
H	-1.32781100	0.27285100	-2.87999400
H	2.19431000	3.08575500	0.00000000
H	-3.83818600	0.00767200	0.00000000
Re	0.22721900	-0.26424400	0.00000000
N	1.57624600	1.08942700	0.00000000

Re-O.S_0

Energy = -417.633128 a.u.

-1 1

C	1.71327200	-0.87086800	2.10894500
C	1.75425500	-0.52384900	-0.20518500
C	1.23999300	-0.26892800	-2.47478800
C	2.25065000	-0.42221500	-1.54701500
H	3.29287900	-0.55981600	-1.84213800
C	0.33351400	-0.66640400	1.85761900
C	2.51334400	-0.81764400	0.95963100
H	3.59490300	-0.98067200	0.96518900
P	-1.57807600	-1.90617500	-0.03683800
H	-1.83487700	-2.64212600	1.17173600
H	-2.93949400	-1.79206500	-0.47392100
H	-1.25505900	-3.06043800	-0.83381000
P	0.91804200	2.09893800	0.34949200
H	0.20923700	3.26183200	0.79270300
H	1.99752600	2.14669200	1.28759600
H	1.59495800	2.72708600	-0.75054000
H	-0.34793800	-1.13894900	2.58586400
H	2.11268400	-1.16656700	3.08458000
H	1.40227300	-0.29679300	-3.55955500
Cl	-2.41065500	1.30233800	0.07471900
Re	-0.21058900	0.01535000	0.05374700
O	0.00231700	-0.15764700	-2.07675000

Re-O.T_1

Energy = -417.635873 a.u.

-1 3

C	2.80010600	-0.34504500	0.00000000
C	0.81510600	-1.63604900	0.00000000
C	-1.40581400	-2.43758400	0.00000000
C	-0.06657600	-2.77364400	0.00000000
H	0.26329200	-3.81488000	0.00000000
C	1.88942700	0.71918600	0.00000000
C	2.22264200	-1.64726300	0.00000000
H	2.82546100	-2.56053000	0.00000000
P	-0.06657600	0.23808700	2.38218600
H	-0.17865700	1.47070300	3.10380700
H	-1.05843600	-0.48555900	3.12652900
H	1.07412500	-0.27977000	3.07828700
P	-0.06657600	0.23808700	-2.38218600
H	-0.17865700	1.47070300	-3.10380700
H	1.07412500	-0.27977000	-3.07828700
H	-1.05843600	-0.48555900	-3.12652900
H	2.29944600	1.73870800	0.00000000
H	3.88548200	-0.20335200	0.00000000
H	-2.20302500	-3.19446200	0.00000000
Cl	-1.25653700	2.48178200	0.00000000
Re	-0.08741800	0.20711000	0.00000000
O	-1.79492000	-1.19000000	0.00000000

Ru-N.S_0

Energy = -411.625419 a.u.

1 1

C	2.58788800	-0.95851500	0.00000000
C	0.41295600	-1.80553800	0.00000000
C	-1.87562300	-2.04560000	0.00000000
C	-0.62155500	-2.72686200	0.00000000
H	-0.50879900	-3.81003800	0.00000000
C	1.83281800	0.21128800	0.00000000
C	1.79111200	-2.10149800	0.00000000
H	2.18367800	-3.11789200	0.00000000
Ru	-0.14632000	0.23387200	0.00000000
P	-0.20224300	0.43176100	2.42788100
H	0.78546500	1.25963000	3.01842300
H	-1.39229800	1.02971200	2.91541200
H	-0.12037900	-0.72271100	3.25451000
P	-0.20224300	0.43176100	-2.42788100
H	0.78546500	1.25963000	-3.01842300
H	-0.12037900	-0.72271100	-3.25451000
H	-1.39229800	1.02971200	-2.91541200
H	2.30644100	1.19423800	0.00000000
H	3.67505300	-0.97075100	0.00000000
H	-2.86669400	-2.50018000	0.00000000
N	-1.73676100	-0.75236600	0.00000000
Cl	-0.20224300	2.62676900	0.00000000

Ru-N.T_1

Energy = -411.579768 a.u.

1 3

C	2.44190800	-1.22330000	0.00000000
C	0.12865500	-1.71665700	0.00000000
C	-2.22168000	-1.52992300	0.00000000
C	-1.06743300	-2.40888300	0.00000000
H	-1.16182700	-3.49565900	0.00000000
C	1.94057500	0.09671900	0.00000000
C	1.46239400	-2.21427600	0.00000000
H	1.69890700	-3.27877900	0.00000000
Ru	-0.03433700	0.34338800	0.00000000
P	-0.07554900	0.12238400	2.43341300
H	-0.01554100	1.32838900	3.17772400
H	-1.23588500	-0.48933000	2.97537200
H	0.95422600	-0.63696500	3.04875100
P	-0.07554900	0.12238400	-2.43341300
H	-0.01554100	1.32838900	-3.17772400
H	0.95422600	-0.63696500	-3.04875100
H	-1.23588500	-0.48933000	-2.97537200
H	2.64547400	0.93344700	0.00000000
H	3.50519900	-1.45550600	0.00000000
H	-3.24732400	-1.91144400	0.00000000
N	-1.98441600	-0.25801200	0.00000000
Cl	-0.07554900	2.69453900	0.00000000

Ru-O.S_0

Energy = -432.352816 a.u.

0 1

C	-1.57258600	0.16944900	-2.31625400
C	-1.73636900	-0.49123000	-0.06911700
C	-1.33261600	-1.11883600	2.16158600
C	-2.28902200	-0.93311400	1.12832900
H	-3.33401200	-1.20742500	1.27417400
C	-0.18195200	0.21006500	-1.92645500
C	-2.41912000	-0.27143900	-1.32485900

H	-3.48771400	-0.43190600	-1.47325000
P	1.38986700	-1.95737700	-0.47818300
H	2.31037800	-1.95905400	-1.56143100
H	2.25089600	-2.35993800	0.57572500
H	0.75517800	-3.21264600	-0.74068400
P	-0.53096000	2.26505500	0.50119600
H	0.35407600	3.33636800	0.20839300
H	-1.74102500	2.79101900	-0.04265000
H	-0.77977300	2.54215900	1.87674400
H	0.55749200	0.12247900	-2.73408200
H	-1.90770300	0.38045500	-3.33212600
H	-1.61012200	-1.59649800	3.11198000
Cl	2.54850300	0.90215300	0.20204800
O	-0.11765100	-0.79261200	2.00307600
Ru	0.19444000	0.05897100	-0.06560900

Ru-O.T_1

Energy = -432.351171 a.u.

0 3

C	2.68467500	-0.74647900	0.00000000
C	0.53161900	-1.71308600	0.00000000
C	-1.78834100	-2.13727900	0.00000000
C	-0.49390300	-2.67541000	0.00000000
H	-0.32161400	-3.75129600	0.00000000
C	1.93695400	0.42092000	0.00000000
C	1.92286500	-1.93863300	0.00000000
H	2.36854700	-2.93386400	0.00000000
Ru	-0.07119600	0.25085800	0.00000000
P	-0.07119600	0.35525300	2.37800800
H	0.37001800	1.56710900	2.97446100
H	-1.32163800	0.21674400	3.04606600
H	0.69125400	-0.57103000	3.14841200
P	-0.07119600	0.35525300	-2.37800800
H	0.37001800	1.56710900	-2.97446100
H	0.69125400	-0.57103000	-3.14841200
H	-1.32163800	0.21674400	-3.04606600
H	2.41007800	1.40519300	0.00000000
H	3.77502300	-0.75067700	0.00000000
H	-2.68491600	-2.76955000	0.00000000
Cl	-0.75100400	2.61049100	0.00000000
O	-1.96925300	-0.86992100	0.00000000

Ir-N.S_0

Energy = -422.051304 a.u.

2 1

C	1.24297300	-0.00057100	2.51455200
C	1.88233500	-0.00125700	0.25627800
C	1.88044300	-0.00196600	-2.05706900
C	2.69003800	-0.00219800	-0.86557700
H	3.77889500	-0.00299300	-0.86688300
C	-0.00102600	0.00021300	1.90149500
C	2.30263200	-0.00130500	1.60409600
H	3.35284800	-0.00183800	1.89486700
P	-0.42592900	-2.44359400	-0.14942300
H	-1.17046200	-2.97661900	0.93033000
H	-1.14176500	-2.84965600	-1.30225600
H	0.75653400	-3.22651900	-0.17878900
P	-0.42118400	2.44430700	-0.15012400
H	-1.16467400	2.97925800	0.92939500
H	0.76292800	3.22472500	-0.17957500
H	-1.13605800	2.85164000	-1.30311700
H	-0.92755900	0.00094500	2.47844900
H	1.36692400	-0.00059200	3.59493400
H	2.22667600	-0.00239900	-3.09258400
N	0.61973600	-0.00100300	-1.77819500
Cl	-2.54056800	0.00214300	0.03344800
Ir	-0.19650000	0.00008400	-0.08643500

Ir-N.T_1

Energy = -422.011590 a.u.

2 3

C	1.35834700	-0.08128000	2.42478800
C	1.75610500	-0.31600800	0.09759700
C	1.51579000	-0.46797200	-2.25603200
C	2.40978800	-0.53127500	-1.10543300
H	3.47511400	-0.73352600	-1.21206200
C	0.04363700	0.12506800	1.95701900
C	2.29719300	-0.32359200	1.42329300
H	3.35175300	-0.50712500	1.62679500
P	-0.69280500	-2.36000400	0.05681600
H	-1.42084100	-2.80974700	1.18586100
H	-1.46250500	-2.79150300	-1.05148800
H	0.45096600	-3.19660000	0.03356800
P	0.33215100	2.42371200	-0.21030000
H	-0.75811500	3.30294500	0.00353000
H	1.32830900	2.88609800	0.68514400

H	0.82230700	2.78123300	-1.49104600
H	-0.76607600	0.30420700	2.67019600
H	1.61487800	-0.05804500	3.48143800
H	1.84437300	-0.62466400	-3.28726700
N	0.28431900	-0.20937000	-1.97805900
Cl	-2.56408200	0.44596600	-0.06176700
Ir	-0.23060200	0.05124200	-0.00900500

Ir-O.S_0

Energy = -442.965646 a.u.

1 1

C	2.75712000	-0.61076900	0.00000000
C	0.67103900	-1.72872700	0.00000000
C	-1.62216300	-2.27707600	0.00000000
C	-0.26176400	-2.74527500	0.00000000
H	-0.03549000	-3.80944400	0.00000000
C	1.87568300	0.53673900	0.00000000
C	2.12156100	-1.83169000	0.00000000
H	2.65271600	-2.78197300	0.00000000
P	-0.26176400	0.42848800	2.35504700
H	0.32182000	1.60648800	2.87764700
H	-1.62524200	0.56755200	2.71062000
H	0.18727100	-0.56435400	3.26996800
P	-0.26176400	0.42848800	-2.35504700
H	0.32182000	1.60648800	-2.87764700
H	0.18727100	-0.56435400	-3.26996800
H	-1.62524200	0.56755200	-2.71062000
H	2.32144200	1.53661800	0.00000000
H	3.83911700	-0.50350800	0.00000000
H	-2.47007500	-2.97035300	0.00000000
Cl	-0.87522200	2.45103700	0.00000000
Ir	0.00622700	0.14328400	0.00000000
O	-1.88400800	-1.03812900	0.00000000

Ir-O.T_1

Energy = -442.941393 a.u.

1 3

C	1.42941100	-0.00002000	2.41786300
C	1.83028900	-0.00000400	0.09106100
C	1.63704500	0.00003400	-2.24967200
C	2.49684300	0.00000700	-1.14489700
H	3.57841200	-0.00000100	-1.25130600
C	0.11555300	-0.00001700	1.99773000
C	2.39268200	-0.00001900	1.38019600
H	3.46580400	-0.00002200	1.55726500
P	-0.32344900	-2.38479200	0.00068700
H	-1.39795600	-2.92686800	0.74719700
H	-0.51603100	-2.97184600	-1.27641700
H	0.79145700	-3.10898400	0.49737100
P	-0.32344200	2.38479200	0.00072300
H	-1.39795000	2.92685700	0.74723800
H	0.79146400	3.10897400	0.49742000
H	-0.51602000	2.97186400	-1.27637400
H	-0.73040900	-0.00001900	2.68493500
H	1.70040000	-0.00002700	3.47138900
H	1.97609500	0.00002000	-3.28816300
Cl	-2.59646300	0.00000500	-0.08868000
Ir	-0.21050600	0.00000000	-0.00062200
O	0.36199800	0.00001300	-2.06624500

Os-N.$SnCl^{3-}$.S_0

Energy = -442.252644 a.u.

1 1

C	-2.260915000	0.000785000	-2.549127000
C	-3.039287000	0.000153000	-0.346509000
C	-3.166732000	-0.000481000	1.960283000
C	-3.905328000	-0.000082000	0.746151000
H	-4.992756000	0.000011000	0.693009000
C	-1.043910000	0.000515000	-1.855358000
C	-3.375878000	0.000578000	-1.711967000
H	-4.402064000	0.000736000	-2.076267000
Os	-0.955888000	-0.000123000	0.137534000
P	-0.858520000	-2.432951000	0.160461000
H	-0.086339000	-3.075532000	-0.839146000
H	-0.327745000	-3.010289000	1.341196000
H	-2.095477000	-3.123525000	0.040520000
P	-0.858495000	2.432713000	0.161648000
H	-0.085956000	3.075641000	-0.837443000
H	-2.095419000	3.123316000	0.041572000
H	-0.328137000	3.009570000	1.342802000
H	-0.109864000	0.000663000	-2.427817000
H	-2.325077000	0.001151000	-3.634159000
H	-3.563592000	-0.000743000	2.973978000
N	-1.873752000	-0.000541000	1.735715000
Sn	1.848369000	-0.000068000	0.019112000
Cl	2.630806000	0.000692000	-2.205508000
Cl	2.810368000	-1.891706000	1.029829000
Cl	2.809722000	1.891621000	1.030447000

Os-N.SnCl^{3-}.T$_1$

Energy = -442.207923 a.u.

1 3

P	-1.040519000	2.541150000	0.088351000
C	-2.085415000	-0.126705000	-2.535311000
C	-3.237379000	-0.361424000	-1.721392000
H	-4.233357000	-0.543437000	-2.122075000
C	-2.931442000	-0.297561000	-0.367742000
C	-3.770136000	-0.377927000	0.769820000
H	-4.843994000	-0.543826000	0.683992000
H	-0.723821000	3.206335000	-1.124003000
H	-2.310628000	3.103278000	0.391516000
H	-0.222986000	3.243498000	1.012358000
C	-1.733397000	0.044592000	1.923780000
C	-3.127238000	-0.197894000	1.994401000
H	-1.208309000	0.200969000	2.872193000
P	-0.829868000	-2.308704000	0.158930000
H	-0.807598000	-2.961952000	-1.101742000
H	0.236544000	-2.968278000	0.823383000
H	-1.948868000	-2.925360000	0.779315000
H	-2.091134000	-0.130834000	-3.626306000
H	-3.672004000	-0.231128000	2.935453000
Os	-0.932163000	0.112760000	0.093551000
Sn	1.853161000	-0.035767000	-0.004317000
Cl	2.689639000	-0.331792000	2.161809000
Cl	2.644117000	-1.805649000	-1.296570000
Cl	2.684106000	1.986979000	-0.835007000
N	-0.989329000	0.105992000	-1.860376000

Os-N.BMe^{2-}.S$_0$

Energy = -498.528956 a.u.

1 1

C	-0.884042000	-0.005490000	2.673570000
C	-1.861788000	-0.000479000	0.556932000
C	-2.218565000	0.004923000	-1.760733000
C	-2.811302000	0.002284000	-0.458794000
H	-3.888262000	0.002578000	-0.281587000
C	0.291915000	-0.004115000	1.900503000
C	-2.073644000	-0.003500000	1.946015000
H	-3.061950000	-0.004229000	2.403010000
Os	0.130444000	0.000169000	-0.137064000
P	-0.007869000	2.404809000	-0.167258000
H	-0.122589000	3.077656000	1.077517000
H	1.041904000	3.152225000	-0.768169000
H	-1.124146000	2.937940000	-0.867433000
P	-0.010655000	-2.404140000	-0.176454000
H	1.039216000	-3.150862000	-0.778056000
H	-0.128548000	-3.081090000	1.065795000
H	-1.126355000	-2.933437000	-0.880463000
H	1.212025000	-0.005468000	2.483721000
H	-0.864883000	-0.007854000	3.761363000
H	-2.817855000	0.007195000	-2.675650000
N	-0.908469000	0.004360000	-1.824235000
B	2.175696000	-0.000785000	0.068839000
C	3.436177000	-0.002783000	0.976542000
H	4.066173000	-0.877185000	0.753000000
H	4.067280000	0.871466000	0.755573000
H	3.242805000	-0.004285000	2.054951000
C	2.300585000	0.002074000	-1.547409000
H	2.894974000	0.893213000	-1.794570000
H	2.894816000	-0.888228000	-1.797867000
H	1.444278000	0.003410000	-2.232871000

Os-N.BMe^{2-}.T$_1$

Energy = -498.483179 a.u.

1 3

C	-1.903053000	0.585503000	2.110773000
C	-2.009584000	-0.215019000	-0.109571000
C	-1.386830000	-0.748292000	-2.295085000
C	-2.458369000	-0.628344000	-1.353786000
H	-3.503272000	-0.802184000	-1.610413000
C	-0.525128000	0.712066000	1.810268000
C	-2.704331000	0.090474000	1.081732000
H	-3.783964000	-0.027291000	1.178889000
Os	0.100936000	0.104753000	0.009438000
P	0.207023000	2.396504000	-0.731617000
H	1.040474000	3.301335000	-0.018212000
H	0.639630000	2.637678000	-2.063183000
H	-1.007276000	3.138156000	-0.722716000
P	-0.023280000	-2.183324000	0.745193000
H	1.112182000	-2.855101000	1.275669000
H	-0.974082000	-2.452118000	1.765833000
H	-0.419337000	-3.118539000	-0.250522000
H	0.090738000	1.208505000	2.569666000
H	-2.324464000	0.884572000	3.068555000
H	-1.531446000	-1.053813000	-3.333510000
N	-0.194716000	-0.449215000	-1.843015000

B	2.325197000	-0.266581000	0.069538000
C	3.050099000	0.504726000	1.229260000
H	3.313215000	-0.239188000	2.000014000
H	4.003363000	0.910614000	0.855720000
H	2.503865000	1.307710000	1.731351000
C	3.015298000	-1.193236000	-0.977546000
H	3.855915000	-1.747252000	-0.532500000
H	2.365780000	-1.888270000	-1.516384000
H	3.459784000	-0.533572000	-1.742071000

Os-N.H$^-$.S_0

Energy = -394.423664 a.u.

1 1

C	0.387057000	-0.146389000	-2.646777000
C	0.238004000	1.373553000	-0.874456000
C	-0.023574000	2.330994000	1.209650000
C	0.207254000	2.580837000	-0.166237000
H	0.336634000	3.571207000	-0.601371000
C	0.146880000	-1.039313000	-1.595513000
C	0.440378000	1.192579000	-2.251662000
H	0.618510000	2.014140000	-2.943902000
Os	-0.071950000	-0.387114000	0.289573000
P	-2.478346000	-0.412438000	0.079045000
H	-3.040797000	-1.268772000	-0.900936000
H	-3.183046000	-0.831259000	1.238254000
H	-3.153407000	0.806380000	-0.206983000
P	2.307842000	-0.666856000	0.591439000
H	2.796009000	-1.958492000	0.914711000
H	3.134119000	-0.338667000	-0.517020000
H	2.912504000	0.111220000	1.615557000
H	0.085283000	-2.104475000	-1.822348000
H	0.516256000	-0.465746000	-3.678016000
H	-0.093040000	3.070201000	2.006202000
N	-0.148428000	1.043535000	1.458682000
H	-0.240254000	-2.053979000	0.570217000

Os-N.H$^-$.T_1

Energy = -394.373277 a.u.

1 3

C	-1.130431000	-2.266070000	-0.996142000
C	-1.435428000	0.071571000	-1.008588000
C	-0.894627000	2.349495000	-0.862438000
C	-1.795379000	1.354257000	-1.377158000
H	-2.620422000	1.602995000	-2.043995000
C	0.017085000	-1.925886000	-0.233793000
C	-1.913037000	-1.192660000	-1.421913000
H	-2.788169000	-1.317161000	-2.059309000
Os	0.336699000	-0.003346000	0.194944000
P	-1.444642000	-0.027158000	1.812519000
H	-2.473657000	-0.982064000	1.604483000
H	-1.103142000	-0.260114000	3.167513000
H	-2.181789000	1.183129000	1.908616000
P	2.677854000	-0.030290000	-0.398180000
H	3.422995000	-1.189030000	-0.056282000
H	3.013324000	0.096704000	-1.775424000
H	3.476885000	0.998117000	0.164308000
H	0.695493000	-2.749622000	0.014125000
H	-1.367313000	-3.291831000	-1.271403000
H	-0.992979000	3.414049000	-1.083538000
N	0.093942000	1.906068000	-0.127777000
H	1.084796000	-0.075885000	1.694678000

Os-N.PMe_3.S_0

Energy = -519.795557 a.u.

2 1

C	1.573586000	0.093898000	2.543124000
C	2.300192000	-0.006387000	0.321208000
C	2.366039000	-0.131363000	-1.985263000
C	3.138700000	-0.074459000	-0.789474000
H	4.226830000	-0.087027000	-0.764390000
C	0.343819000	0.072406000	1.877678000
C	2.668718000	0.053503000	1.677479000
H	3.703855000	0.063826000	2.015670000
Os	0.198835000	-0.008697000	-0.108857000
P	0.245212000	-2.460936000	-0.059994000
H	-0.647937000	-3.156681000	-0.916788000
H	1.486060000	-3.026168000	-0.454302000
H	0.011754000	-3.108892000	1.179598000
P	0.409622000	2.429811000	-0.222555000
H	-0.706651000	3.237945000	-0.562372000
H	0.867099000	3.068970000	0.958402000
H	1.359860000	2.866607000	-1.182473000
H	-0.570164000	0.105298000	2.479302000
H	1.667164000	0.138307000	3.625120000
H	2.735321000	-0.188194000	-3.008362000
N	1.082541000	-0.104680000	-1.724031000
P	-2.364913000	0.036633000	0.002044000
C	-3.129858000	1.486248000	0.863596000

H	-2.863622000	2.421504000	0.364130000
H	-4.219977000	1.384371000	0.842676000
H	-2.806661000	1.532588000	1.908038000
C	-3.179812000	-1.426998000	0.791855000
H	-4.266560000	-1.293591000	0.770912000
H	-2.939000000	-2.345904000	0.249506000
H	-2.864567000	-1.530255000	1.834752000
C	-3.030836000	0.088385000	-1.727672000
H	-4.125654000	0.096673000	-1.690369000
H	-2.686972000	0.989106000	-2.243684000
H	-2.701553000	-0.788784000	-2.291610000

Os-N.PMe$_3$.T$_1$

Energy = -519.738808 a.u.

2 3

C	2.135767000	-0.390470000	2.189692000
C	2.194326000	-0.416144000	-0.184240000
C	1.588192000	-0.141247000	-2.441247000
C	2.637038000	-0.445650000	-1.499950000
H	3.665485000	-0.637880000	-1.804195000
C	0.776337000	-0.062715000	1.967574000
C	2.903361000	-0.572254000	1.038557000
H	3.970855000	-0.790800000	1.069581000
Os	0.184906000	0.119691000	0.052407000
P	0.079835000	-2.333440000	-0.020647000
H	-1.123940000	-3.010978000	0.307399000
H	0.376980000	-2.889740000	-1.292371000
H	1.005059000	-2.988727000	0.829695000
P	0.825341000	2.500992000	0.075879000
H	-0.144167000	3.438116000	0.522061000
H	1.927089000	2.816183000	0.911748000
H	1.214917000	3.048489000	-1.173789000
H	0.153113000	0.078814000	2.856833000
H	2.562947000	-0.490833000	3.184924000
H	1.735255000	-0.121224000	-3.522721000
N	0.429685000	0.123332000	-1.905918000
P	-2.346146000	-0.003168000	0.027372000
C	-2.990055000	1.732825000	-0.102885000
H	-2.620151000	2.208182000	-1.015429000
H	-4.085327000	1.689001000	-0.147475000
H	-2.700628000	2.320631000	0.772277000
C	-3.161567000	-0.714801000	1.524248000
H	-4.249152000	-0.644698000	1.409731000
H	-2.895495000	-1.766911000	1.658099000
H	-2.864011000	-0.156306000	2.416376000
C	-3.047713000	-0.882246000	-1.436034000
H	-4.133493000	-0.738588000	-1.458081000
H	-2.609900000	-0.475976000	-2.351950000
H	-2.845659000	-1.956105000	-1.387564000

Os-N.H$_2$O.S$_0$

Energy = -469.914259 a.u.

2 1

C	0.000035000	1.133109000	2.484084000
C	-0.000250000	1.710866000	0.215293000
C	-0.000325000	1.656898000	-2.095502000
C	-0.000374000	2.488911000	-0.937470000
H	-0.000524000	3.576278000	-0.966392000
C	0.000136000	-0.121734000	1.872593000
C	-0.000205000	2.169841000	1.550645000
H	-0.000323000	3.226411000	1.813019000
Os	0.000029000	-0.371267000	-0.088881000
P	2.465256000	-0.301601000	-0.086793000
H	3.174428000	-1.527380000	0.034937000
H	3.045599000	0.251631000	-1.257297000
H	3.052205000	0.468954000	0.949018000
P	-2.465178000	-0.302254000	-0.086575000
H	-3.174170000	-1.528210000	0.034385000
H	-3.052202000	0.467561000	0.949741000
H	-3.045594000	0.251630000	-1.256734000
H	0.000289000	-1.041417000	2.472272000
H	0.000137000	1.283380000	3.560306000
H	-0.000422000	1.972191000	-3.137945000
N	-0.000151000	0.392806000	-1.765165000
O	0.000398000	-2.595158000	0.012036000
H	-0.783416000	-3.171449000	-0.059049000
H	0.784426000	-3.171190000	-0.058785000

Os-N. H$_2$O.T$_1$

Energy = -469.858201 a.u.

2 3

C	-0.000772000	1.587141000	2.237464000
C	-0.000517000	1.644508000	-0.136591000
C	-0.000049000	1.079492000	-2.437586000
C	-0.000545000	2.135463000	-1.454439000
H	-0.000908000	3.191411000	-1.722695000
C	-0.000236000	0.190005000	1.975818000
C	-0.000896000	2.383051000	1.098882000

H -0.001222000 3.471723000 1.131784000
Os 0.000112000 -0.345670000 0.036573000
P 2.483024000 -0.260242000 -0.002677000
H 3.124265000 -1.501744000 0.246340000
H 3.056886000 0.146631000 -1.234543000
H 3.097494000 0.601597000 0.940576000
P -2.482786000 -0.261570000 -0.003095000
H -3.123433000 -1.503119000 0.247211000
H -3.097651000 0.600929000 0.939299000
H -3.056854000 0.143776000 -1.235366000
H 0.000055000 -0.480542000 2.842841000
H -0.001026000 2.006112000 3.240857000
H 0.000071000 1.254444000 -3.514900000
N 0.000295000 -0.121259000 -1.931981000
O 0.000581000 -2.595688000 0.126060000
H 0.000785000 -3.176302000 0.909482000
H 0.000812000 -3.160477000 -0.669739000

Os-N.NH$_3$.S$_0$

Energy = -450.071533 a.u.

2 1

C 0.001932000 1.016425000 2.525823000
C 0.003065000 1.708259000 0.288288000
C 0.002932000 1.762602000 -2.020147000
C 0.004433000 2.542695000 -0.828241000
H 0.006378000 3.630464000 -0.808830000
C -0.000286000 -0.214863000 1.866482000
C 0.003846000 2.098156000 1.642807000
H 0.005722000 3.139203000 1.961760000
Os -0.000663000 -0.371618000 -0.113967000
P 2.461372000 -0.288458000 -0.105638000
H 3.185835000 -1.508532000 -0.023948000
H 3.041136000 0.310145000 -1.254172000
H 3.040371000 0.454778000 0.954677000
P -2.462491000 -0.280150000 -0.105401000
H -3.190984000 -1.497834000 -0.023891000
H -3.038982000 0.464825000 0.955059000
H -3.040310000 0.320549000 -1.253821000
H -0.002003000 -1.141008000 2.454482000
H 0.002134000 1.120599000 3.607623000
H 0.003494000 2.119104000 -3.049133000
N 0.000684000 0.484165000 -1.739320000
N -0.004411000 -2.629496000 -0.032006000
H 0.810256000 -3.050943000 0.422853000
H -0.820791000 -3.048470000 0.422058000
H -0.004509000 -3.003091000 -0.988430000

Os-N.NH$_3$.T$_1$

Energy = -450.011868 a.u.

2 3

C 0.002206000 1.535533000 2.271074000
C 0.001604000 1.643547000 -0.096816000
C 0.000260000 1.129118000 -2.411165000
C 0.001602000 2.165110000 -1.406354000
H 0.002526000 3.225859000 -1.656138000
C 0.000716000 0.141678000 1.976952000
C 0.002707000 2.359092000 1.153176000
H 0.003814000 3.446542000 1.215342000
Os -0.000199000 -0.362517000 0.031071000
P 2.473141000 -0.214891000 -0.023501000
H 3.185750000 -1.426197000 0.184336000
H 3.016894000 0.245230000 -1.250248000
H 3.064592000 0.645459000 0.935898000
P -2.473456000 -0.209958000 -0.022358000
H -3.188808000 -1.419888000 0.184034000
H -3.062672000 0.650482000 0.938340000
H -3.016550000 0.253045000 -1.248312000
H 0.000113000 -0.546755000 2.829712000
H 0.002870000 1.928816000 3.284967000
H 0.000105000 1.330288000 -3.484047000
N -0.000698000 -0.086147000 -1.938737000
N -0.003702000 -2.643981000 0.103842000
H 0.807978000 -3.052585000 0.575555000
H -0.812788000 -3.050391000 0.581834000
H -0.007737000 -3.039421000 -0.841695000

Os-N.NH^{2-}.S$_0$

Energy = -449.817503 a.u.

1 1

C 0.003264000 1.216692000 2.448150000
C 0.004351000 1.730868000 0.175842000
C 0.003560000 1.589678000 -2.128615000
C 0.006014000 2.466867000 -1.004856000
H 0.008725000 3.553425000 -1.081879000
C -0.000067000 -0.073833000 1.904373000
C 0.005771000 2.234459000 1.491406000
H 0.008516000 3.294295000 1.743641000
Os -0.001023000 -0.403079000 -0.070701000

P 2.414268000 -0.380116000 -0.091802000
H 3.095006000 -1.624778000 0.023709000
H 3.026476000 0.147505000 -1.259410000
H 3.068751000 0.366477000 0.923133000
P -2.416096000 -0.369053000 -0.091348000
H -3.102361000 -1.610678000 0.024042000
H -3.067228000 0.380298000 0.923710000
H -3.026048000 0.161439000 -1.258835000
H -0.002149000 -0.925800000 2.585772000
H 0.003840000 1.403985000 3.519411000
H 0.004214000 1.905343000 -3.172284000
N 0.000446000 0.316272000 -1.817866000
H -0.830633000 -2.945504000 0.133881000
N -0.005607000 -2.355384000 0.041331000
H 0.816855000 -2.949118000 0.133596000

Os-N.NH^{2-}.T_1

Energy = -449.768633 a.u.

1 3

C 0.001967000 1.403328000 2.318964000
C 0.001859000 1.679388000 -0.021212000
C 0.000790000 1.249819000 -2.321983000
C 0.002142000 2.251612000 -1.287475000
H 0.003308000 3.319454000 -1.505269000
C 0.000381000 0.033218000 1.959338000
C 0.002783000 2.305777000 1.251718000
H 0.004012000 3.385873000 1.398237000
Os -0.000422000 -0.414151000 0.001800000
P 2.418958000 -0.240639000 -0.027437000
H 3.192521000 -1.404358000 0.226417000
H 2.991832000 0.205899000 -1.248205000
H 2.994858000 0.671465000 0.895528000
P -2.419481000 -0.235897000 -0.026684000
H -3.195047000 -1.398305000 0.227046000
H -2.993610000 0.677004000 0.896598000
H -2.991794000 0.211963000 -1.247232000
H -0.000266000 -0.687298000 2.786773000
H 0.002482000 1.738178000 3.354580000
H 0.000741000 1.497138000 -3.386192000
N -0.000366000 0.003219000 -1.926264000
H -0.003558000 -3.027328000 -0.795795000
N -0.002752000 -2.441523000 0.041346000
H -0.003266000 -3.036914000 0.870831000

Os-N.I$^-$.S_0

Energy = -405.273057 a.u.

1 1

C -1.861462000 -0.001319000 2.476985000
C -2.405545000 0.000158000 0.210526000
C -2.339543000 0.001518000 -2.094761000
C -3.177255000 0.000835000 -0.948245000
H -4.264762000 0.000946000 -0.984500000
C -0.589824000 -0.001070000 1.892051000
C -2.886765000 -0.000587000 1.535032000
H -3.945591000 -0.000679000 1.788268000
Os -0.308556000 0.000093000 -0.080980000
P -0.162488000 2.426988000 -0.113653000
H 0.612665000 3.031365000 0.906757000
H 0.431024000 2.972534000 -1.280279000
H -1.364342000 3.184232000 -0.036742000
P -0.163878000 -2.426724000 -0.115753000
H 0.612082000 -3.032249000 0.903366000
H -1.366244000 -3.183043000 -0.037774000
H 0.427711000 -2.972227000 -1.283389000
H 0.294363000 -0.001655000 2.532658000
H -2.024707000 -0.002045000 3.551439000
H -2.656125000 0.002199000 -3.136396000
N -1.068357000 0.001248000 -1.775499000
I 2.426991000 -0.000309000 0.012663000

Os-N.I$^-$.T_1

Energy = -405.224712 a.u.

1 3

C -1.956410000 -0.000894000 2.377788000
C -2.317462000 -0.000157000 0.044453000
C -1.989418000 0.000741000 -2.278969000
C -2.940033000 0.000253000 -1.197172000
H -4.018098000 0.000224000 -1.355798000
C -0.601633000 -0.000555000 1.961045000
C -2.891569000 -0.000673000 1.344114000
H -3.966912000 -0.000771000 1.519314000
Os -0.244380000 -0.000042000 -0.014995000
P -0.470252000 2.422493000 -0.044603000
H 0.671267000 3.233154000 0.183395000
H -0.963926000 2.966495000 -1.259605000
H -1.382613000 2.963292000 0.899038000
P -0.469256000 -2.422755000 -0.045779000
H 0.672679000 -3.232823000 0.182213000

H -1.381545000 -2.964478000 0.897408000
H -0.962316000 -2.966729000 -1.261052000
H 0.161865000 -0.000438000 2.745630000
H -2.253043000 -0.001230000 3.424617000
H -2.289388000 0.001073000 -3.329498000
N -0.728290000 0.000591000 -1.941327000
I 2.446316000 0.000243000 -0.001294000

Os-N.OH$^-$.S_0

Energy = -469.681929 a.u.

1 1

C -0.399646000 0.978024000 2.511738000
C -0.679145000 1.572310000 0.273817000
C -0.704087000 1.597900000 -2.028748000
C -1.014110000 2.327978000 -0.851226000
H -1.444603000 3.327783000 -0.843476000
C 0.090248000 -0.166713000 1.877503000
C -0.833216000 1.960626000 1.618990000
H -1.239354000 2.921526000 1.931589000
Os 0.143720000 -0.347545000 -0.109620000
P 2.436813000 0.467673000 -0.123153000
H 3.397154000 -0.540359000 0.147789000
H 2.917099000 1.024089000 -1.337765000
H 2.795035000 1.483107000 0.801908000
P -2.093199000 -1.280150000 -0.095090000
H -2.226439000 -2.695844000 -0.036441000
H -2.947217000 -0.895047000 0.971814000
H -2.904796000 -0.985003000 -1.222491000
H 0.474221000 -0.997224000 2.473260000
H -0.432011000 1.090586000 3.592480000
H -0.850714000 1.932014000 -3.054778000
N -0.192572000 0.415345000 -1.771451000
O 1.054593000 -2.086058000 0.011456000
H 0.535703000 -2.904740000 0.076917000

Os-N.OH$^-$.T_1

Energy = -469.624408 a.u.

1 3

C 0.004518000 1.227744000 2.421571000
C 0.004049000 1.666060000 0.101165000
C 0.001663000 1.399028000 -2.228914000
C 0.004871000 2.325644000 -1.122175000
H 0.007375000 3.407099000 -1.260490000
C 0.000796000 -0.114526000 1.969289000
C 0.006170000 2.200031000 1.417960000
H 0.008783000 3.267557000 1.637655000
Os -0.000971000 -0.411145000 -0.017818000
P 2.432731000 -0.258321000 -0.093489000
H 3.141943000 -1.487298000 -0.080747000
H 2.964800000 0.373141000 -1.247464000
H 3.073735000 0.457446000 0.950757000
P -2.434126000 -0.248662000 -0.091042000
H -3.147604000 -1.475186000 -0.080776000
H -3.072010000 0.466877000 0.955272000
H -2.964721000 0.387371000 -1.243174000
H -0.001264000 -0.891106000 2.743763000
H 0.005844000 1.492146000 3.477119000
H 0.001580000 1.728508000 -3.270917000
N -0.001302000 0.127213000 -1.932784000
O -0.005192000 -2.382272000 -0.120919000
H -0.005534000 -2.930964000 0.684561000

Os-N.Br$^-$.S_0

Energy = -407.057486 a.u.

1 1

C -1.544507000 -0.137973000 2.489421000
C -2.134026000 0.056405000 0.241823000
C -2.114949000 0.252650000 -2.054484000
C -2.930161000 0.184416000 -0.894814000
H -4.017210000 0.229661000 -0.904855000
C -0.285855000 -0.128566000 1.878786000
C -2.588213000 -0.035288000 1.572784000
H -3.641193000 -0.024535000 1.849001000
Os -0.048507000 0.005991000 -0.094389000
P 0.239121000 2.422750000 0.023646000
H 0.994860000 2.913077000 1.117133000
H 0.931299000 2.987200000 -1.077544000
H -0.915207000 3.250898000 0.082793000
P -0.082638000 -2.418836000 -0.248291000
H 1.119652000 -3.080284000 0.108710000
H -1.042065000 -3.114252000 0.535651000
H -0.339354000 -2.958322000 -1.536728000
H 0.614594000 -0.201639000 2.492160000
H -1.686610000 -0.215269000 3.564088000
H -2.448957000 0.352843000 -3.085673000
N -0.838817000 0.175651000 -1.762036000
Br 2.492214000 -0.086651000 0.009476000

Os-N.Br$^-$.T_1

Energy = -407.004438 a.u.

1 3

C	1.671873000	-0.000291000	2.395195000
C	2.057706000	-0.000055000	0.064127000
C	1.754272000	0.000221000	-2.265680000
C	2.693589000	0.000083000	-1.171323000
H	3.773348000	0.000071000	-1.319194000
C	0.321947000	-0.000227000	1.962355000
C	2.618174000	-0.000223000	1.371831000
H	3.691446000	-0.000254000	1.559498000
Os	-0.008702000	0.000001000	-0.016230000
P	0.193745000	-2.430895000	-0.059982000
H	-0.990988000	-3.195505000	0.090653000
H	0.739653000	-2.969431000	-1.254319000
H	1.034264000	-3.006734000	0.927938000
P	0.193953000	2.430887000	-0.059594000
H	-0.990798000	3.195575000	0.090505000
H	1.034021000	3.006576000	0.928798000
H	0.740505000	2.969481000	-1.253609000
H	-0.455846000	-0.000246000	2.732653000
H	1.956412000	-0.000384000	3.445293000
H	2.068908000	0.000304000	-3.312011000
N	0.489399000	0.000175000	-1.946018000
Br	-2.511033000	0.000066000	-0.003599000

Os-N.F$^-$.S_0

Energy = -493.714786 a.u.

1 1

C	-0.000023000	0.893213000	2.566237000
C	-0.000033000	1.691696000	0.370113000
C	-0.000039000	1.896053000	-1.919900000
C	-0.000047000	2.601538000	-0.693163000
H	-0.000068000	3.685570000	-0.600905000
C	0.000010000	-0.301729000	1.846934000
C	-0.000044000	2.018881000	1.740091000
H	-0.000066000	3.042101000	2.111986000
Os	0.000007000	-0.346258000	-0.144123000
P	2.430246000	-0.505214000	-0.133820000
H	2.914352000	-1.825555000	0.053859000
H	3.113907000	-0.101546000	-1.310724000
H	3.140928000	0.215154000	0.861608000
P	-2.430225000	-0.505303000	-0.133823000
H	-2.914284000	-1.825677000	0.053750000
H	-3.140926000	0.214958000	0.861670000
H	-3.113909000	-0.101560000	-1.310688000
H	0.000026000	-1.269276000	2.354933000
H	-0.000027000	0.939799000	3.651953000
H	-0.000046000	2.316664000	-2.923349000
N	-0.000011000	0.593742000	-1.728486000
F	0.000044000	-2.307930000	-0.022064000

Os-N.F$^-$.T_1

Energy = -493.651870 a.u.

1 3

C	-0.001325000	1.323061000	2.382294000
C	-0.002958000	1.666767000	0.041184000
C	-0.003287000	1.324789000	-2.287075000
C	-0.004589000	2.285536000	-1.205814000
H	-0.006502000	3.362497000	-1.375750000
C	0.000951000	-0.032910000	1.972061000
C	-0.003419000	2.252766000	1.341956000
H	-0.005275000	3.328599000	1.515687000
Os	0.000728000	-0.384411000	-0.003126000
P	2.450916000	-0.334360000	-0.077191000
H	3.042922000	-1.620483000	0.005435000
H	3.027835000	0.196026000	-1.259595000
H	3.134363000	0.382780000	0.938052000
P	-2.449652000	-0.341344000	-0.075624000
H	-3.038339000	-1.628989000	0.006944000
H	-3.134687000	0.373901000	0.939887000
H	-3.028070000	0.187785000	-1.257852000
H	0.002643000	-0.805384000	2.748483000
H	-0.001442000	1.625483000	3.427256000
H	-0.004320000	1.626992000	-3.337295000
N	-0.000984000	0.064777000	-1.952917000
F	0.003473000	-2.339101000	0.042366000

Os-N.CO.S_0

Energy = -506.798069 a.u.

2 1

C	1.143568000	-0.000733000	2.508444000
C	1.826788000	-0.000758000	0.262464000
C	1.834524000	-0.000458000	-2.049204000
C	2.639415000	-0.000937000	-0.866670000
H	3.727719000	-0.001389000	-0.872214000
C	-0.102480000	-0.000171000	1.872647000
C	2.217443000	-0.001067000	1.616348000

H	3.259788000	-0.001521000	1.933254000
Os	-0.288603000	0.000151000	-0.108664000
P	-0.184677000	-2.476861000	-0.087904000
H	-1.397063000	-3.194344000	0.076840000
H	0.350473000	-3.048801000	-1.270685000
H	0.633897000	-3.026625000	0.931026000
P	-0.182443000	2.477044000	-0.087500000
H	-1.394413000	3.195637000	0.075452000
H	0.635115000	3.026059000	0.932654000
H	0.355022000	3.048605000	-1.269417000
H	-1.010671000	0.000153000	2.487181000
H	1.261860000	-0.000855000	3.589046000
H	2.171037000	-0.000443000	-3.086265000
N	0.566665000	0.000016000	-1.746153000
C	-2.387295000	0.000840000	-0.032975000
O	-3.518823000	0.001114000	-0.035079000

Os-N. CO.T_1

Energy = -506.745154 a.u.

2 3

C	1.488624000	-0.001243000	2.366923000
C	1.773493000	-0.000172000	0.041144000
C	1.503637000	0.000871000	-2.338228000
C	2.435939000	0.000354000	-1.230317000
H	3.516473000	0.000509000	-1.376747000
C	0.102254000	-0.000876000	1.941686000
C	2.406270000	-0.000806000	1.334284000
H	3.483877000	-0.000985000	1.488639000
Os	-0.253516000	0.000011000	0.005206000
P	-0.257145000	-2.480891000	-0.040721000
H	-1.473980000	-3.110057000	0.326565000
H	0.015032000	-3.057086000	-1.308305000
H	0.684026000	-3.119727000	0.806935000
P	-0.256632000	2.481030000	-0.039078000
H	-1.474295000	3.110265000	0.325339000
H	0.682492000	3.119310000	0.811258000
H	0.018908000	3.057750000	-1.305696000
H	-0.651772000	-0.001082000	2.735624000
H	1.775717000	-0.001843000	3.416357000
H	1.804813000	0.001332000	-3.388286000
N	0.259992000	0.000889000	-1.976839000
C	-2.314115000	0.000185000	-0.029287000
O	-3.450497000	0.000327000	-0.051211000

Os-N.PF_3.S_0

Energy = -699.601674 a.u.

2 1

C	1.729227000	0.004863000	2.463521000
C	2.294299000	0.000703000	0.188580000
C	2.193125000	-0.003021000	-2.125291000
C	3.048298000	-0.001211000	-0.979410000
H	4.134988000	-0.001230000	-1.036984000
C	0.459440000	0.003564000	1.877866000
C	2.758102000	0.003096000	1.520326000
H	3.815680000	0.003605000	1.780684000
Os	0.181677000	0.000080000	-0.086784000
P	0.296151000	-2.473944000	-0.066533000
H	-0.892744000	-3.217564000	0.147975000
H	0.788349000	-3.038783000	-1.271446000
H	1.166809000	-3.013056000	0.914264000
P	0.292168000	2.474203000	-0.072325000
H	-0.893890000	3.215346000	0.165127000
H	1.180293000	3.015618000	0.891407000
H	0.759792000	3.039710000	-1.286667000
H	-0.432166000	0.004431000	2.519122000
H	1.895681000	0.006894000	3.537670000
H	2.486505000	-0.004721000	-3.175038000
N	0.939337000	-0.002298000	-1.766406000
P	-2.358533000	-0.001067000	-0.018088000
F	-3.103170000	1.226502000	-0.698150000
F	-2.987466000	0.000492000	1.443838000
F	-3.102017000	-1.231002000	-0.695137000

Os-N. PF_3.T_1

Energy = -699.547410 a.u.

2 3

C	1.982678000	-0.001168000	2.348310000
C	2.210743000	-0.000176000	0.002454000
C	1.875885000	0.000869000	-2.363168000
C	2.834183000	0.000305000	-1.282981000
H	3.910858000	0.000252000	-1.453858000
C	0.595028000	-0.000793000	1.959108000
C	2.868556000	-0.000844000	1.289612000
H	3.950614000	-0.001022000	1.410378000
Os	0.209841000	0.000091000	0.008277000
P	0.244623000	-2.483954000	-0.029280000
H	-0.970322000	-3.155345000	0.262380000
H	0.611943000	-3.051925000	-1.276482000

H 1.150204000 -3.090029000 0.878810000
P 0.244914000 2.484143000 -0.027767000
H -0.970382000 3.155296000 0.262995000
H 1.149516000 3.089880000 0.881524000
H 0.613430000 3.052760000 -1.274319000
H -0.143793000 -0.000991000 2.767720000
H 2.302878000 -0.001675000 3.387753000
H 2.147300000 0.001273000 -3.420757000
N 0.640074000 0.000836000 -1.962769000
P -2.290601000 0.000042000 -0.003401000
F -3.006769000 1.234871000 -0.711894000
F -3.027891000 -0.000656000 1.410408000
F -3.006134000 -1.234648000 -0.712859000

Os-N.iso1.S_0

Energy = -408.815829 a.u.

1 1

Os 0.239018000 -0.000083000 0.020432000
P 0.380151000 2.424898000 0.042102000
C -0.323623000 -0.000086000 -1.882535000
C -2.427317000 0.000707000 -1.393696000
H -3.486919000 0.000999000 -1.639142000
C -1.887375000 0.000618000 -0.110215000
C -2.644158000 0.000957000 1.068273000
H -3.732463000 0.001315000 1.090919000
Cl 2.622184000 -0.000852000 0.025842000
H 0.986461000 3.027010000 -1.090570000
H -0.816728000 3.180364000 0.155738000
H 1.161606000 2.974256000 1.090988000
C -0.496759000 0.000356000 1.853362000
C -1.829727000 0.000824000 2.211590000
H 0.325886000 0.000169000 2.581797000
P 0.378093000 -2.425120000 0.042428000
H 0.984930000 -3.027997000 -1.089554000
H 1.158027000 -2.975054000 1.092149000
H -0.819592000 -3.179454000 0.155055000
H -2.188825000 0.001059000 3.236699000
H 0.572729000 -0.000456000 -2.522203000
N -1.515357000 0.000238000 -2.400378000

Os-N. iso1.T_1

Energy = -408.771424 a.u.

1 3

Os 0.293014000 -0.000094000 0.008438000
P 0.074141000 2.428979000 -0.007702000
C -0.195687000 0.000955000 -1.997918000
C -2.314066000 0.000787000 -1.342311000
H -3.383450000 0.000939000 -1.551423000
C -1.759553000 0.000104000 -0.050136000
C -2.440423000 -0.000470000 1.185027000
H -3.527550000 -0.000468000 1.263417000
Cl 2.628714000 0.000361000 0.045123000
H -0.519411000 3.011400000 -1.157585000
H -0.709286000 2.988317000 1.034771000
H 1.281904000 3.165066000 0.102105000
C -0.233211000 -0.000974000 1.998094000
C -1.594486000 -0.001059000 2.309313000
H 0.498746000 -0.001394000 2.811679000
P 0.074285000 -2.429134000 -0.009488000
H 1.282225000 -3.164895000 0.100612000
H -0.709564000 -2.989243000 1.032250000
H -0.518465000 -3.011209000 -1.159967000
H -1.981317000 -0.001505000 3.326151000
H 0.554004000 0.001321000 -2.799801000
N -1.460982000 0.001277000 -2.395020000

Os-N.iso2.S_0

Energy = -408.808825 a.u.

1 1

Os -0.247063000 0.000014000 -0.072957000
P -0.360728000 2.431630000 -0.053643000
C 0.131733000 0.000272000 1.871222000
C 1.406720000 0.000274000 2.389713000
C 1.883409000 -0.000026000 0.246638000
C 2.736266000 -0.000157000 -0.883037000
H 3.819311000 -0.000241000 -0.791659000
Cl -2.627308000 -0.000044000 -0.044830000
H -1.109397000 2.998851000 1.008749000
H 0.850006000 3.169260000 0.022265000
H -0.984083000 3.032622000 -1.178436000
C 0.654127000 -0.000118000 -1.805657000
C 2.015023000 -0.000212000 -2.074857000
H -0.126803000 -0.000154000 -2.583760000
P -0.360752000 -2.431694000 -0.053304000
H -1.107742000 -2.998759000 1.010353000
H -0.985988000 -3.032720000 -1.177030000
H 0.850041000 -3.169418000 0.020723000
H 1.654385000 0.000450000 3.447118000

H 2.445548000 -0.000302000 -3.071622000
H -0.779260000 0.000375000 2.475067000
N 2.396224000 0.000064000 1.466452000

Os-N. iso2.T_1

Energy = -408.766672 a.u.

1 3

Os -0.312108000 0.000549000 -0.013587000
P -0.019285000 2.421601000 -0.013952000
C 0.099006000 -0.000401000 1.985216000
C 1.459961000 -0.002112000 2.317978000
C 1.756012000 -0.001919000 0.114038000
C 2.464858000 -0.002409000 -1.113232000
H 3.552897000 -0.003570000 -1.142945000
Cl -2.646643000 0.001392000 -0.055795000
H 0.676552000 2.965076000 1.096274000
H 0.694145000 2.969184000 -1.110805000
H -1.212824000 3.188966000 -0.020379000
C 0.272444000 0.000209000 -1.982106000
C 1.645611000 -0.001256000 -2.252131000
H -0.434978000 0.001070000 -2.817175000
P -0.024232000 -2.421107000 -0.014732000
H -1.219268000 -3.186119000 -0.021242000
H 0.688147000 -2.969871000 -1.111676000
H 0.670568000 -2.966014000 1.095434000
H 1.844465000 -0.002803000 3.335280000
H 2.057925000 -0.001546000 -3.258790000
H -0.648621000 0.000179000 2.783218000
N 2.358504000 -0.002858000 1.309374000

PMe_3.Os-N.S_0

Energy = -644.815633 a.u.

1 1

C -0.000050000 1.450268000 2.514445000
C 0.000035000 1.984885000 0.248649000
C 0.000117000 1.937387000 -2.050525000
C 0.000021000 2.768290000 -0.907250000
H 0.000010000 3.856020000 -0.934075000
C -0.000077000 0.182943000 1.917080000
C 0.000024000 2.472941000 1.572408000
H 0.000032000 3.533160000 1.819728000
Os -0.000001000 -0.094311000 -0.041060000
P 2.465843000 -0.294411000 -0.103778000
P -2.465850000 -0.294369000 -0.103833000
H -0.000161000 -0.717619000 2.536079000
H -0.000106000 1.609132000 3.589592000
H 0.000138000 2.249497000 -3.093062000
N 0.000066000 0.661836000 -1.723511000
Cl -0.000054000 -2.505639000 0.167283000
C -3.000577000 -1.259379000 -1.586365000
H -4.090408000 -1.365009000 -1.596614000
H -2.676515000 -0.745833000 -2.495947000
H -2.536638000 -2.248650000 -1.556090000
C -3.424566000 1.284951000 -0.198773000
H -4.495243000 1.069732000 -0.279191000
H -3.246615000 1.883274000 0.699118000
H -3.111418000 1.861325000 -1.073675000
C -3.193014000 -1.193540000 1.336913000
H -4.268549000 -1.332851000 1.186487000
H -2.709156000 -2.168590000 1.435046000
H -3.032138000 -0.618936000 2.253828000
C 3.424603000 1.284849000 -0.199286000
H 4.495282000 1.069542000 -0.279437000
H 3.111620000 1.860807000 -1.074521000
H 3.246531000 1.883609000 0.698288000
C 3.000534000 -1.259861000 -1.586041000
H 4.090335000 -1.365813000 -1.596097000
H 2.536298000 -2.248989000 -1.555691000
H 2.676769000 -0.746349000 -2.495750000
C 3.193051000 -1.193116000 1.337237000
H 2.709615000 -2.168379000 1.435340000
H 4.268688000 -1.331947000 1.187091000
H 3.031684000 -0.618512000 2.254063000

PMe_3.Os-N.T_1

Energy = -644.760426 a.u.

1 3

C 0.000328000 1.554027000 2.422988000
C -0.000057000 1.902943000 0.090495000
C -0.000330000 1.589499000 -2.236152000
C -0.000168000 2.534010000 -1.145128000
H -0.000161000 3.613822000 -1.297006000
C 0.000304000 0.199079000 1.992332000
C 0.000119000 2.485806000 1.391378000
H 0.000077000 3.562136000 1.562242000
Os -0.000007000 -0.148702000 0.033206000
P 2.493227000 -0.195495000 -0.077732000
P -2.493256000 -0.195577000 -0.077557000

H	0.000448000	-0.578133000	2.764633000
H	0.000505000	1.844621000	3.471642000
H	-0.000434000	1.903365000	-3.283769000
N	-0.000290000	0.326299000	-1.912961000
Cl	0.000156000	-2.534670000	0.109117000
C	-3.056863000	-1.128258000	-1.568342000
H	-4.150865000	-1.164533000	-1.598645000
H	-2.677087000	-0.641162000	-2.470042000
H	-2.655296000	-2.144178000	-1.527512000
C	-3.367416000	1.430867000	-0.167049000
H	-4.447847000	1.263886000	-0.228370000
H	-3.146798000	2.024695000	0.724166000
H	-3.040910000	1.983081000	-1.052067000
C	-3.266371000	-1.066147000	1.357756000
H	-4.346846000	-1.156621000	1.204170000
H	-2.827387000	-2.062730000	1.453943000
H	-3.079589000	-0.504806000	2.277673000
C	3.367348000	1.430980000	-0.167004000
H	4.447742000	1.264030000	-0.229007000
H	3.040332000	1.983609000	-1.051573000
H	3.147220000	2.024385000	0.724616000
C	3.056680000	-1.127953000	-1.568719000
H	4.150686000	-1.163648000	-1.599535000
H	2.655674000	-2.144084000	-1.527591000
H	2.676215000	-0.641165000	-2.470297000
C	3.266485000	-1.066339000	1.357336000
H	2.827310000	-2.062836000	1.453541000
H	4.346901000	-1.157043000	1.203474000
H	3.080070000	-0.505029000	2.277346000
H	-0.000037000	1.677938000	3.579269000
H	0.000044000	2.268582000	-3.110038000
N	0.000002000	0.653256000	-1.743048000
Cl	-0.000009000	-2.594922000	0.142982000
C	-3.084525000	-1.189263000	-1.582722000
H	-4.176629000	-1.279681000	-1.565307000
H	-2.774459000	-0.648577000	-2.481874000
H	-2.631007000	-2.184405000	-1.603822000
C	-3.440783000	1.287866000	-0.101675000
H	-4.515495000	1.082913000	-0.167761000
H	-3.231470000	1.850941000	0.812574000
H	-3.132896000	1.897411000	-0.956321000
C	-3.208688000	-1.236535000	1.318665000
H	-4.288242000	-1.359040000	1.175784000
H	-2.727563000	-2.216880000	1.373983000
H	-3.024142000	-0.701825000	2.255264000
C	3.440785000	1.287851000	-0.101652000
H	4.515497000	1.082896000	-0.167740000
H	3.132899000	1.897401000	-0.956295000
H	3.231475000	1.850923000	0.812600000
C	3.084528000	-1.189276000	-1.582703000
H	4.176632000	-1.279700000	-1.565281000
H	2.631004000	-2.184417000	-1.603806000
H	2.774470000	-0.648588000	-2.481856000
C	3.208674000	-1.236550000	1.318685000
H	2.727543000	-2.216892000	1.374002000
H	4.288228000	-1.359061000	1.175810000
H	3.024126000	-0.701839000	2.255284000
Re	-0.000001000	-0.097969000	-0.054023000

PMe_3.Re-N.S_0

Energy = -633.072986 a.u.

0 1

C	-0.000033000	1.492483000	2.505526000
C	0.000006000	1.992071000	0.233174000
C	0.000044000	1.949597000	-2.067821000
C	0.000066000	2.777565000	-0.939756000
H	0.000085000	3.867316000	-0.972680000
C	-0.000012000	0.209795000	1.928466000
C	-0.000031000	2.504955000	1.547807000
H	-0.000027000	3.569571000	1.785004000
P	2.457147000	-0.287025000	-0.086117000
P	-2.457149000	-0.287013000	-0.086134000
H	0.000000000	-0.669241000	2.583360000

PMe_3.Re-N.T_1

Energy = -633.018292 a.u.

0 3

C	0.000004000	1.429925000	2.488902000
C	-0.000006000	1.948167000	0.172825000
C	-0.000001000	1.802076000	-2.160056000
C	-0.000046000	2.678456000	-1.039546000
H	-0.000078000	3.765784000	-1.119077000
C	0.000002000	0.155196000	1.995087000
C	-0.000008000	2.451908000	1.477332000
H	-0.000026000	3.517427000	1.711809000
P	2.484674000	-0.201917000	-0.030983000
P	-2.484670000	-0.201931000	-0.030980000
H	-0.000013000	-0.712225000	2.662033000

H	-0.000004000	1.671838000	3.552716000
H	-0.000019000	2.119231000	-3.205250000
N	-0.000005000	0.531011000	-1.840306000
Cl	0.000011000	-2.610166000	0.023291000
C	-3.220720000	-0.963068000	-1.555601000
H	-4.315699000	-0.964559000	-1.509492000
H	-2.886813000	-0.398349000	-2.430674000
H	-2.855706000	-1.990116000	-1.649058000
C	-3.334873000	1.439950000	0.090441000
H	-4.423318000	1.313182000	0.087685000
H	-3.020784000	1.935412000	1.013184000
H	-3.032183000	2.065603000	-0.753623000
C	-3.249161000	-1.183852000	1.344437000
H	-4.340772000	-1.206759000	1.251018000
H	-2.855077000	-2.203636000	1.313620000
H	-2.972731000	-0.732585000	2.301681000
C	3.334878000	1.439963000	0.090451000
H	4.423322000	1.313195000	0.087697000
H	3.032190000	2.065622000	-0.753610000
H	3.020786000	1.935420000	1.013196000
C	3.220724000	-0.963039000	-1.555611000
H	4.315704000	-0.964525000	-1.509505000
H	2.855716000	-1.990089000	-1.649073000
H	2.886812000	-0.398317000	-2.430679000
C	3.249170000	-1.183846000	1.344425000
H	2.855085000	-2.203630000	1.313603000
H	4.340780000	-1.206753000	1.251002000
H	2.972744000	-0.732585000	2.301673000
Re	0.000001000	-0.181282000	-0.074584000

H	-3.192831000	-2.258295000	0.000000000
H	-0.331900000	3.814074000	0.000000000
N	0.335691000	1.838440000	0.000000000
Cl	2.050456000	-1.475065000	0.000000000
C	1.934997000	0.675257000	-2.981215000
H	2.041483000	0.631833000	-4.070408000
H	1.986259000	1.716965000	-2.652118000
H	2.747286000	0.116614000	-2.509351000
C	-0.948219000	0.865195000	-3.448844000
H	-0.706703000	0.816940000	-4.516053000
H	-1.938757000	0.429941000	-3.288671000
H	-0.970047000	1.913702000	-3.138658000
C	0.319487000	-1.757363000	-3.204675000
H	0.536672000	-1.700883000	-4.276555000
H	1.082589000	-2.362705000	-2.708876000
H	-0.658920000	-2.226713000	-3.064489000
C	-0.948219000	0.865195000	3.448844000
H	-0.706703000	0.816940000	4.516053000
H	-0.970047000	1.913702000	3.138658000
H	-1.938757000	0.429941000	3.288671000
C	1.934997000	0.675257000	2.981215000
H	2.041483000	0.631833000	4.070408000
H	2.747286000	0.116614000	2.509351000
H	1.986259000	1.716965000	2.652118000
C	0.319487000	-1.757363000	3.204675000
H	1.082589000	-2.362705000	2.708876000
H	0.536672000	-1.700883000	4.276555000
H	-0.658920000	-2.226713000	3.064489000
Ru	0.121995000	-0.011838000	0.000000000

PMe_3.Ru-N.S_0

Energy = -647.595797 a.u.

1 1

C	-2.511907000	-1.410630000	0.000000000
C	-1.818654000	0.812699000	0.000000000
C	-0.592599000	2.755543000	0.000000000
C	-1.900604000	2.197127000	0.000000000
H	-2.821434000	2.778715000	0.000000000
C	-1.121010000	-1.533274000	0.000000000
C	-2.912065000	-0.079275000	0.000000000
H	-3.951146000	0.248753000	0.000000000
P	0.319487000	-0.062189000	2.466808000
P	0.319487000	-0.062189000	-2.466808000
H	-0.636540000	-2.511255000	0.000000000

PMe_3.Ru-N.T_1

Energy = -647.551316 a.u.

1 3

C	0.000053000	1.409759000	2.472578000
C	0.000006000	1.842673000	0.154014000
C	-0.000074000	1.626778000	-2.189100000
C	0.000002000	2.520243000	-1.047661000
H	0.000012000	3.606547000	-1.153573000
C	0.000002000	0.080431000	1.984790000
C	0.000031000	2.377041000	1.474805000
H	0.000055000	3.447737000	1.683138000
P	2.490079000	-0.177834000	-0.078749000
P	-2.490082000	-0.177830000	-0.078728000
H	0.000040000	-0.744647000	2.704581000

H	0.000091000	1.658043000	3.532504000
H	-0.000035000	1.997184000	-3.219887000
N	-0.000014000	0.357545000	-1.935887000
Cl	0.000001000	-2.592177000	0.073613000
C	-3.055787000	-1.096746000	-1.579087000
H	-4.150240000	-1.123316000	-1.614026000
H	-2.668945000	-0.608174000	-2.476933000
H	-2.662229000	-2.115881000	-1.542325000
C	-3.363429000	1.450860000	-0.161119000
H	-4.443584000	1.284016000	-0.231329000
H	-3.151418000	2.038659000	0.736246000
H	-3.032773000	2.011372000	-1.039383000
C	-3.285015000	-1.054957000	1.343132000
H	-4.365651000	-1.131138000	1.181247000
H	-2.858060000	-2.057527000	1.430879000
H	-3.099975000	-0.507016000	2.271594000
C	3.363425000	1.450855000	-0.161152000
H	4.443580000	1.284011000	-0.231371000
H	3.032763000	2.011366000	-1.039414000
H	3.151423000	2.038656000	0.736214000
C	3.055773000	-1.096757000	-1.579109000
H	4.150226000	-1.123329000	-1.614055000
H	2.662213000	-2.115891000	-1.542341000
H	2.668927000	-0.608188000	-2.476955000
C	3.285021000	-1.054957000	1.343108000
H	2.858065000	-2.057526000	1.430862000
H	4.365655000	-1.131138000	1.181217000
H	3.099986000	-0.507012000	2.271569000
Ru	-0.000001000	-0.213159000	0.030734000

H	0.000031000	1.540327000	3.611098000
H	0.000009000	2.267952000	-3.079911000
N	-0.000006000	0.687626000	-1.727807000
Cl	-0.000012000	-2.440784000	0.172201000
C	-2.953828000	-1.299777000	-1.599562000
H	-4.043398000	-1.408426000	-1.636333000
H	-2.612601000	-0.800605000	-2.510642000
H	-2.493898000	-2.288850000	-1.535795000
C	-3.431370000	1.284644000	-0.253529000
H	-4.500994000	1.061946000	-0.335561000
H	-3.270700000	1.903887000	0.633123000
H	-3.124204000	1.837531000	-1.145339000
C	-3.194725000	-1.180175000	1.347970000
H	-4.268403000	-1.332672000	1.192596000
H	-2.709690000	-2.152280000	1.465433000
H	-3.053447000	-0.584362000	2.254451000
C	3.431374000	1.284625000	-0.253523000
H	4.500995000	1.061921000	-0.335568000
H	3.124200000	1.837523000	-1.145323000
H	3.270715000	1.903859000	0.633138000
C	2.953817000	-1.299790000	-1.599565000
H	4.043387000	-1.408455000	-1.636329000
H	2.493872000	-2.288856000	-1.535806000
H	2.612604000	-0.800607000	-2.510644000
C	3.194715000	-1.180198000	1.347969000
H	2.709675000	-2.152300000	1.465431000
H	4.268393000	-1.332701000	1.192595000
H	3.053442000	-0.584386000	2.254451000
Ir	-0.000001000	-0.089790000	-0.034253000

PMe_3.Ir-N.S_0

Energy = -658.058097 a.u.

2 1

C	0.000009000	1.401534000	2.533178000
C	0.000010000	1.985620000	0.267706000
C	0.000008000	1.946107000	-2.038017000
C	0.000053000	2.774614000	-0.868908000
H	0.000072000	3.862825000	-0.886464000
C	-0.000006000	0.146975000	1.929264000
C	-0.000005000	2.439168000	1.605904000
H	0.000017000	3.495774000	1.870427000
P	2.502040000	-0.303190000	-0.116923000
P	-2.502044000	-0.303174000	-0.116924000
H	0.000021000	-0.769936000	2.520081000

PMe_3.Ir-N.T_1

Energy = -658.021234 a.u.

2 3

C	-0.000067000	1.439075000	2.449103000
C	0.000008000	1.847836000	0.122843000
C	0.000056000	1.627191000	-2.220159000
C	0.000073000	2.526839000	-1.084069000
H	0.000092000	3.610482000	-1.194514000
C	-0.000013000	0.104912000	1.978136000
C	-0.000055000	2.397990000	1.441774000
H	-0.000057000	3.470047000	1.635123000
P	2.509038000	-0.155940000	-0.077486000
P	-2.509039000	-0.155935000	-0.077515000
H	-0.000026000	-0.717815000	2.699123000

H	-0.000094000	1.690109000	3.507194000
H	0.000075000	1.965313000	-3.259610000
N	0.000014000	0.365843000	-1.929442000
Cl	-0.000002000	-2.530605000	0.038579000
C	-3.040184000	-1.082520000	-1.578462000
H	-4.135785000	-1.088370000	-1.613996000
H	-2.650242000	-0.604696000	-2.480285000
H	-2.670802000	-2.109798000	-1.529403000
C	-3.311966000	1.497588000	-0.152985000
H	-4.396590000	1.345807000	-0.204581000
H	-3.083861000	2.083199000	0.741338000
H	-2.995565000	2.045963000	-1.043583000
C	-3.233984000	-1.023067000	1.379072000
H	-4.319818000	-1.084978000	1.241591000
H	-2.822485000	-2.032521000	1.456485000
H	-3.025605000	-0.470096000	2.299036000
C	3.311966000	1.497583000	-0.152946000
H	4.396590000	1.345803000	-0.204533000
H	2.995571000	2.045959000	-1.043545000
H	3.083853000	2.083192000	0.741376000
C	3.040197000	-1.082523000	-1.578430000
H	4.135799000	-1.088374000	-1.613952000
H	2.670813000	-2.109800000	-1.529376000
H	2.650265000	-0.604696000	-2.480256000
C	3.233967000	-1.023076000	1.379107000
H	2.822466000	-2.032530000	1.456515000
H	4.319802000	-1.084988000	1.241638000
H	3.025579000	-0.470106000	2.299071000
Ir	0.000000000	-0.174241000	0.028007000

PPh_3.Os-N.S_0

Energy = -1795.211440 a.u.

1 1

C	0.000163000	-1.515741000	-2.641773000
C	0.000029000	-2.164968000	-0.408753000
C	0.000019000	-2.231783000	1.887534000
C	0.000015000	-3.004406000	0.705012000
H	0.000021000	-4.091789000	0.675945000
C	0.000083000	-0.281104000	-1.983780000
C	0.000114000	-2.585128000	-1.752030000
H	0.000137000	-3.631174000	-2.052850000
Os	-0.000007000	-0.102445000	-0.013462000
P	2.519929000	0.082010000	0.012081000
P	-2.519874000	0.082008000	0.012031000
H	0.000042000	0.653491000	-2.547594000
H	0.000245000	-1.623586000	-3.723647000
H	0.000032000	-2.592861000	2.914287000
N	-0.000010000	-0.942398000	1.624026000
Cl	-0.000059000	2.308004000	-0.061965000
C	-3.156146000	1.366432000	-1.163456000
C	-3.853432000	2.486612000	-0.687267000
C	-2.924923000	1.246267000	-2.544962000
C	-4.315194000	3.461513000	-1.576642000
H	-4.035378000	2.610926000	0.374252000
C	-3.392824000	2.218184000	-3.430456000
H	-2.385889000	0.391275000	-2.941055000
C	-4.088886000	3.330649000	-2.947653000
H	-4.849925000	4.324942000	-1.190836000
H	-3.212324000	2.106271000	-4.496247000
H	-4.448995000	4.089748000	-3.636381000
C	-3.178453000	0.575868000	1.672741000
C	-4.501126000	0.255697000	2.027440000
C	-2.393637000	1.327336000	2.561006000
C	-5.022232000	0.672716000	3.253932000
H	-5.128190000	-0.317846000	1.352252000
C	-2.920762000	1.743708000	3.786550000
H	-1.380402000	1.604981000	2.295798000
C	-4.232704000	1.415539000	4.137043000
H	-6.045302000	0.417588000	3.516208000
H	-2.304072000	2.327261000	4.464584000
H	-4.639565000	1.738740000	5.091307000
C	-3.446439000	-1.482186000	-0.370807000
C	-4.198239000	-1.657711000	-1.541558000
C	-3.394491000	-2.530329000	0.566364000
C	-4.869520000	-2.862955000	-1.777839000
H	-4.288370000	-0.856579000	-2.265976000
C	-4.070261000	-3.727647000	0.331281000
H	-2.848638000	-2.404011000	1.495895000
C	-4.805486000	-3.900527000	-0.846719000
H	-5.452811000	-2.979377000	-2.687164000
H	-4.031522000	-4.521610000	1.072453000
H	-5.334819000	-4.831808000	-1.028283000
C	3.156358000	1.366931000	-1.162771000
C	2.924940000	1.247644000	-2.544322000
C	3.854040000	2.486631000	-0.686028000
C	3.393004000	2.219945000	-3.429302000
H	2.385639000	0.393037000	-2.940877000
C	4.315972000	3.461924000	-1.574888000

H	4.036186000	2.610271000	0.375535000
C	4.089441000	3.331935000	-2.945942000
H	3.212333000	2.108709000	-4.495134000
H	4.851015000	4.324962000	-1.188639000
H	4.449659000	4.091338000	-3.634278000
C	3.178307000	0.575154000	1.673094000
C	4.500559000	0.253950000	2.028393000
C	2.393675000	1.327252000	2.561004000
C	5.021418000	0.670527000	3.255150000
H	5.127501000	-0.320048000	1.353486000
C	2.920557000	1.743194000	3.786790000
H	1.380796000	1.605745000	2.295299000
C	4.232074000	1.413961000	4.137901000
H	6.044165000	0.414589000	3.517897000
H	2.304026000	2.327252000	4.464533000
H	4.638745000	1.736827000	5.092360000
C	3.446419000	-1.482060000	-0.371440000
C	4.198084000	-1.657046000	-1.542364000
C	3.394547000	-2.530635000	0.565242000
C	4.869341000	-2.862171000	-1.779282000
H	4.288019000	-0.855573000	-2.266425000
C	4.070305000	-3.727841000	0.329530000
H	2.848765000	-2.404760000	1.494875000
C	4.805417000	-3.900164000	-0.848619000
H	5.452520000	-2.978189000	-2.688730000
H	4.031640000	-4.522159000	1.070326000
H	5.334734000	-4.831361000	-1.030664000

PPh_3.Os-N.T_1

Energy = -1795.160193 a.u.

1 3

C	-0.001300000	-2.565515000	-1.306532000
C	0.001152000	-1.717390000	0.892445000
C	0.000639000	-0.301317000	2.758979000
C	0.001765000	-1.654181000	2.281418000
H	0.002276000	-2.519382000	2.945187000
C	-0.002611000	-1.182630000	-1.609160000
C	0.000739000	-2.863331000	0.052640000
H	0.001230000	-3.883339000	0.434270000
Os	0.000098000	0.096010000	-0.060555000
P	2.548018000	0.052476000	-0.015044000
P	-2.547139000	0.054239000	-0.014285000
H	-0.007312000	-0.919411000	-2.672719000
H	-0.002520000	-3.341133000	-2.069473000
H	0.000325000	-0.045635000	3.821323000
N	-0.000206000	0.628957000	1.842468000
Cl	0.005179000	2.236473000	-1.107301000
C	-3.321935000	0.902852000	-1.472532000
C	-4.572907000	1.524450000	-1.321791000
C	-2.715513000	0.885222000	-2.736929000
C	-5.204347000	2.110982000	-2.421075000
H	-5.057854000	1.560334000	-0.352037000
C	-3.351680000	1.470352000	-3.834139000
H	-1.740544000	0.434063000	-2.871793000
C	-4.597089000	2.084429000	-3.679145000
H	-6.169318000	2.592374000	-2.288865000
H	-2.866946000	1.454527000	-4.806405000
H	-5.087700000	2.545741000	-4.531714000
C	-3.252541000	0.941617000	1.448123000
C	-4.377884000	0.468752000	2.142211000
C	-2.694787000	2.182684000	1.801652000
C	-4.926899000	1.220691000	3.185684000
H	-4.838549000	-0.475544000	1.872502000
C	-3.253997000	2.932275000	2.837577000
H	-1.829917000	2.566915000	1.271232000
C	-4.366745000	2.451557000	3.535335000
H	-5.796811000	0.843799000	3.716593000
H	-2.817249000	3.891872000	3.099962000
H	-4.796948000	3.035724000	4.344241000
C	-3.298902000	-1.640377000	-0.018380000
C	-3.893826000	-2.153697000	-1.181455000
C	-3.255224000	-2.443089000	1.135235000
C	-4.433450000	-3.443827000	-1.189472000
H	-3.951875000	-1.550511000	-2.081309000
C	-3.804083000	-3.726787000	1.126479000
H	-2.808616000	-2.064584000	2.049089000
C	-4.391341000	-4.232570000	-0.037889000
H	-4.895053000	-3.824411000	-2.096443000
H	-3.778227000	-4.328278000	2.031307000
H	-4.820227000	-5.230817000	-0.043302000
C	3.318327000	0.905971000	-1.472690000
C	2.725517000	0.856983000	-2.742892000
C	4.550061000	1.563288000	-1.317176000
C	3.356044000	1.446521000	-3.840710000
H	1.765889000	0.374916000	-2.881940000
C	5.175801000	2.154809000	-2.417293000
H	5.024562000	1.622987000	-0.343552000
C	4.582285000	2.097152000	-3.680674000

H	2.882203000	1.405281000	-4.817597000
H	6.125795000	2.664147000	-2.281389000
H	5.068478000	2.562137000	-4.533772000
C	3.256077000	0.934603000	1.449052000
C	4.387217000	0.461800000	2.133884000
C	2.695735000	2.171374000	1.813326000
C	4.939078000	1.209172000	3.179063000
H	4.850075000	-0.478862000	1.855408000
C	3.257815000	2.916539000	2.850973000
H	1.826682000	2.555763000	1.290025000
C	4.376107000	2.435653000	3.539619000
H	5.813366000	0.832318000	3.702750000
H	2.818913000	3.872815000	3.121766000
H	4.808491000	3.016316000	4.349886000
C	3.299305000	-1.642344000	-0.024988000
C	3.891884000	-2.153209000	-1.190273000
C	3.257808000	-2.447465000	1.127048000
C	4.431474000	-3.443337000	-1.202062000
H	3.948104000	-1.548012000	-2.088898000
C	3.806516000	-3.731174000	1.114475000
H	2.813298000	-2.070684000	2.042654000
C	4.391485000	-4.234544000	-0.052112000
H	4.891419000	-3.821948000	-2.110702000
H	3.782401000	-4.334579000	2.018075000
H	4.820292000	-5.232804000	-0.060441000

PPh_3.Re-N.S_0

Energy = -1783.458862 a.u.

0 1

C	0.000006000	1.601138000	-2.620148000
C	0.000026000	2.230752000	-0.381851000
C	0.000040000	2.315415000	1.917706000
C	0.000057000	3.079594000	0.745093000
H	0.000080000	4.169441000	0.717458000
C	0.000002000	0.354360000	-1.972830000
C	0.000021000	2.666505000	-1.721241000
H	0.000033000	3.714817000	-2.020804000
P	-2.506675000	-0.063170000	0.006689000
P	2.506676000	-0.063176000	0.006673000
H	-0.000001000	-0.562887000	-2.571461000
H	0.000003000	1.727627000	-3.702547000
H	0.000045000	2.687963000	2.941851000
N	0.000010000	1.004660000	1.662490000
Cl	0.000007000	-2.334461000	0.104110000
C	3.129630000	-1.433481000	-1.093396000
C	3.805215000	-2.546231000	-0.573658000
C	2.893421000	-1.373394000	-2.477125000
C	4.236509000	-3.574213000	-1.418202000
H	3.990677000	-2.624575000	0.491916000
C	3.331058000	-2.396217000	-3.320358000
H	2.366170000	-0.524878000	-2.901766000
C	4.003531000	-3.502807000	-2.792672000
H	4.751403000	-4.432857000	-0.994654000
H	3.140827000	-2.329624000	-4.388818000
H	4.337833000	-4.303409000	-3.447697000
C	3.241953000	-0.478737000	1.670299000
C	4.557932000	-0.116359000	2.002077000
C	2.481212000	-1.203968000	2.600480000
C	5.099853000	-0.467309000	3.241374000
H	5.164461000	0.443700000	1.297227000
C	3.027491000	-1.557851000	3.837576000
H	1.468521000	-1.502476000	2.354553000
C	4.335325000	-1.188669000	4.163097000
H	6.118838000	-0.175782000	3.483856000
H	2.426015000	-2.121199000	4.546576000
H	4.756415000	-1.460481000	5.127959000
C	3.535830000	1.410141000	-0.502736000
C	4.479425000	1.377154000	-1.539473000
C	3.373495000	2.602897000	0.222728000
C	5.233119000	2.514612000	-1.852832000
H	4.641934000	0.466449000	-2.105108000
C	4.131899000	3.733268000	-0.083770000
H	2.653657000	2.649207000	1.032522000
C	5.062680000	3.694904000	-1.127551000
H	5.957857000	2.469052000	-2.662059000
H	3.993135000	4.645049000	0.492059000
H	5.651126000	4.576528000	-1.369241000
C	-3.129639000	-1.433540000	-1.093292000
C	-2.893431000	-1.373534000	-2.477024000
C	-3.805253000	-2.546243000	-0.573492000
C	-3.331088000	-2.396396000	-3.320199000
H	-2.366169000	-0.525049000	-2.901714000
C	-4.236568000	-3.574265000	-1.417978000
H	-3.990722000	-2.624520000	0.492086000
C	-4.003585000	-3.502942000	-2.792452000
H	-3.140855000	-2.329868000	-4.388664000
H	-4.751484000	-4.432871000	-0.994382000
H	-4.337902000	-4.303575000	-3.447431000

C	-3.241928000	-0.478640000	1.670348000
C	-4.557850000	-0.116120000	2.002193000
C	-2.481217000	-1.203952000	2.600493000
C	-5.099744000	-0.467007000	3.241520000
H	-5.164356000	0.444001000	1.297373000
C	-3.027471000	-1.557774000	3.837616000
H	-1.468572000	-1.502573000	2.354512000
C	-4.335249000	-1.188448000	4.163205000
H	-6.118685000	-0.175367000	3.484054000
H	-2.426020000	-2.121188000	4.546586000
H	-4.756318000	-1.460213000	5.128090000
C	-3.535848000	1.410099000	-0.502819000
C	-4.479444000	1.377011000	-1.539552000
C	-3.373554000	2.602907000	0.222567000
C	-5.233173000	2.514424000	-1.852988000
H	-4.641920000	0.466264000	-2.105128000
C	-4.131996000	3.733233000	-0.084007000
H	-2.653721000	2.649294000	1.032361000
C	-5.062773000	3.694770000	-1.127786000
H	-5.957908000	2.468786000	-2.662214000
H	-3.993263000	4.645056000	0.491763000
H	-5.651248000	4.576358000	-1.369536000
Re	0.000005000	0.158022000	0.024521000

PPh_3.Re-N.T_1

Energy = -1783.408454 a.u.

0 3

C	-0.153977000	1.854004000	-2.345222000
C	-0.161669000	2.113562000	0.001454000
C	0.036757000	1.730217000	2.295292000
C	-0.157237000	2.702289000	1.277113000
H	-0.222645000	3.773301000	1.474269000
C	0.054581000	0.528094000	-1.995987000
C	-0.272420000	2.743542000	-1.247498000
H	-0.395813000	3.820485000	-1.372095000
P	-2.528823000	-0.085195000	0.006983000
P	2.551950000	-0.060238000	-0.010930000
H	0.382560000	-0.167450000	-2.776872000
H	-0.169430000	2.210344000	-3.376483000
H	0.088566000	1.969665000	3.361299000
N	0.182702000	0.494179000	1.875220000
Cl	-0.014425000	-2.438959000	-0.076650000
C	3.333596000	-0.531309000	-1.635422000
C	4.431774000	0.149247000	-2.181095000
C	2.815557000	-1.646895000	-2.316065000
C	4.997001000	-0.271770000	-3.390058000
H	4.853367000	1.008609000	-1.670103000
C	3.387483000	-2.069080000	-3.517697000
H	1.968951000	-2.187951000	-1.903025000
C	4.477524000	-1.380849000	-4.061001000
H	5.845828000	0.269019000	-3.801340000
H	2.977459000	-2.935721000	-4.030254000
H	4.918313000	-1.708021000	-4.999414000
C	3.292809000	-1.293770000	1.171481000
C	4.519832000	-1.915921000	0.889777000
C	2.635081000	-1.587125000	2.376220000
C	5.082820000	-2.813437000	1.800938000
H	5.039342000	-1.709127000	-0.040610000
C	3.204860000	-2.482860000	3.285528000
H	1.682701000	-1.114283000	2.596139000
C	4.426838000	-3.098640000	3.001808000
H	6.031301000	-3.290916000	1.567689000
H	2.684413000	-2.704684000	4.213976000
H	4.863015000	-3.800453000	3.708504000
C	3.375716000	1.542272000	0.446841000
C	3.171776000	2.670406000	-0.365735000
C	4.173306000	1.664690000	1.593457000
C	3.769153000	3.890203000	-0.045433000
H	2.540307000	2.599204000	-1.245690000
C	4.761260000	2.892107000	1.918686000
H	4.340167000	0.807581000	2.237321000
C	4.564908000	4.005567000	1.099504000
H	3.605207000	4.752528000	-0.686944000
H	5.374174000	2.971589000	2.813055000
H	5.025314000	4.957743000	1.351187000
C	-3.241295000	-1.442016000	-1.057729000
C	-2.678119000	-1.698703000	-2.317286000
C	-4.349312000	-2.196162000	-0.643870000
C	-3.221240000	-2.678608000	-3.150979000
H	-1.808733000	-1.137164000	-2.642268000
C	-4.886967000	-3.182229000	-1.476767000
H	-4.795606000	-2.026687000	0.330266000
C	-4.327126000	-3.424560000	-2.733248000
H	-2.770676000	-2.865362000	-4.122615000
H	-5.741909000	-3.761718000	-1.137362000
H	-4.744046000	-4.193477000	-3.378911000
C	-3.262126000	-0.435668000	1.683504000
C	-4.519469000	0.054465000	2.072666000

C	-2.555831000	-1.272910000	2.562281000
C	-5.055785000	-0.278531000	3.320074000
H	-5.085501000	0.698943000	1.407647000
C	-3.098953000	-1.611053000	3.804357000
H	-1.583092000	-1.660038000	2.279407000
C	-4.347033000	-1.112828000	4.188803000
H	-6.028151000	0.113563000	3.607938000
H	-2.540107000	-2.260801000	4.473035000
H	-4.764186000	-1.371870000	5.158835000
C	-3.453288000	1.426969000	-0.569988000
C	-4.115619000	1.457332000	-1.805210000
C	-3.471486000	2.577273000	0.236814000
C	-4.782259000	2.613617000	-2.225619000
H	-4.120599000	0.582009000	-2.445672000
C	-4.146759000	3.725508000	-0.178489000
H	-2.954173000	2.580092000	1.190923000
C	-4.802685000	3.749078000	-1.414031000
H	-5.288439000	2.618818000	-3.187728000
H	-4.155018000	4.603836000	0.462312000
H	-5.325484000	4.645254000	-1.738845000
Re	0.029069000	0.001394000	0.005935000

PPh_3.Ru-N.S_0

Energy = -1797.993951 a.u.

1 1

C	-1.347308000	-2.721545000	0.000000000
C	-2.136493000	-0.533277000	0.000000000
C	-2.330367000	1.752362000	0.000000000
C	-3.036821000	0.519010000	0.000000000
H	-4.121458000	0.425448000	0.000000000
C	-0.164554000	-1.983867000	0.000000000
C	-2.470249000	-1.900159000	0.000000000
H	-3.496931000	-2.264404000	0.000000000
P	0.073716000	0.013307000	2.530265000
P	0.073716000	0.013307000	-2.530265000
H	0.815380000	-2.461597000	0.000000000
H	-1.382856000	-3.808687000	0.000000000
H	-2.758568000	2.754981000	0.000000000
N	-1.037778000	1.579574000	0.000000000
Cl	2.319861000	-0.010404000	0.000000000
C	1.332327000	-1.180089000	-3.183639000
C	2.467199000	-0.717667000	-3.866491000
C	1.186556000	-2.561827000	-2.966790000
C	3.427910000	-1.620086000	-4.332271000
H	2.613719000	0.343479000	-4.033316000
C	2.144719000	-3.460488000	-3.438461000
H	0.322152000	-2.948317000	-2.435561000
C	3.269875000	-2.991036000	-4.122978000
H	4.302388000	-1.244469000	-4.856207000
H	2.012323000	-4.525921000	-3.269882000
H	4.018261000	-3.689749000	-4.486228000
C	0.591193000	1.671608000	-3.177145000
C	0.302014000	2.028119000	-4.506956000
C	1.321305000	2.559413000	-2.372495000
C	0.730558000	3.255408000	-5.015944000
H	-0.255434000	1.353004000	-5.148698000
C	1.748389000	3.786666000	-2.887657000
H	1.576423000	2.289472000	-1.354680000
C	1.452385000	4.138526000	-4.206631000
H	0.501093000	3.518712000	-6.044856000
H	2.315856000	4.464504000	-2.255903000
H	1.784448000	5.093669000	-4.604254000
C	-1.505632000	-0.324737000	-3.450723000
C	-1.735406000	-1.505137000	-4.172614000
C	-2.518125000	0.652004000	-3.409148000
C	-2.956531000	-1.710907000	-4.825033000
H	-0.962625000	-2.260502000	-4.256657000
C	-3.732061000	0.446539000	-4.065090000
H	-2.348904000	1.590373000	-2.889986000
C	-3.958307000	-0.740605000	-4.770528000
H	-3.113210000	-2.627357000	-5.387474000
H	-4.496536000	1.218604000	-4.036103000
H	-4.901872000	-0.898744000	-5.285414000
C	1.332327000	-1.180089000	3.183639000
C	1.186556000	-2.561827000	2.966790000
C	2.467199000	-0.717667000	3.866491000
C	2.144719000	-3.460488000	3.438461000
H	0.322152000	-2.948317000	2.435561000
C	3.427910000	-1.620086000	4.332271000
H	2.613719000	0.343479000	4.033316000
C	3.269875000	-2.991036000	4.122978000
H	2.012323000	-4.525921000	3.269882000
H	4.302388000	-1.244469000	4.856207000
H	4.018261000	-3.689749000	4.486228000
C	0.591193000	1.671608000	3.177145000
C	0.302014000	2.028119000	4.506956000
C	1.321305000	2.559413000	2.372495000
C	0.730558000	3.255408000	5.015944000

H	-0.255434000	1.353004000	5.148698000
C	1.748389000	3.786666000	2.887657000
H	1.576423000	2.289472000	1.354680000
C	1.452385000	4.138526000	4.206631000
H	0.501093000	3.518712000	6.044856000
H	2.315856000	4.464504000	2.255903000
H	1.784448000	5.093669000	4.604254000
C	-1.505632000	-0.324737000	3.450723000
C	-1.735406000	-1.505137000	4.172614000
C	-2.518125000	0.652004000	3.409148000
C	-2.956531000	-1.710907000	4.825033000
H	-0.962625000	-2.260502000	4.256657000
C	-3.732061000	0.446539000	4.065090000
H	-2.348904000	1.590373000	2.889986000
C	-3.958307000	-0.740605000	4.770528000
H	-3.113210000	-2.627357000	5.387474000
H	-4.496536000	1.218604000	4.036103000
H	-4.901872000	-0.898744000	5.285414000
Ru	-0.092774000	-0.017777000	0.000000000

PPh_3.Ru-N.T_1

Energy = -1797.952746 a.u.

1 3

C	-0.000112000	2.556615000	1.220333000
C	0.000049000	1.613437000	-0.940093000
C	-0.000126000	0.124690000	-2.757387000
C	-0.000010000	1.498494000	-2.316538000
H	-0.000017000	2.340082000	-3.011416000
C	-0.000285000	1.190146000	1.571127000
C	0.000053000	2.794056000	-0.149596000
H	0.000086000	3.796290000	-0.577692000
P	2.552664000	-0.049648000	0.022463000
P	-2.552636000	-0.049765000	0.022442000
H	-0.000750000	0.947353000	2.638710000
H	-0.000191000	3.362243000	1.952061000
H	-0.000233000	-0.157701000	-3.814635000
N	-0.000095000	-0.772641000	-1.824050000
Cl	0.000732000	-2.241211000	1.247968000
C	-3.365255000	-0.782460000	1.523860000
C	-4.672084000	-1.288424000	1.413624000
C	-2.732082000	-0.792065000	2.774128000
C	-5.331819000	-1.784601000	2.539705000
H	-5.178315000	-1.303672000	0.453897000
C	-3.396672000	-1.287055000	3.899368000
H	-1.714228000	-0.438326000	2.875798000
C	-4.697090000	-1.783671000	3.785152000
H	-6.340076000	-2.176770000	2.439299000
H	-2.890582000	-1.295100000	4.860769000
H	-5.210156000	-2.175493000	4.659019000
C	-3.248956000	-1.038681000	-1.378521000
C	-4.348541000	-0.607939000	-2.138410000
C	-2.704587000	-2.313655000	-1.613443000
C	-4.886868000	-1.437238000	-3.127513000
H	-4.799949000	0.362157000	-1.960079000
C	-3.253617000	-3.139671000	-2.595142000
H	-1.859235000	-2.665101000	-1.030603000
C	-4.341236000	-2.702262000	-3.358048000
H	-5.738114000	-1.093430000	-3.708842000
H	-2.828403000	-4.125036000	-2.764425000
H	-4.763549000	-3.346177000	-4.124649000
C	-3.288958000	1.647061000	-0.097174000
C	-3.855769000	2.254201000	1.035172000
C	-3.250584000	2.366299000	-1.305319000
C	-4.375560000	3.549880000	0.958878000
H	-3.906992000	1.718044000	1.977066000
C	-3.780207000	3.656088000	-1.380766000
H	-2.822790000	1.917813000	-2.196230000
C	-4.341223000	4.253327000	-0.247298000
H	-4.816220000	4.002031000	1.843154000
H	-3.760181000	4.190635000	-2.326854000
H	-4.755315000	5.256019000	-0.307247000
C	3.364931000	-0.783084000	1.523684000
C	2.732479000	-0.790416000	2.774353000
C	4.670633000	-1.291808000	1.413082000
C	3.396694000	-1.285852000	3.899590000
H	1.715448000	-0.434374000	2.876357000
C	5.329994000	-1.788492000	2.539184000
H	5.176293000	-1.308807000	0.453091000
C	4.696020000	-1.785277000	3.784991000
H	2.891178000	-1.292056000	4.861307000
H	6.337379000	-2.182821000	2.438483000
H	5.208785000	-2.177476000	4.658865000
C	3.248984000	-1.037990000	-1.378894000
C	4.348786000	-0.607041000	-2.138359000
C	2.704412000	-2.312731000	-1.614620000
C	4.887101000	-1.435881000	-3.127853000
H	4.800378000	0.362847000	-1.959374000
C	3.253434000	-3.138297000	-2.596704000

H	1.858914000	-2.664345000	-1.032098000
C	4.341252000	-2.700665000	-3.359197000
H	5.738515000	-1.091916000	-3.708843000
H	2.828054000	-4.123483000	-2.766611000
H	4.763557000	-3.344226000	-4.126101000
C	3.289193000	1.647158000	-0.096428000
C	3.856574000	2.253617000	1.035994000
C	3.250573000	2.366989000	-1.304219000
C	4.376638000	3.549215000	0.960132000
H	3.908051000	1.716997000	1.977607000
C	3.780465000	3.656691000	-1.379238000
H	2.822415000	1.919010000	-2.195206000
C	4.342018000	4.253260000	-0.245682000
H	4.817742000	4.000825000	1.844463000
H	3.760233000	4.191691000	-2.325066000
H	4.756315000	5.255887000	-0.305294000
Ru	-0.000048000	-0.155435000	0.097163000

PPh_3.Ir-N.S_0

Energy = -1808.490246 a.u.

2 1

C	-0.000030000	1.368088000	-2.699267000
C	0.000004000	2.114618000	-0.486874000
C	0.000037000	2.241114000	1.811619000
C	0.000028000	2.982697000	0.588125000
H	0.000038000	4.068212000	0.524345000
C	-0.000018000	0.160379000	-2.008955000
C	-0.000015000	2.469878000	-1.849657000
H	-0.000018000	3.504312000	-2.188402000
P	-2.568176000	-0.088969000	0.018750000
P	2.568176000	-0.088965000	0.018725000
H	-0.000016000	-0.800544000	-2.521076000
H	-0.000046000	1.432297000	-3.783980000
H	0.000052000	2.634507000	2.827646000
N	0.000022000	0.963829000	1.592593000
Cl	0.000011000	-2.282353000	-0.088253000
C	3.166156000	-1.351250000	-1.180367000
C	3.831657000	-2.494548000	-0.709153000
C	2.949880000	-1.202780000	-2.563613000
C	4.284264000	-3.463000000	-1.610008000
H	4.001949000	-2.637576000	0.351971000
C	3.406642000	-2.171870000	-3.457111000
H	2.444707000	-0.325719000	-2.957539000
C	4.075248000	-3.305215000	-2.981143000
H	4.799946000	-4.341440000	-1.233381000
H	3.246671000	-2.040343000	-4.523566000
H	4.430346000	-4.059194000	-3.677477000
C	3.156450000	-0.593060000	1.690531000
C	4.477617000	-0.277464000	2.063040000
C	2.355921000	-1.352931000	2.559033000
C	4.980017000	-0.712011000	3.290725000
H	5.117802000	0.298875000	1.402898000
C	2.866439000	-1.781571000	3.786630000
H	1.346879000	-1.632441000	2.280148000
C	4.175746000	-1.460994000	4.155416000
H	6.000921000	-0.465784000	3.567942000
H	2.241964000	-2.371759000	4.451051000
H	4.569923000	-1.796626000	5.110256000
C	3.403396000	1.520811000	-0.325496000
C	4.057939000	1.789448000	-1.538424000
C	3.388681000	2.509004000	0.678954000
C	4.671352000	3.029793000	-1.747441000
H	4.130794000	1.032906000	-2.310815000
C	4.005699000	3.741859000	0.465864000
H	2.939122000	2.302302000	1.645644000
C	4.642536000	4.008542000	-0.752129000
H	5.188746000	3.218042000	-2.683784000
H	4.009258000	4.486294000	1.257351000
H	5.131536000	4.964934000	-0.913122000
C	-3.166162000	-1.351336000	-1.180250000
C	-2.949895000	-1.202955000	-2.563507000
C	-3.831669000	-2.494598000	-0.708958000
C	-3.406667000	-2.172100000	-3.456940000
H	-2.444727000	-0.325916000	-2.957491000
C	-4.284287000	-3.463106000	-1.609749000
H	-4.001959000	-2.637555000	0.352176000
C	-4.075274000	-3.305411000	-2.980894000
H	-3.246702000	-2.040642000	-4.523405000
H	-4.799973000	-4.341518000	-1.233063000
H	-4.430380000	-4.059434000	-3.677177000
C	-3.156413000	-0.592965000	1.690599000
C	-4.477526000	-0.277242000	2.063189000
C	-2.355902000	-1.352909000	2.559056000
C	-4.979890000	-0.711732000	3.290910000
H	-5.117700000	0.299151000	1.403083000
C	-2.866384000	-1.781493000	3.786687000
H	-1.346906000	-1.632521000	2.280107000
C	-4.175636000	-1.460786000	4.155555000

H	-6.000753000	-0.465406000	3.568189000
H	-2.241924000	-2.371740000	4.451071000
H	-4.569785000	-1.796375000	5.110422000
C	-3.403424000	1.520768000	-0.325583000
C	-4.058067000	1.789260000	-1.538490000
C	-3.388650000	2.509071000	0.678758000
C	-4.671519000	3.029571000	-1.747594000
H	-4.130963000	1.032633000	-2.310794000
C	-4.005709000	3.741889000	0.465583000
H	-2.939011000	2.302483000	1.645435000
C	-4.642646000	4.008427000	-0.752390000
H	-5.188986000	3.217710000	-2.683919000
H	-4.009221000	4.486411000	1.256989000
H	-5.131677000	4.964793000	-0.913449000
Ir	0.000003000	0.070227000	-0.034311000

PPh_3.Ir-N.T_1

Energy = -1808.467917 a.u.

2 3

C	-0.000011000	1.491696000	-2.575897000
C	0.000009000	2.066090000	-0.295642000
C	0.000022000	2.009806000	2.038979000
C	0.000030000	2.832378000	0.857292000
H	0.000043000	3.920491000	0.887583000
C	-0.000007000	0.198313000	-2.008670000
C	0.000001000	2.522764000	-1.640815000
H	0.000005000	3.577740000	-1.910391000
P	-2.558391000	-0.072165000	-0.002520000
P	2.558391000	-0.072171000	-0.002514000
H	-0.000016000	-0.675943000	-2.663615000
H	-0.000019000	1.669369000	-3.649173000
H	0.000027000	2.407465000	3.056706000
N	0.000004000	0.727482000	1.827458000
Cl	-0.000012000	-2.356016000	0.129603000
C	3.125833000	-1.358310000	-1.183809000
C	3.784275000	-2.500878000	-0.695176000
C	2.901793000	-1.227020000	-2.568390000
C	4.234714000	-3.478106000	-1.584021000
H	3.956597000	-2.629492000	0.367088000
C	3.358961000	-2.204784000	-3.449660000
H	2.381705000	-0.361829000	-2.967465000
C	4.024286000	-3.334881000	-2.958928000
H	4.753333000	-4.351125000	-1.199030000
H	3.194774000	-2.088423000	-4.517042000
H	4.373231000	-4.100548000	-3.645613000
C	3.172264000	-0.529194000	1.669190000
C	4.455761000	-0.093643000	2.063843000
C	2.434389000	-1.378049000	2.514077000
C	4.988294000	-0.513896000	3.281983000
H	5.047952000	0.547755000	1.420291000
C	2.977369000	-1.789561000	3.731562000
H	1.451986000	-1.727117000	2.220458000
C	4.250070000	-1.357349000	4.120023000
H	5.982505000	-0.186817000	3.572296000
H	2.405017000	-2.448709000	4.377615000
H	4.666562000	-1.677564000	5.070764000
C	3.364443000	1.525237000	-0.410354000
C	4.066728000	1.738354000	-1.611497000
C	3.308018000	2.564047000	0.547390000
C	4.694882000	2.961912000	-1.847379000
H	4.164909000	0.947351000	-2.345075000
C	3.944012000	3.780193000	0.307785000
H	2.801473000	2.406822000	1.493606000
C	4.632100000	3.985927000	-0.893841000
H	5.253069000	3.108338000	-2.767467000
H	3.913673000	4.562761000	1.060505000
H	5.131189000	4.932569000	-1.079899000
C	-3.125824000	-1.358173000	-1.183961000
C	-2.901726000	-1.226755000	-2.568520000
C	-3.784305000	-2.500778000	-0.695463000
C	-3.358880000	-2.204423000	-3.449902000
H	-2.381598000	-0.361538000	-2.967489000
C	-4.234730000	-3.477909000	-1.584420000
H	-3.956667000	-2.629492000	0.366783000
C	-4.024247000	-3.334554000	-2.959305000
H	-3.194648000	-2.087963000	-4.517266000
H	-4.753381000	-4.350956000	-1.199533000
H	-4.373182000	-4.100147000	-3.646078000
C	-3.172250000	-0.529391000	1.669131000
C	-4.455724000	-0.093849000	2.063867000
C	-2.434392000	-1.378396000	2.513882000
C	-4.988250000	-0.514253000	3.281960000
H	-5.047903000	0.547662000	1.420417000
C	-2.977363000	-1.790057000	3.731320000
H	-1.452009000	-1.727462000	2.220192000
C	-4.250040000	-1.357850000	4.119867000
H	-5.982442000	-0.187176000	3.572339000
H	-2.405024000	-2.449318000	4.377269000

H	-4.666526000	-1.678182000	5.070571000
C	-3.364460000	1.525281000	-0.410180000
C	-4.066708000	1.738539000	-1.611320000
C	-3.308108000	2.563962000	0.547709000
C	-4.694889000	2.962110000	-1.847062000
H	-4.164839000	0.947631000	-2.345006000
C	-3.944129000	3.780122000	0.308242000
H	-2.801602000	2.406624000	1.493926000
C	-4.632173000	3.985998000	-0.893384000
H	-5.253045000	3.108643000	-2.767152000
H	-3.913846000	4.562588000	1.061070000
H	-5.131285000	4.932650000	-1.079333000
Ir	-0.000001000	0.053951000	-0.044232000