

Supporting Information

Probing the mechanism of adaptive aromaticity in metallapyridiniums

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1. The geometries of metallapyridiniums (M.X) in the singlet and triplet states.

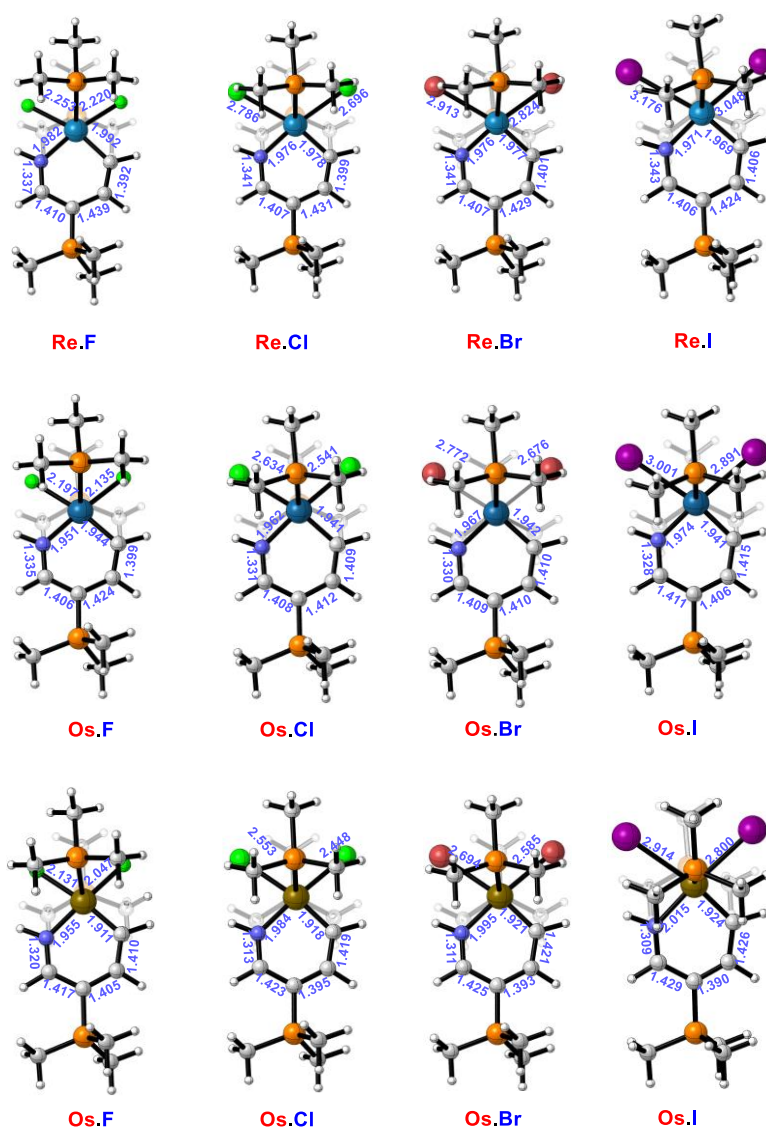


Fig. S1. Selected bond lengths (Å, blue) of M.X in the singlet state.

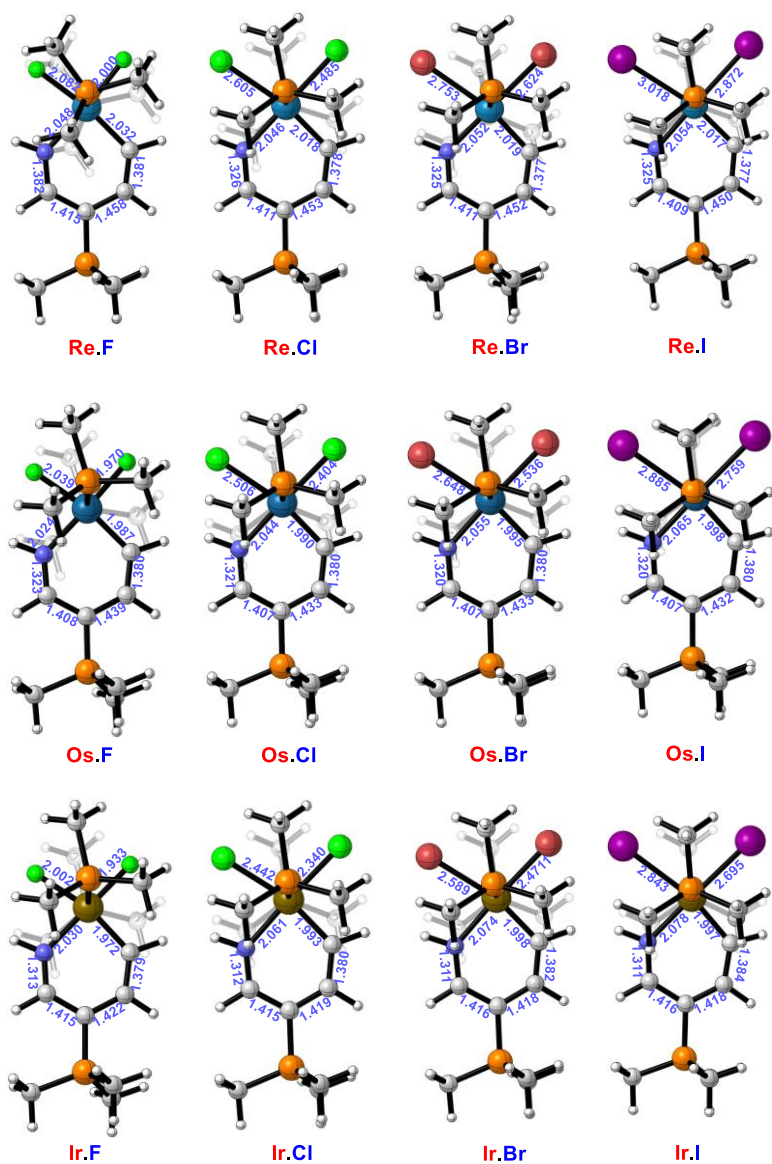


Fig. S2. Selected bond lengths (Å, blue) of M.X in the triplet state.

2. $\Delta E_{ST}(E_T - E_S)$ values of M.X.

Table S1. ΔE_{ST} values (kcal/mol) calculated of M.X. Level of theory: (U)PBE0/6-311G++(d, p)~SDD/(U)B3LYP/6-31G(d)~LanL2DZ.

	Re.F	Os.F	Ir.F	Re.Cl	Os.Cl	Ir.Cl
ΔE_{ST}	-17.6	-4.7	13.3	-14.0	0.1	11.5
	Re.Br	Os.Br	Ir.Br	Re.I	Os.I	Ir.I
ΔE_{ST}	-14.8	-1.2	7.1	-12.9	-0.9	3.2

3. Position of the ghost atom (Bq) for NICS calculation.

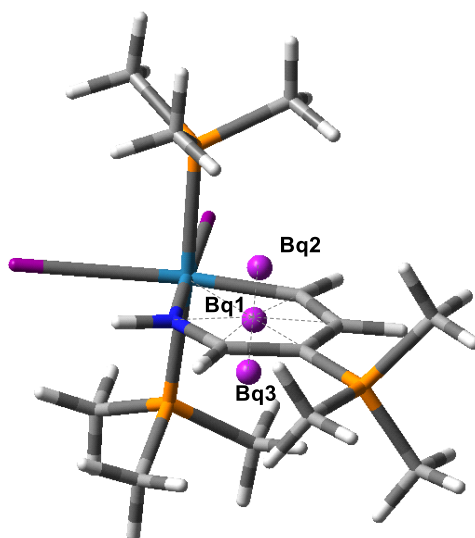


Fig. S3. Method used in NICS(1)_{zz} calculations. Bq1 is placed at the geometry centers of six-membered rings (6MRs). The distances of Bq2-Bq1 and Bq3-Bq1 are 1 Å. The NICS(1)_{zz} of a metallapyridinium is computed by the average value of the out-of-plane (ZZ) components obtained from Bq2 and Bq3.

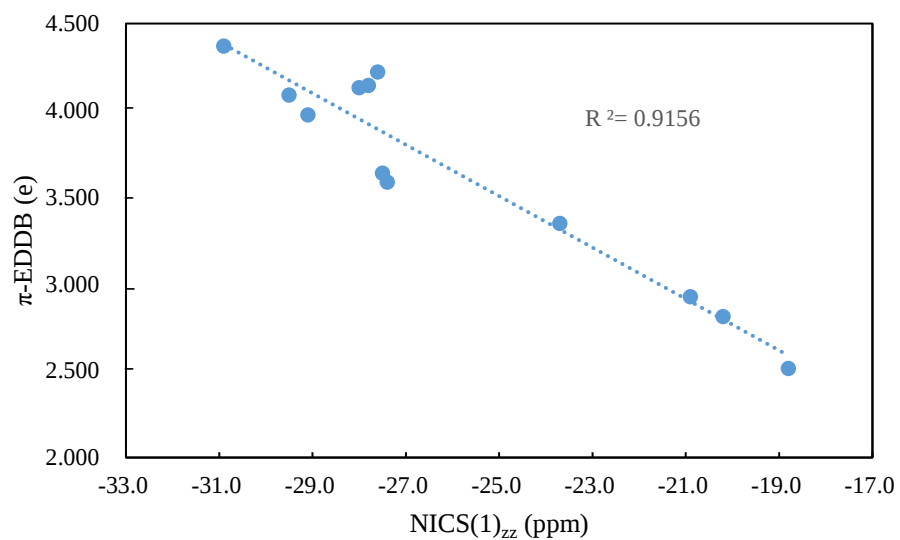
4. Correlation between NICS(1)_{zz}, π -EDDB, and HOMA values of M.X.

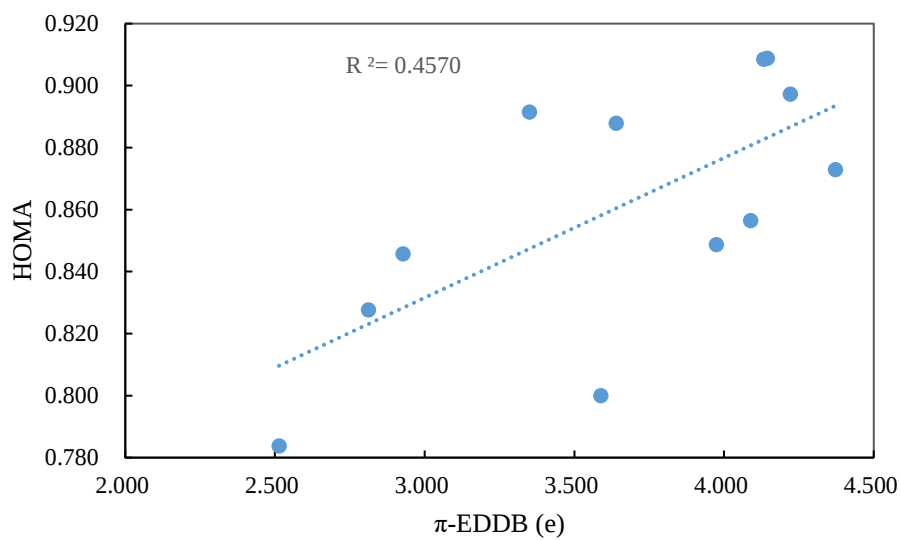
The essence of aromaticity is the delocalization of electrons. We use π -EDDB analysis as a benchmark in this work, the linear relationship between π -EDDB and NICS(1)_{zz} / π -EDDB and HOMA are provided in Fig. S4. As shown in Fig. S4a, the coefficient of determination (R^2) is 0.916 between NICS(1)_{zz} and π -EDDB, the HOMA/ π -EDDB correlation is relatively weaker (R^2 : 0.457) in the lowest singlet state. As shown in Fig. S4b, the coefficient of determination (R^2) is 0.863 between NICS(1)_{zz} and π -EDDB, the HOMA/ π -EDDB correlation is relatively weaker (R^2 : 0.395) in the triplet state. As the parameters of HOMA are limited and M-C bond cannot be considered, errors may be caused when evaluating the organometallic system. It has been reported that π -EDDB and NICS(1)_{zz} have a good linear relationship. So π -EDDB, NICS(1)_{zz} and ACID criteria are mainly used as the criteria to evaluate the aromaticity of M.X in this work.

Table S2 HOMA of **M.X** in the lowest singlet and triplet states. Level of theory: (U)B3LYP/6-31G(d)~LanL2DZ.

	HOMA(singlet)	HOMA(triplet)
Re.F	0.800	0.580
Os.F	0.888	0.800
Ir.F	0.891	0.863
Re.Cl	0.849	0.838
Os.Cl	0.908	0.685
Ir.Cl	0.846	0.891
Re.Br	0.856	0.692
Os.Br	0.909	0.838
Ir.Br	0.828	0.877
Re.I	0.873	0.714
Os.I	0.897	0.843
Ir.I	0.784	0.878

(a) Singlet





(b) Triplet

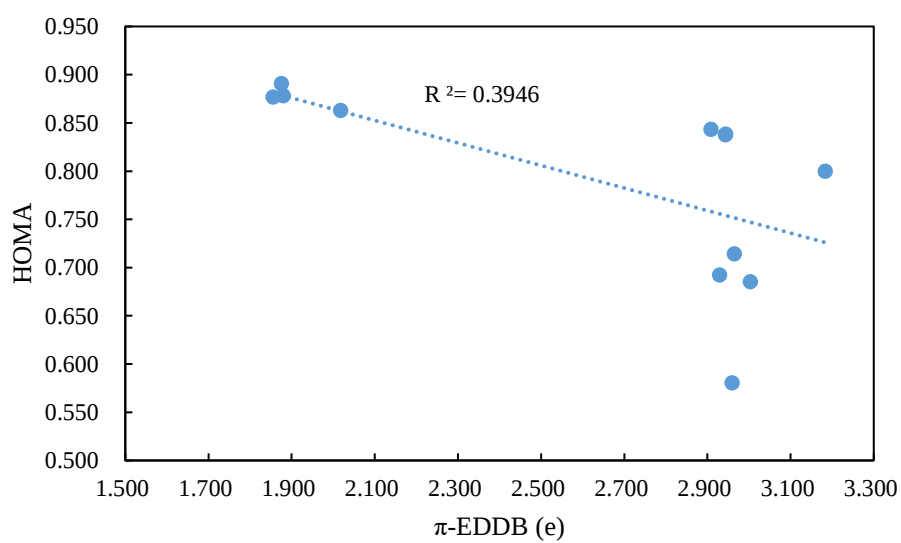
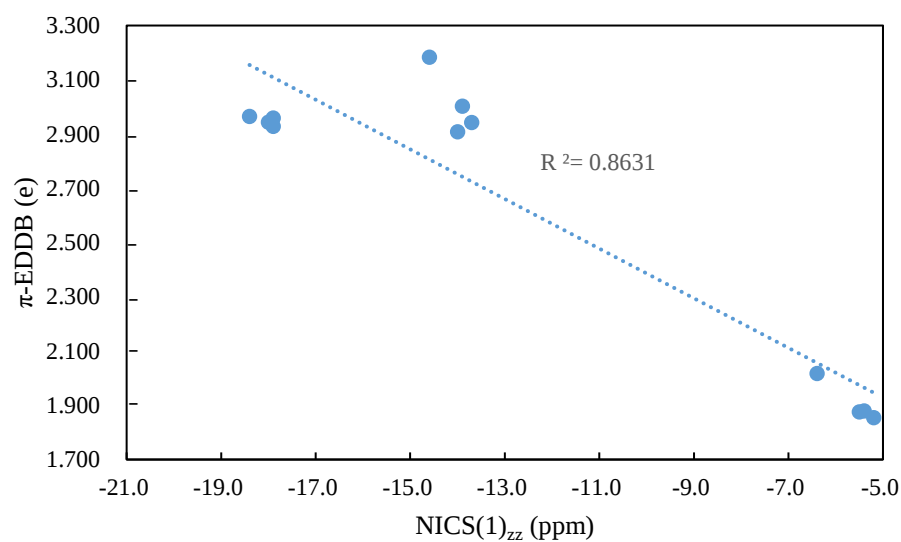


Fig. S4. Correlation between NICS(1)_{zz}, π -EDDB, and HOMA values of **M.X**.

5. NICS(1)_{zz} grids of M.F, M.Cl, M.Br, and M.I in the singlet and triplet states.

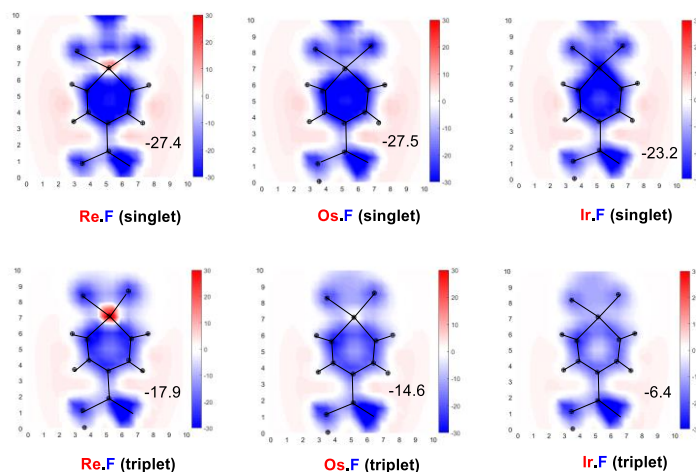


Fig. S5. NICS(1)_{zz} grids of complexes **M.F** in the singlet and triplet states (values provided on the right-bottom of each graph were calculated at 1.0 Å above the geometrical ring centers). Each grid covers a 10 × 10 Å square area parallel to molecular planes. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ).

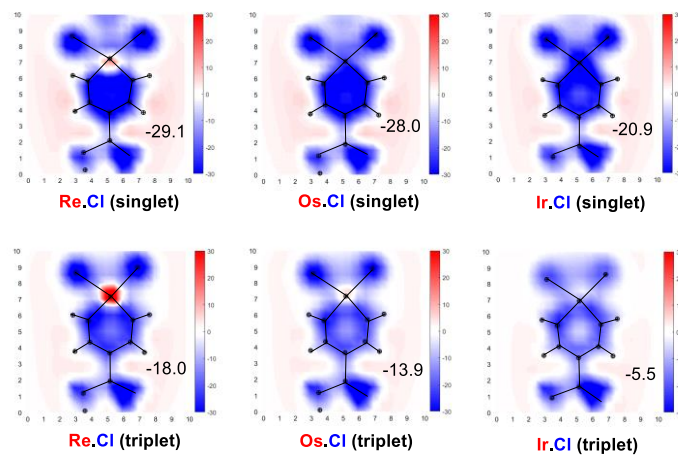


Fig. S6. NICS(1)_{zz} grids of complexes **M.Cl** in the singlet and triplet states (values provided on the right-bottom of each graph were calculated at 1.0 Å above the geometrical ring centers). Each grid covers a 10 × 10 Å square area parallel to molecular planes. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ).

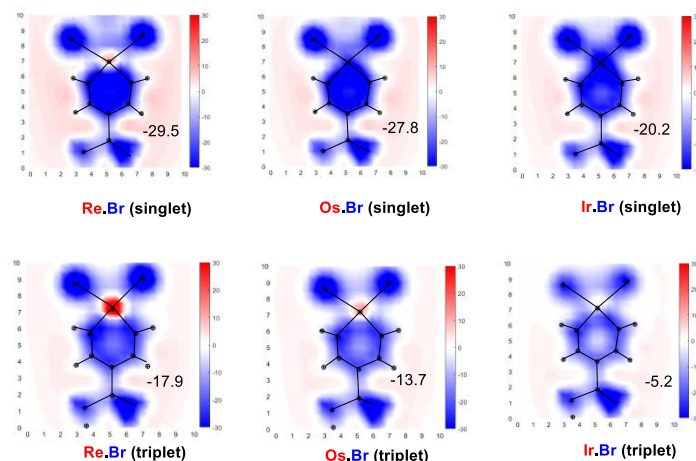


Fig. S7. NICS(1)_{zz} grids of complexes **M.Br** in the singlet and triplet states (values provided on the right-bottom of each graph were calculated at 1.0 Å above the geometrical ring centers). Each grid covers a 10 × 10 Å square area parallel to molecular planes. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ).

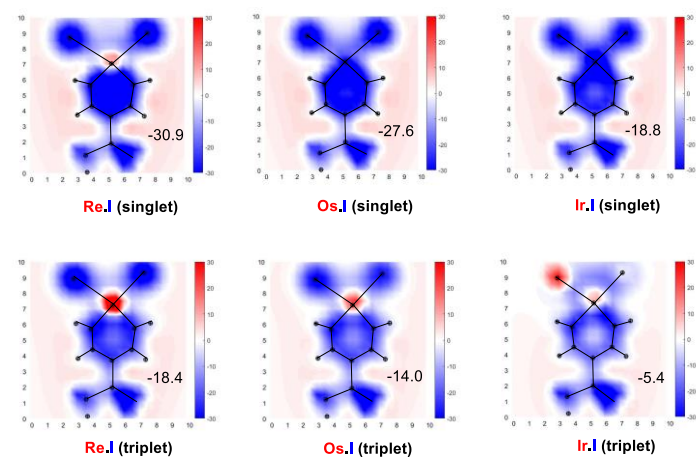


Fig. S8. NICS(1)_{zz} grids of complexes **M.I** in the singlet and triplet states (values provided on the right-bottom of each graph were calculated at 1.0 Å above the geometrical ring centers). Each grid covers a 10 × 10 Å square area parallel to molecular planes. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ).

6. ACID plot of individual molecular orbitals, NICS(1)_{zz} and EDDB values of pyridinium

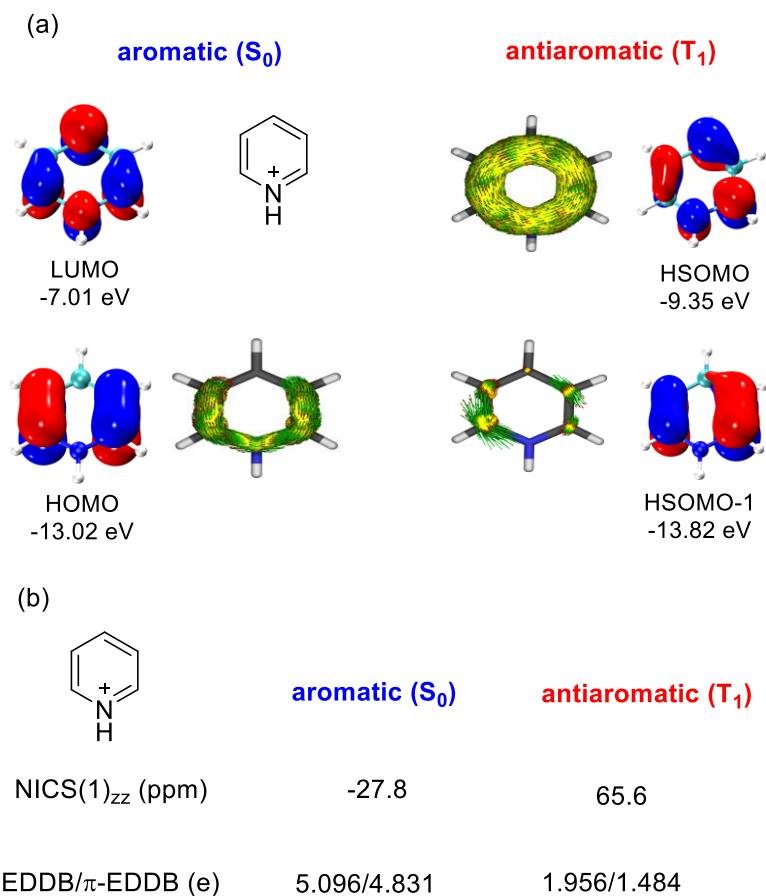


Fig. S9. (a) ACID plot of individual molecular orbitals, (b) NICS(1)_{zz} and EDDB values of pyridinium. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ.

7. ACID plots of M.F, M.Br and M.I in the singlet and triplet states.

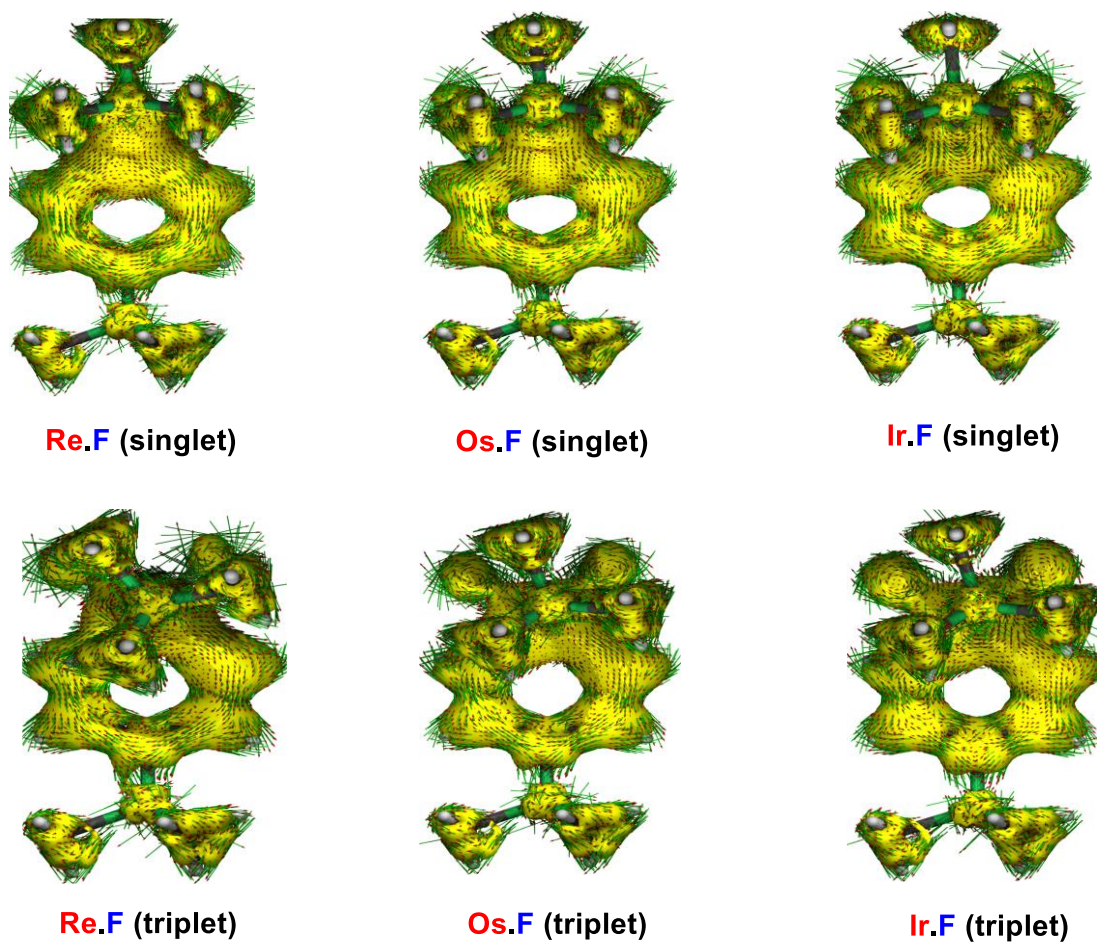


Fig. S10. ACID plots of **M.F** in the singlet and triplet states. Isovalue for density surfaces: 0.035 a.u. High-resolution plots are in **Figs. S27-S32**. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ.

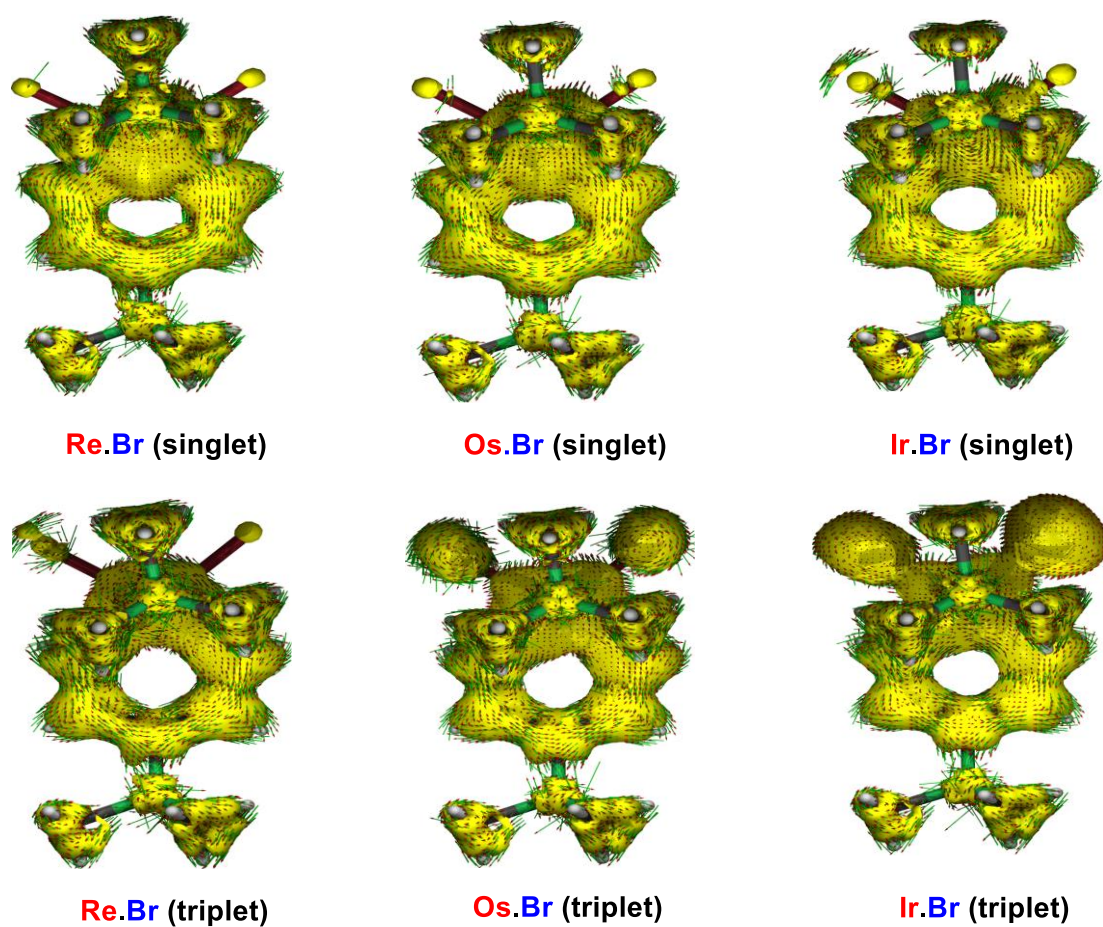


Fig. S11. ACID plots of **M.Br** in the singlet and triplet states. Isovalue for density surfaces: 0.035 a.u. High-resolution plots are in **Figs. S39-S44**. Level of theory: (U)CAM-B3LYP/def2-TZVP//(U)B3LYP/6-31G(d)~LanL2DZ.

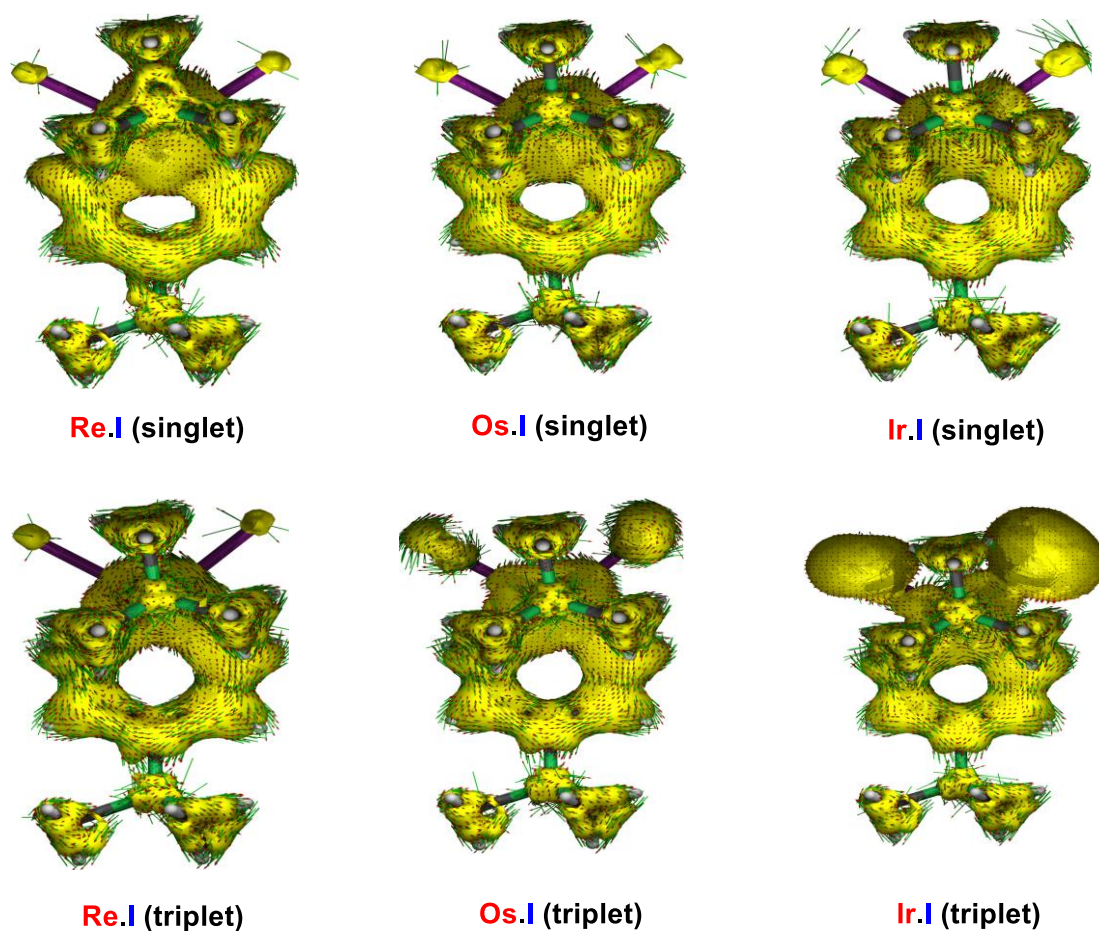


Fig. S12. ACID plots of **M.I** in the singlet and triplet states. Isovalue for density surfaces: 0.035 a.u. High-resolution plots are in **Figs. S45-S50**. Level of theory: (U)CAM-B3LYP/def2-TZVP//(U)B3LYP/6-31G(d)~LanL2DZ.

8. EDDB and π -EDDB analyses of M.X in the lowest singlet and triplet states.

Table S3 EDDB and π -EDDB analyses of M.X. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ.

	EDDB (e)	π -EDDB (e)		EDDB (e)	π -EDDB (e)
Re.F (S_1)	4.212	3.588	Re.F (T_0)	3.492	2.959
Os.F (S_1)	4.232	3.639	Os.F (T_0)	3.759	3.183
Ir.F (S_0)	3.959	3.350	Ir.F (T_1)	2.596	2.017
Re.Cl (S_1)	4.571	3.974	Re.Cl (T_0)	3.500	2.944
Os.Cl (S_0)	4.760	4.132	Os.Cl (T_1)	3.602	3.003
Ir.Cl (S_0)	3.528	2.927	Ir.Cl (T_1)	2.419	1.875
Re.Br (S_1)	4.697	4.088	Re.Br (T_0)	3.488	2.929
Os.Br (S_1)	4.775	4.144	Os.Br (T_0)	3.539	2.943
Ir.Br (S_0)	3.405	2.812	Ir.Br (T_1)	2.393	1.855
Re.I (S_1)	4.997	4.371	Re.I (T_0)	3.535	2.965
Os.I (S_1)	4.854	4.221	Os.I (T_0)	3.504	2.908
Ir.I (S_0)	3.082	2.513	Ir.I (T_1)	2.451	1.879

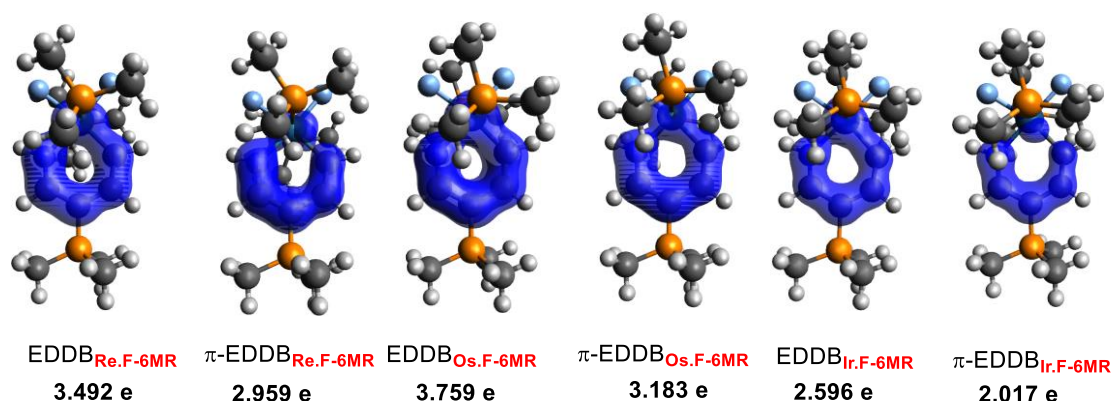


Fig. S13. Dissected EDDB and π -EDDB calculated for the 6MR of M.F in the lowest triplet state. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ.

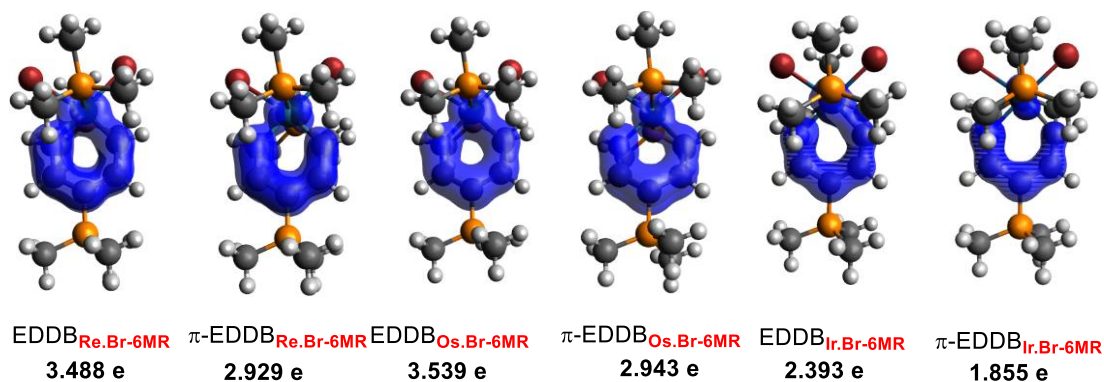


Fig. S14. Dissected EDDB and π -EDDB calculated for the 6MR of **M.Br** in the lowest triplet state. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ.

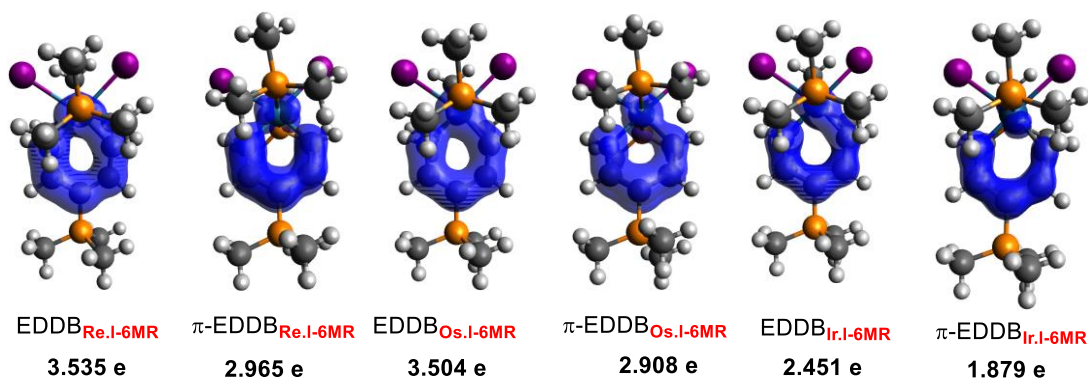


Fig. S15. Dissected EDDB and π -EDDB calculated for the 6MR of **M.I** in the lowest triplet state. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)~LanL2DZ.

9. Biorthogonalized molecular orbitals and spin density distributions of M.X.

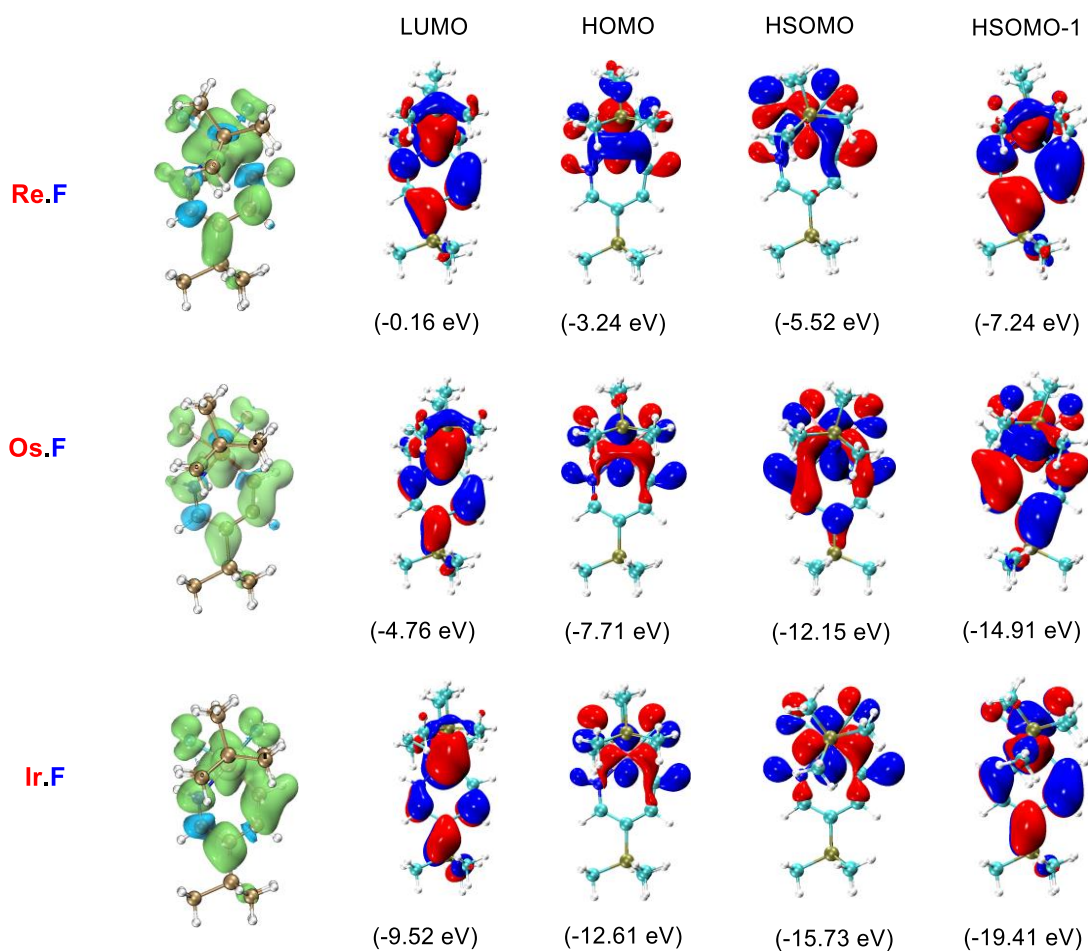


Fig. S16. Frontier molecular orbital HOMO/LUMO of **M.F** in the lowest singlet state and

biorthogonalized SOMOs (isovalue: 0.030 a.u.) and spin density distributions (isovalue: 0.001 a.u.) of **M.F** in the lowest triplet state. Level of theory: (U)B3LYP/6-31G(d)~LanL2DZ.

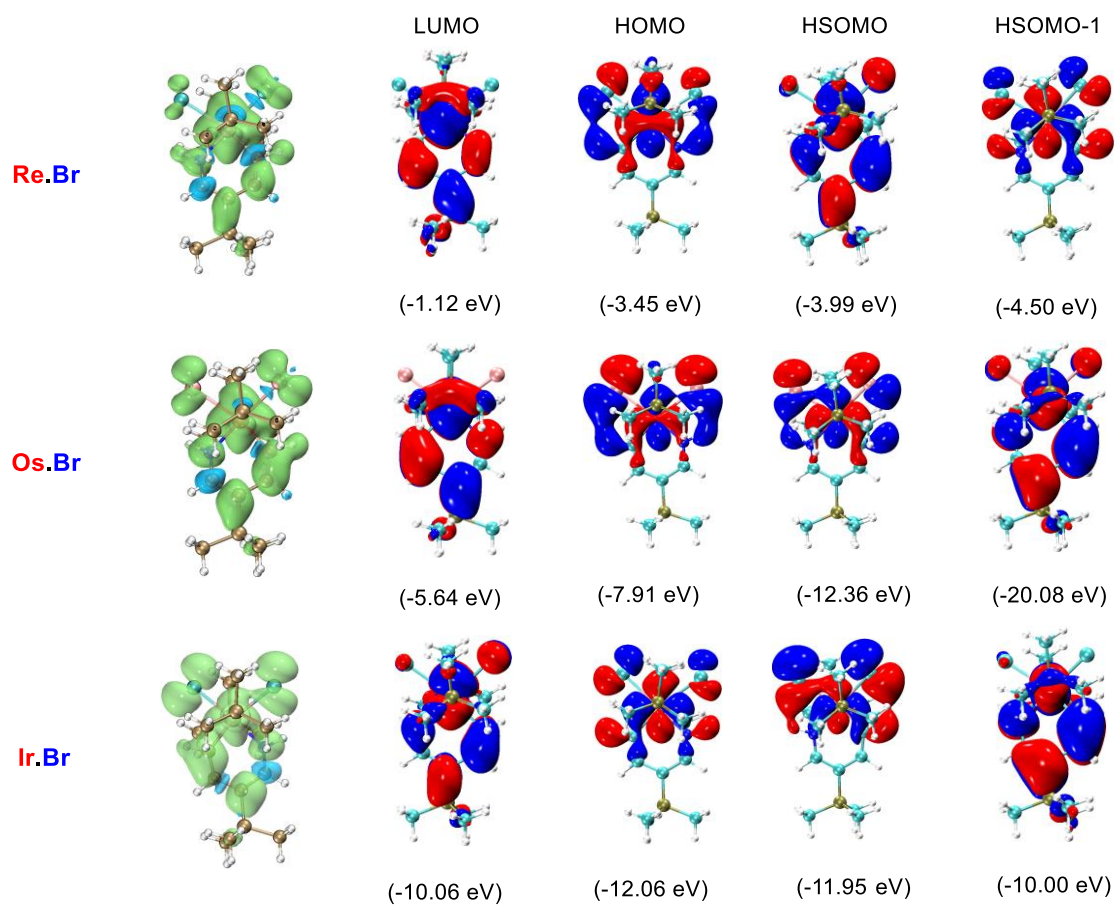


Fig. S17. Frontier molecular orbital HOMO/LUMO of **M.Br** in the lowest singlet state and biorthogonalized SOMOs (isovalue: 0.030 a.u.) and spin density distributions (isovalue: 0.001 a.u.) of **M.Br** in the lowest triplet state. Level of theory: (U)B3LYP/6-31G(d)~LanL2DZ.

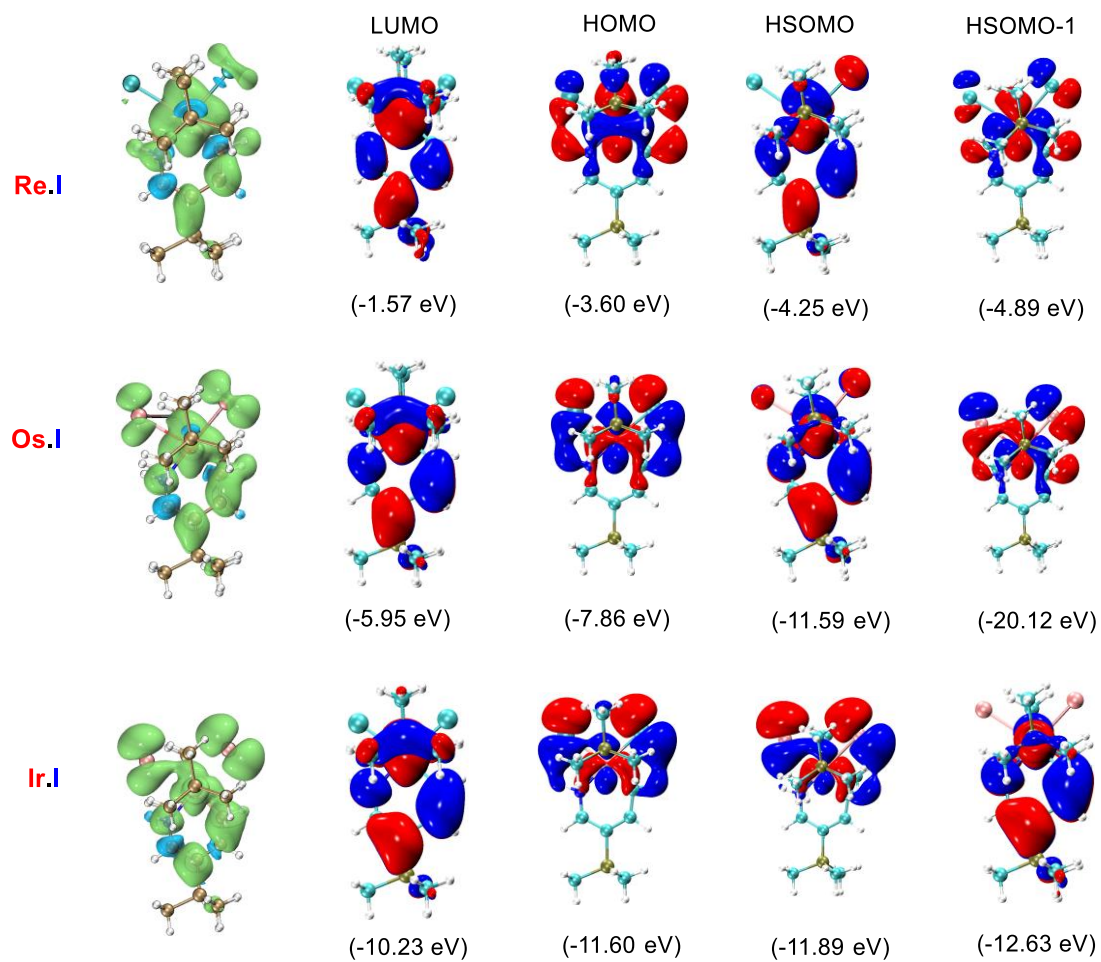


Fig. S18. Frontier molecular orbital HOMO/LUMO of **M.I** in the lowest singlet state and biorthogonalized SOMOs (isovalue: 0.030 a.u.) and spin density distributions (isovalue: 0.001 a.u.) of **M.I** in the lowest triplet state. Level of theory: (U)B3LYP/6-31G(d)~LanL2DZ.

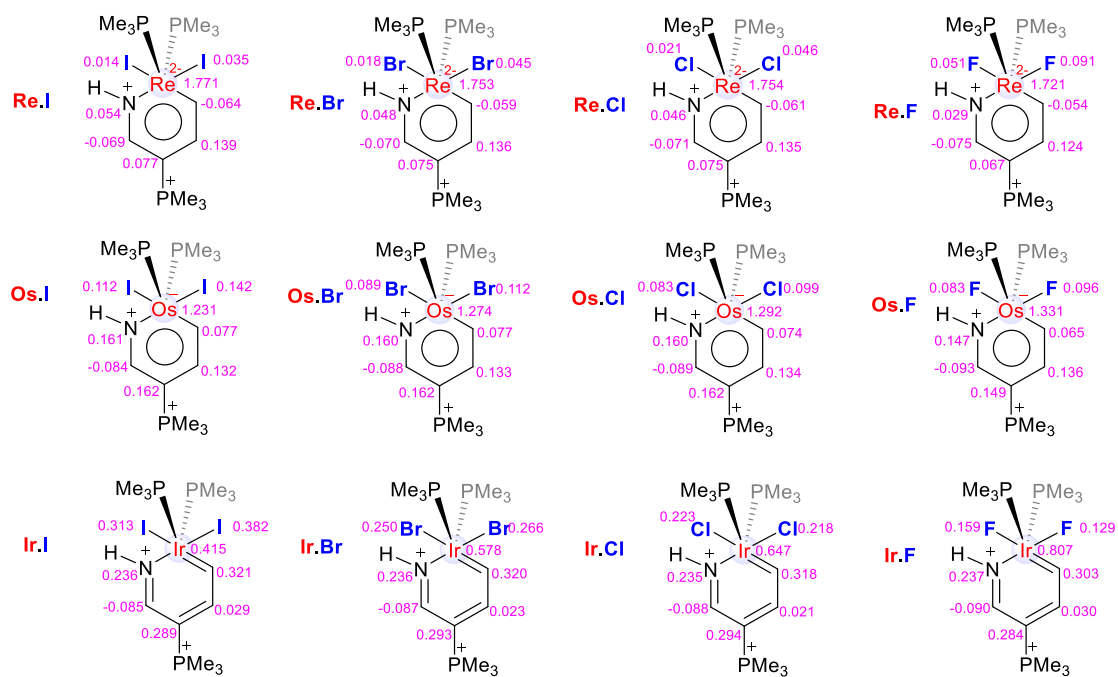


Fig. S19. Atomic Mulliken spin populations (in e) in metallapyridiniums. Level of theory: (U)B3LYP/6-31G(d)~LanL2DZ.

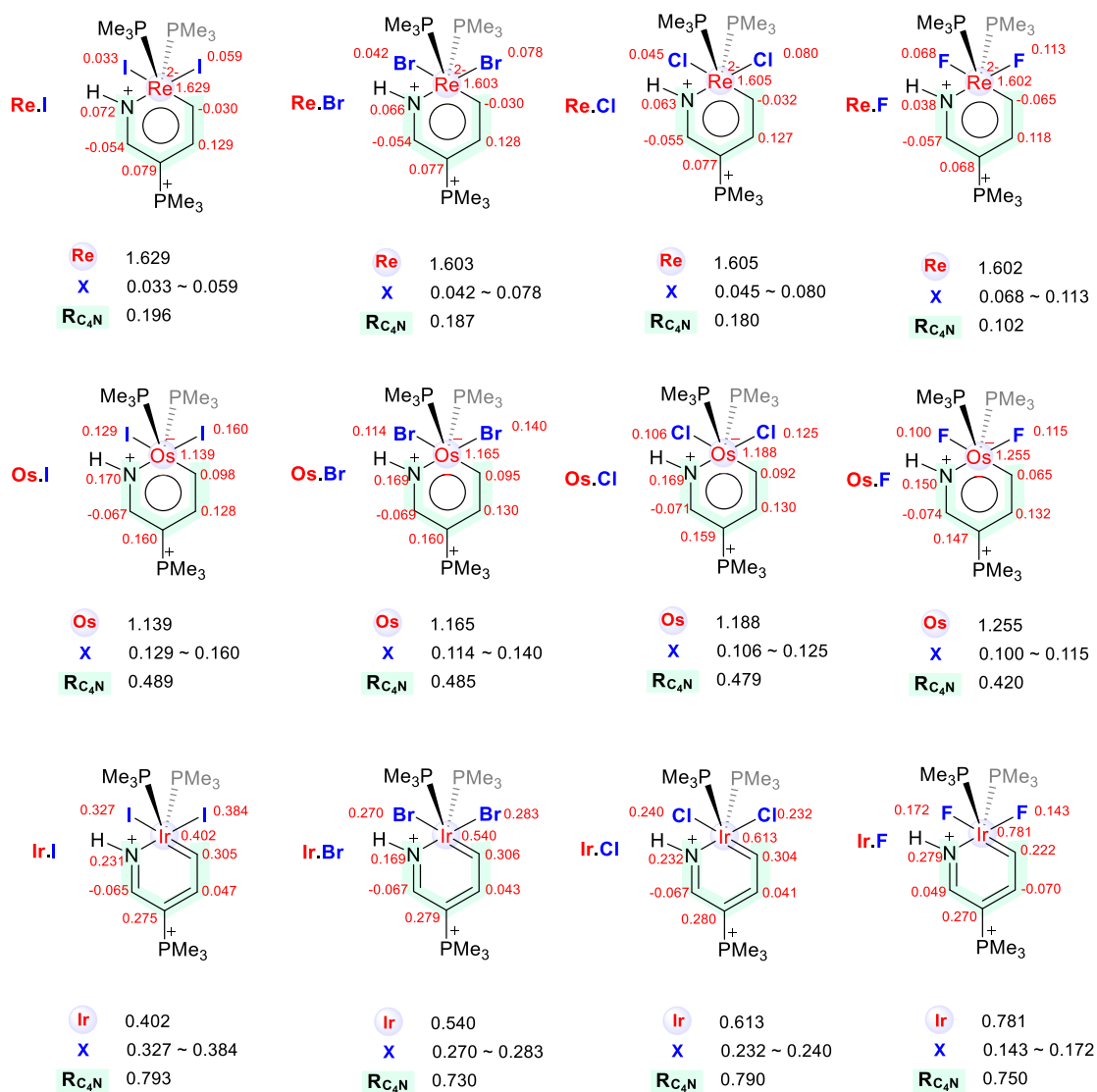
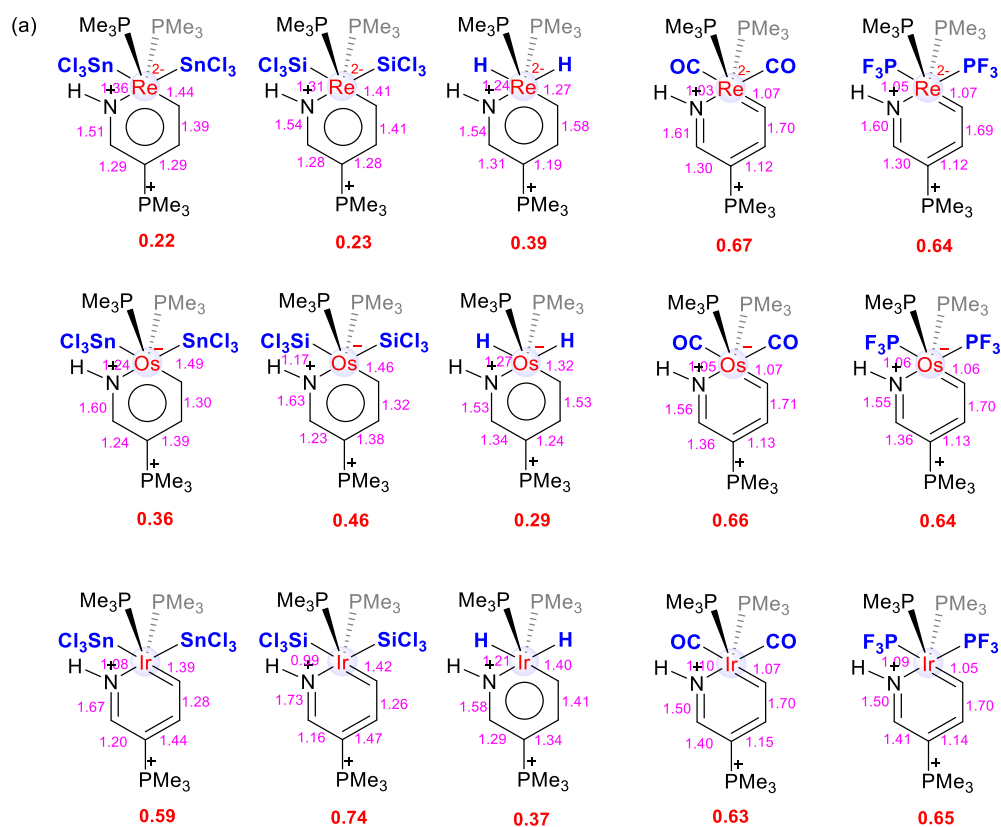


Fig. S20 Spin populations in NPA (in e) in metallapyridiniums (X: different ligands). Level of theory: (U)B3LYP/6-31G(d)~LanL2DZ.

10. The bond order difference and EDDB analyses of M.X in the lowest singlet and triplet states for ligand effect.



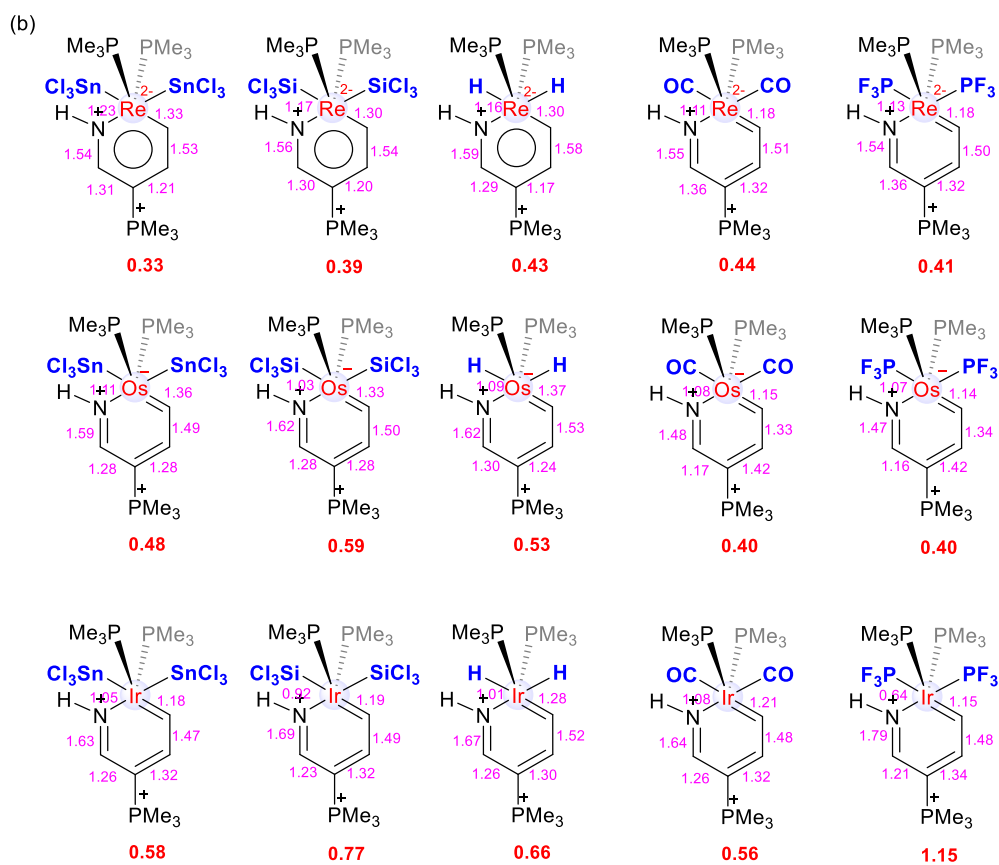


Fig. S21. The bond order difference (ΔFBO) (red) of **M.X** in the lowest singlet (a) and triplet state (b) for ligand effect. Level of theory: (U)B3LYP/6-31G(d)~LanL2DZ.

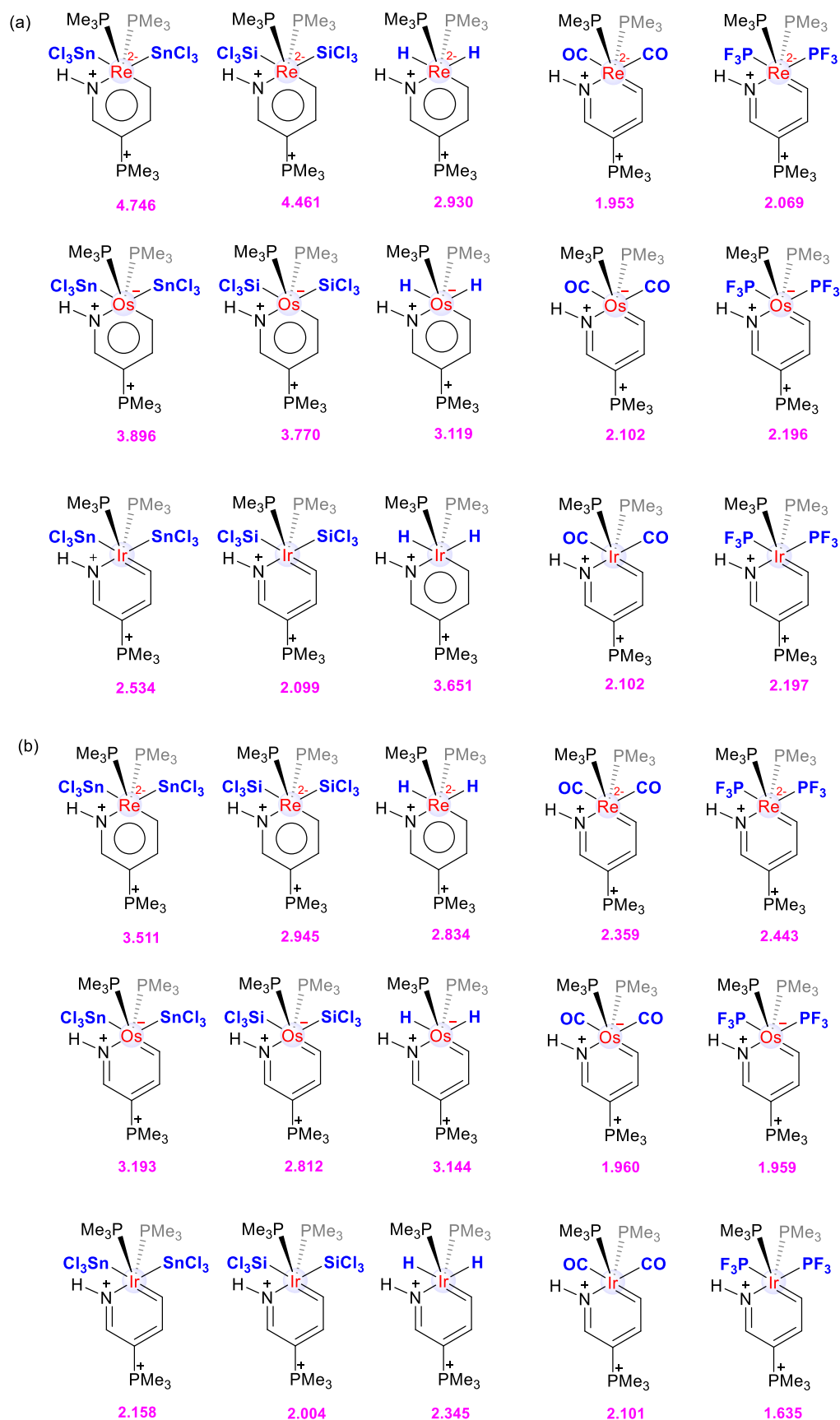


Fig. S22. EDDB values (in e) (pink) of **M.X** in the lowest singlet (a) and triplet state (b) for ligand effect. Level of theory: (U)CAM-B3LYP/def2-TZVP//((U)B3LYP/6-31G(d)-LanL2DZ).

11. A summary and correlation between fuzzy atom bond order difference (Δ FBO), NICS(1)_{zz}, and EDDB values in the lowest singlet and triplet states for ligand effect.

Table S4. Fuzzy atom bond order difference (Δ FBO), NICS(1)_{zz}, and EDDB values of **M.X** in the singlet state for ligand effect.

Species (Singlet)	NICS(1) _{zz} (ppm)	Δ FBO	EDDB (e)
Re.SnCl₃	-31.40	0.22	4.746
Re.SiCl₃	-32.30	0.23	4.461
Re.H	-19.60	0.39	2.930
Re.CO	-1.10	0.67	1.953
Re.PF₃	-0.90	0.64	2.069
Os.SnCl₃	-24.00	0.36	3.896
Os.SiCl₃	-23.30	0.46	3.777
Os.H	-21.50	0.29	3.119
Os.CO	-1.50	0.66	2.102
Os.PF₃	-0.10	0.64	2.196
Ir.SnCl₃	-15.20	0.59	2.534
Ir-SiCl₃	-11.70	0.74	2.099
Ir.H	-21.70	0.37	3.651
Ir.CO	-2.00	0.63	2.102
Ir.PF₃	-0.40	0.65	2.197

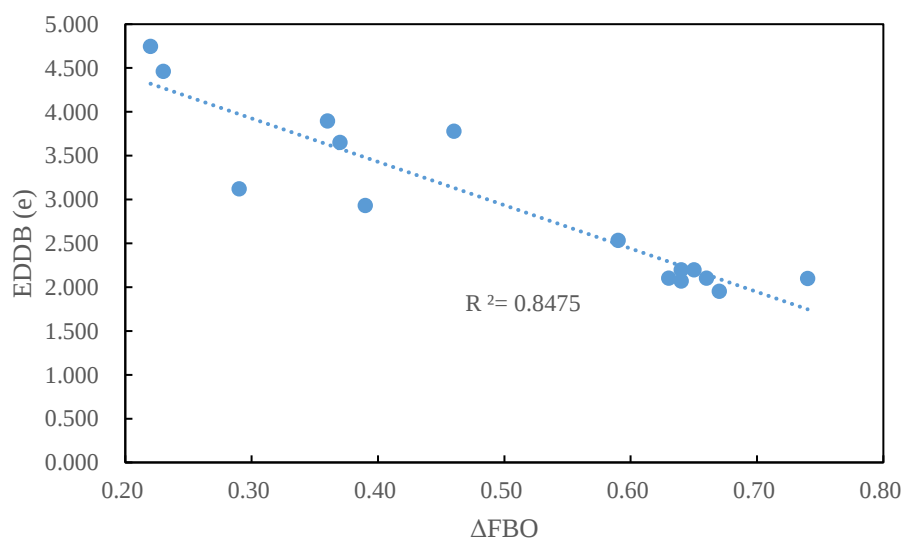
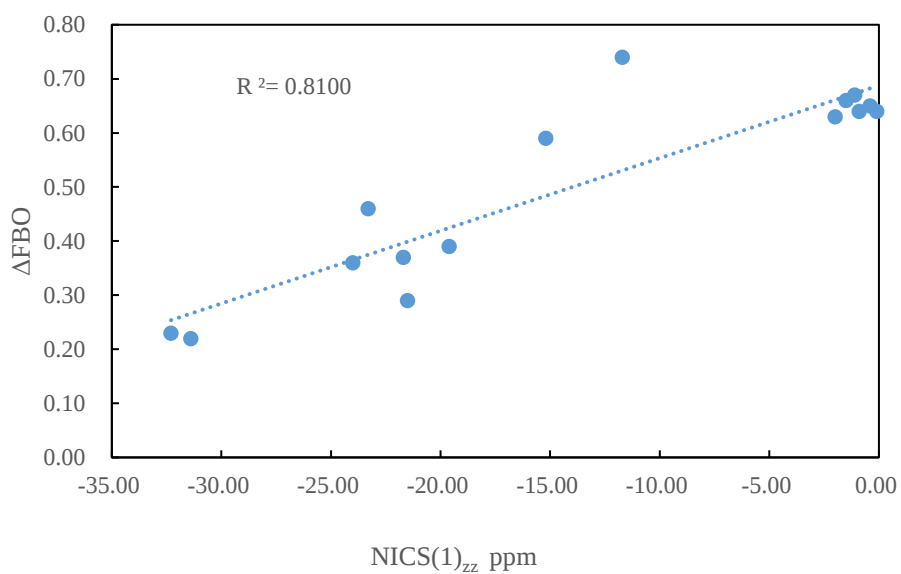
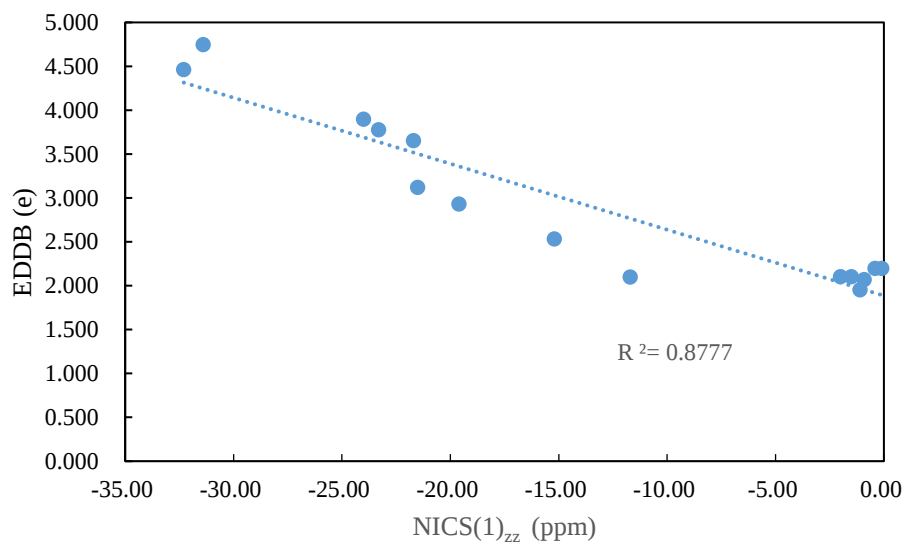


Fig. S23. Correlation between NICS(1)_{zz}, Δ FBO and EDDB values of **M.X** in the singlet state.

Table S5. Fuzzy atom bond order difference (Δ FBO), NICS(1)_{zz}, and EDDB values of **M.X** in the triplet state for ligand effect.

Species (Triplet)	NICS(1) _{zz} (ppm)	FBO	EDDB (e)
Re.SnCl₃	-17.80	0.33	3.511
Re.SiCl₃	-17.90	0.39	2.945
Re.H	-15.10	0.43	2.834
Re.CO	-5.50	0.44	2.359
Re.PF₃	-4.80	0.41	2.443
Os.SnCl₃	-10.50	0.48	3.193
Os.SiCl₃	-12.60	0.59	2.812
Os.H	-12.40	0.53	3.144
Os.CO	0.30	0.40	1.960
Os.PF₃	1.70	0.40	1.959
Ir.SnCl₃	-1.30	0.58	2.158
Ir.SiCl₃	-3.30	0.77	2.004
Ir.H	-5.20	0.66	2.345
Ir.CO	-2.50	0.56	2.101
Ir.PF₃	1.30	1.15	1.635

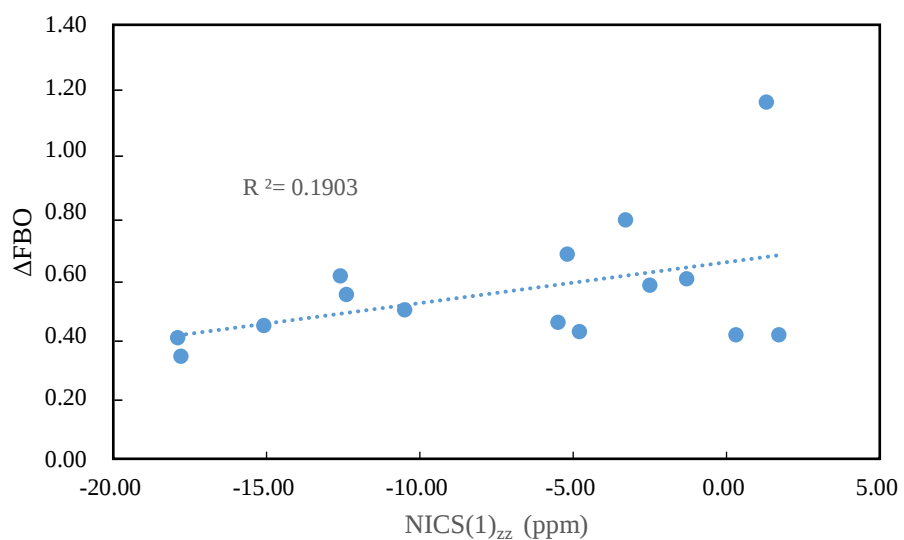
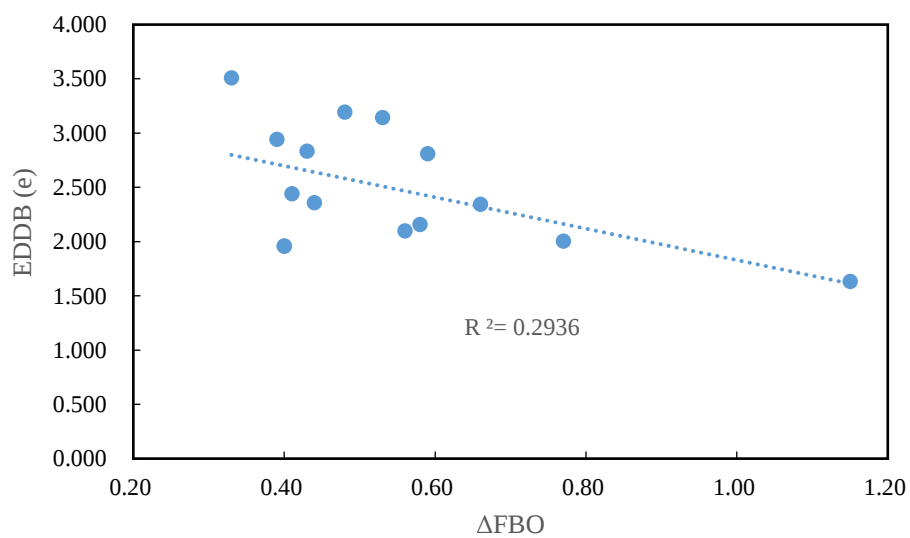
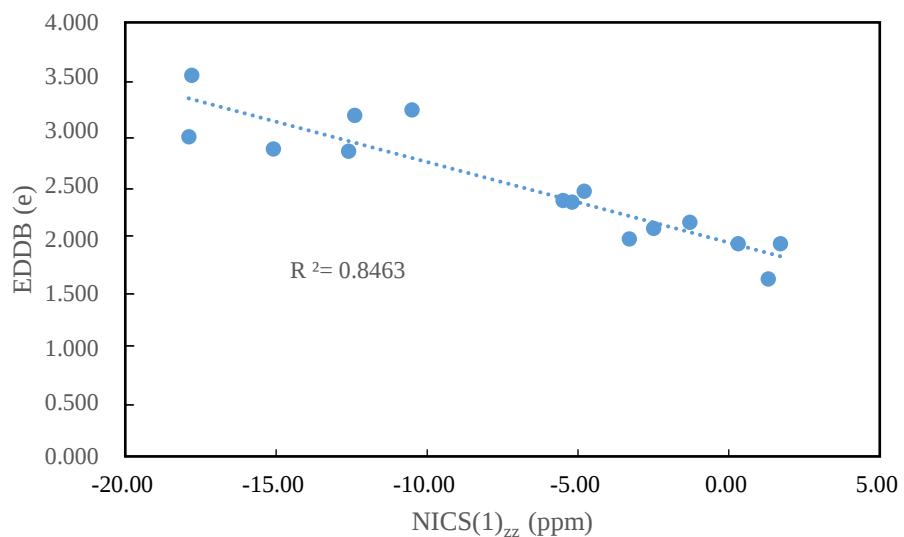


Fig. S24. Correlation between NICS(1)_{zz}, ΔFBO and EDDB values of **M.X** in the triplet state.

12. Atomic Mulliken spin populations in metallapyridiniums for ligand effect.

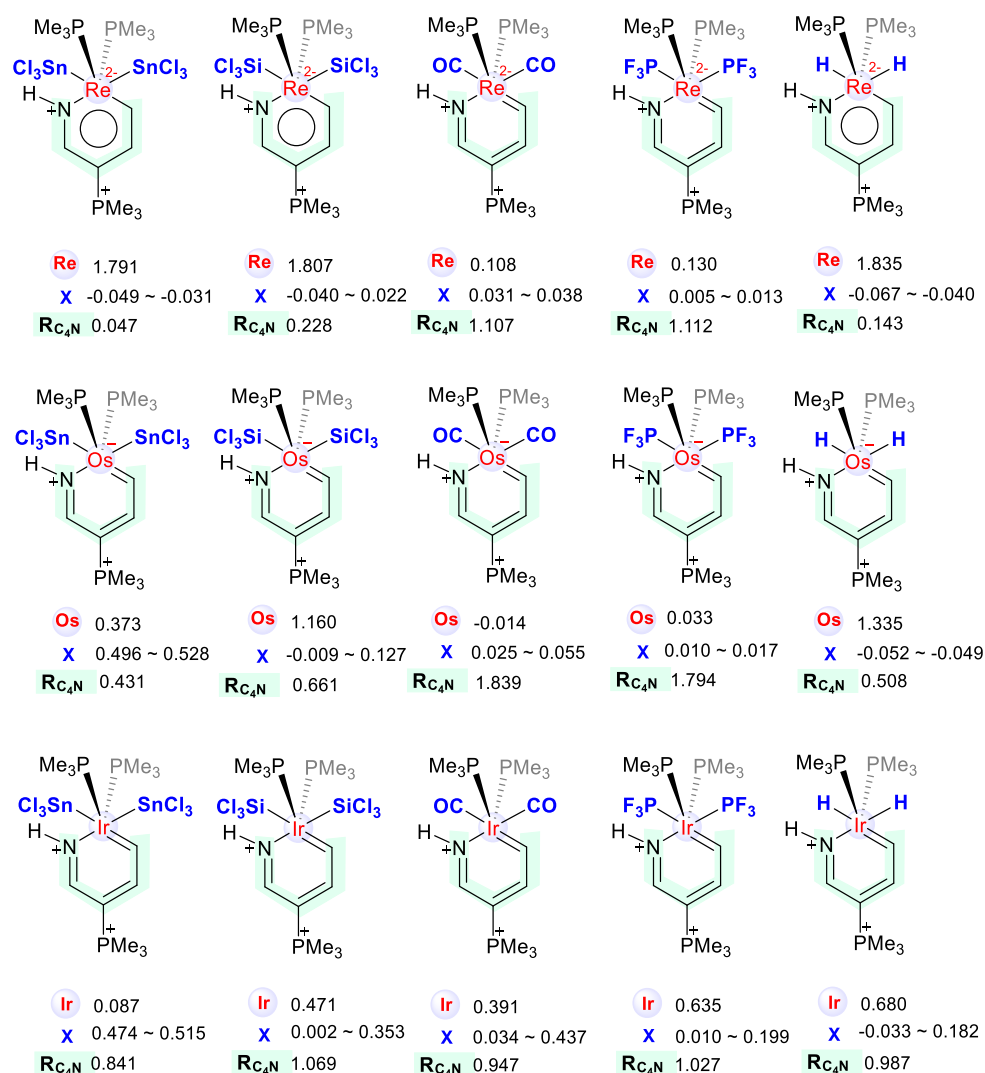


Fig. S25. Atomic Mulliken spin populations (in e) in metallapyridiniums for ligand effect. Level of theory: (U)B3LYP/6-31G(d)~LanL2DZ.

13. Ligand effect on the adaptive aromaticity in metallapyridiniums.

(a)

	BMe ₂	NH ₂	OH	PMe ₃	H ₂ O	NH ₃
Re ²⁻	0.3/-9.3	0.6/-11.2	2.0/-15.0	-0.9/-13.9	-6.2/-5.2	-3.2/-4.2
Os ⁻	1.3/-11.3	-1.1/-7.9	-26.5/-15.8	-1.0/+2.8	-4.5/NA	-3.4/NA
Ir	1.3/-2.4	-19.5/-2.2	-22.9/-5.6	-0.6/+0.5	-3.7/NA	-2.7/-16.0

(b)

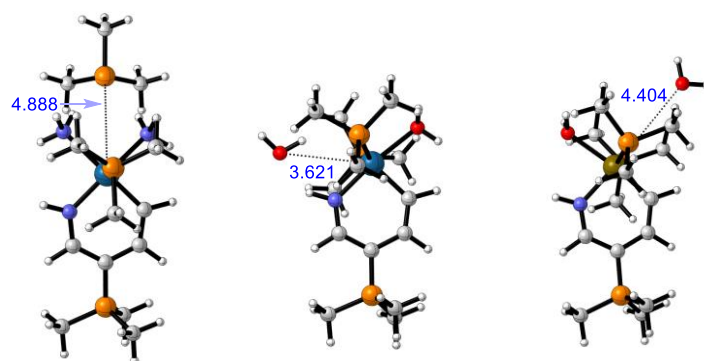


Fig. S26. (a) Ligand expansion on NICS(1)_{zz} values of metallapyridiniums in the lowest singlet and triplet states. NA denotes the broken structures in which the NICS(1)_{zz} values can not be computed. Level of theory: (U)CAM-B3LYP/def2-TZVP//(U)B3LYP/6-31G(d)~LanL2DZ. (b) The 3D broken structures and the bond distance after the ligands dissociated (Å, blue).

14. High-resolution ACID plots of M.X.

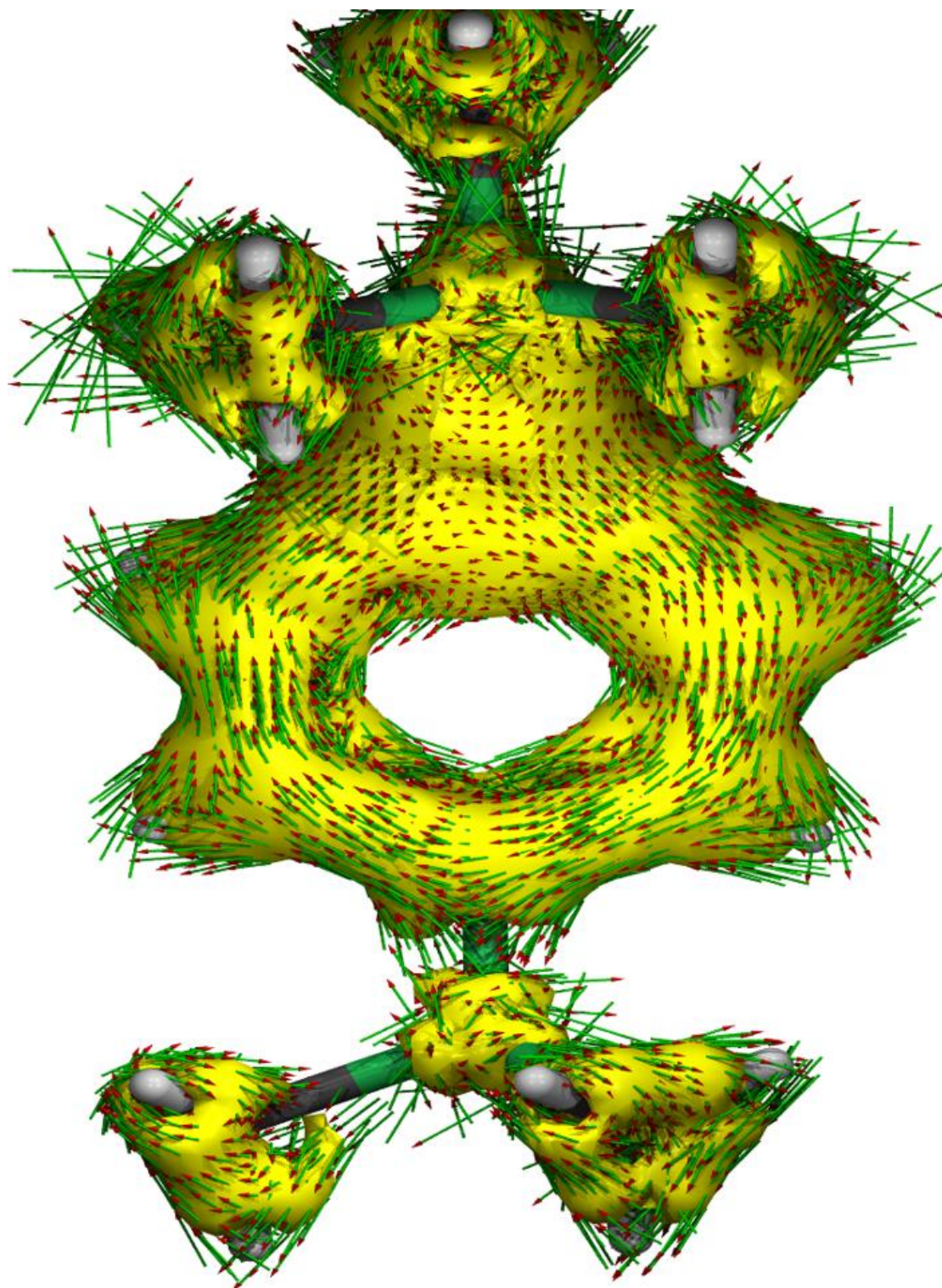


Fig. S27. ACID plot of $\text{Re}(\rho)$ in the singlet state. Isovalue for ACID is 0.035 a.u.

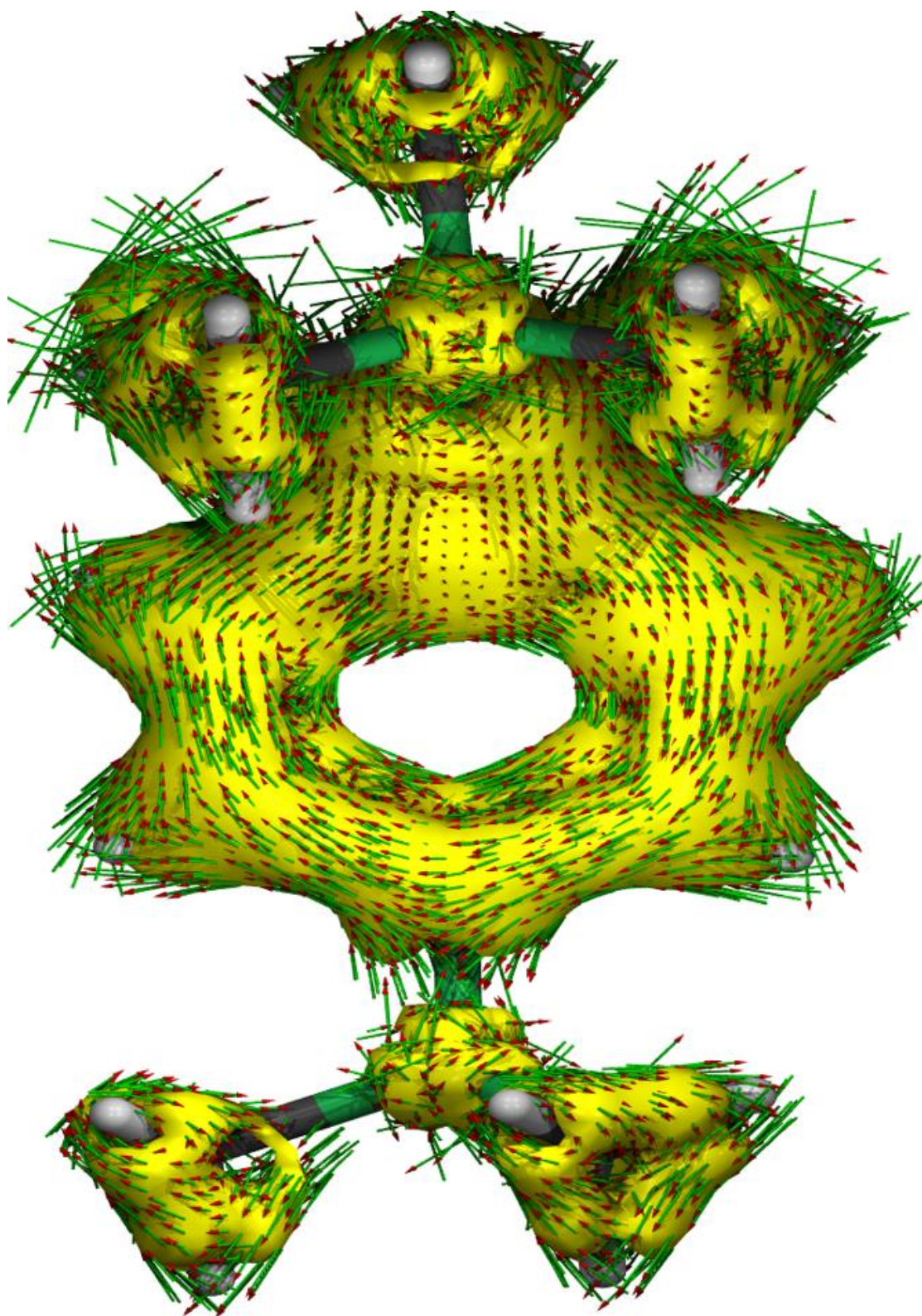


Fig. S28. ACID plot of Os.F in the singlet state. Isovalue for ACID is 0.035 a.u.

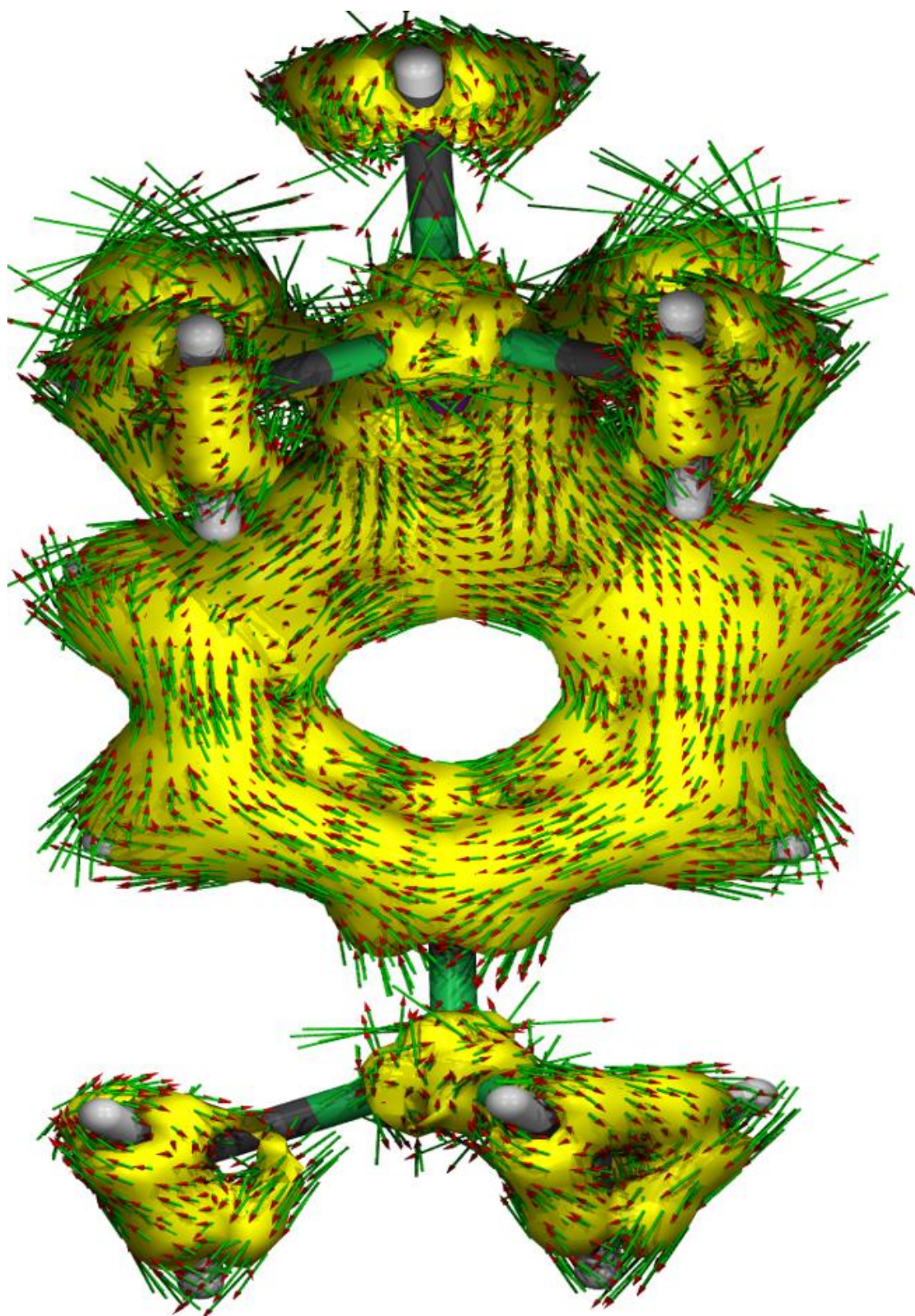


Fig. S29. ACID plot of Ir.F in the singlet state. Isovalue for ACID is 0.035 a.u.

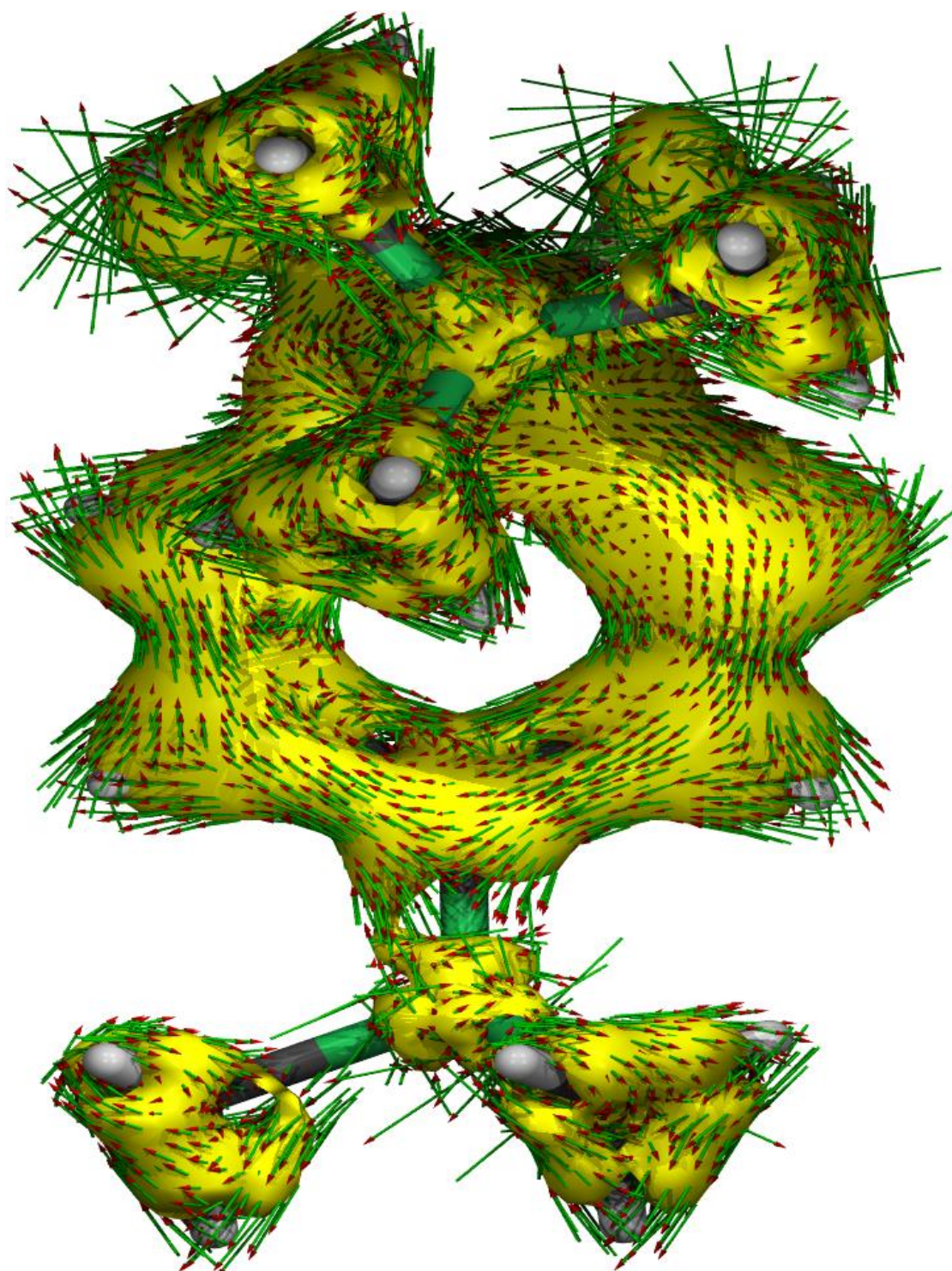


Fig. S30. ACID plot of Re.F in the triplet state. Isovalue for ACID is 0.035 a.u.

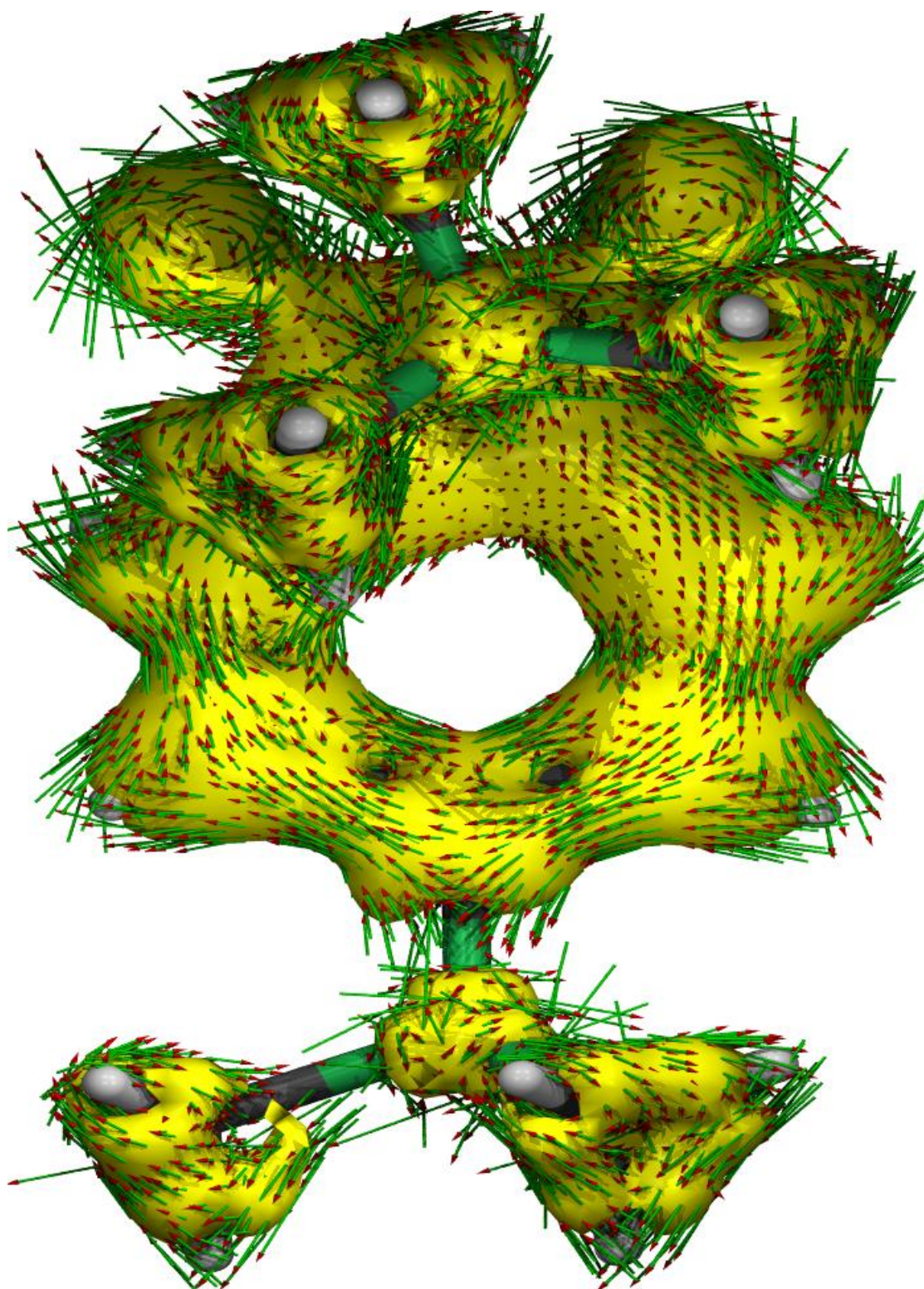


Fig. S31. ACID plot of **Os.F** in the triplet state. Isovalue for ACID is 0.035 a.u.

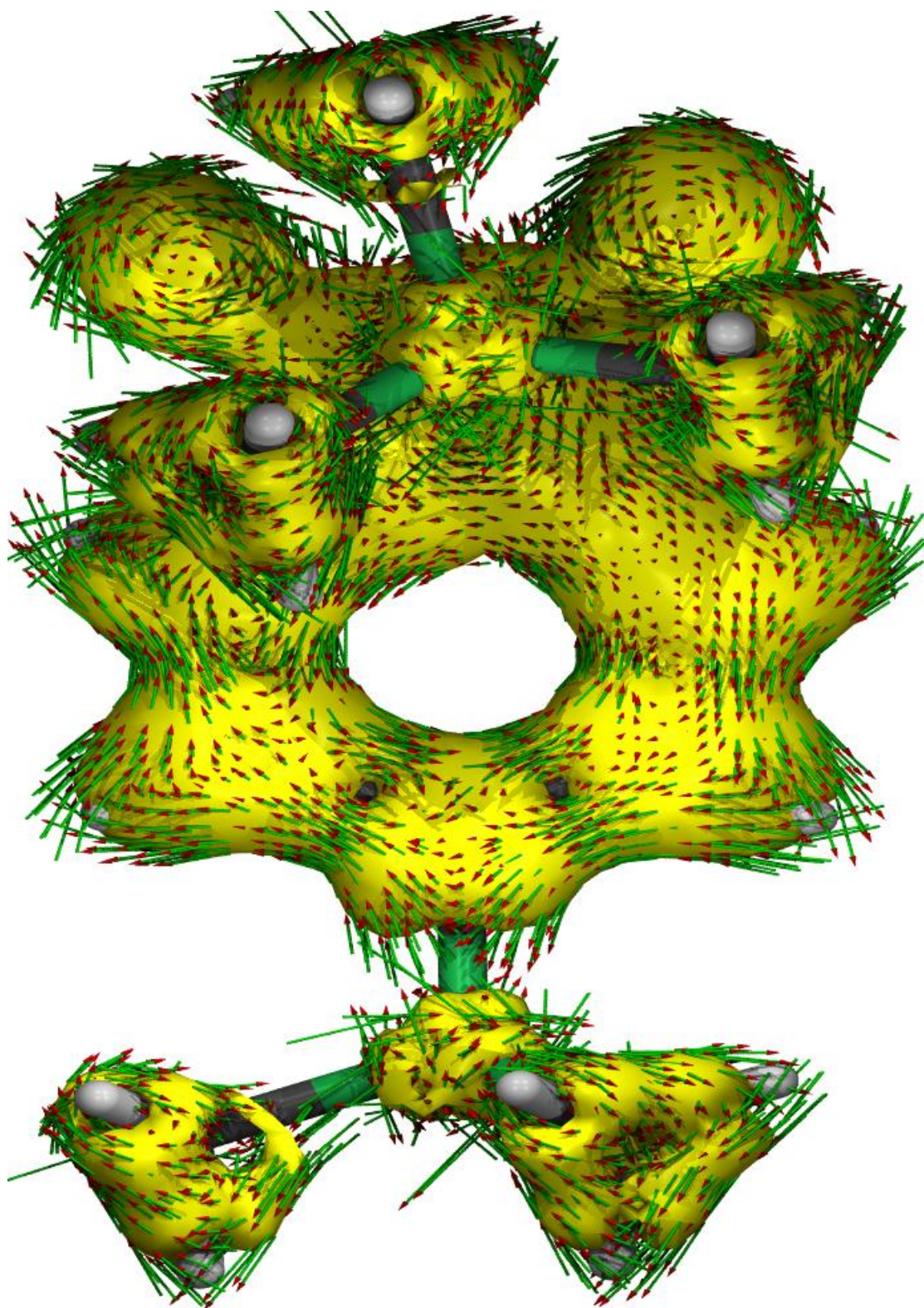


Fig. S32. ACID plot of **Ir.F** in the triplet state. Isovalue for ACID is 0.035 a.u.

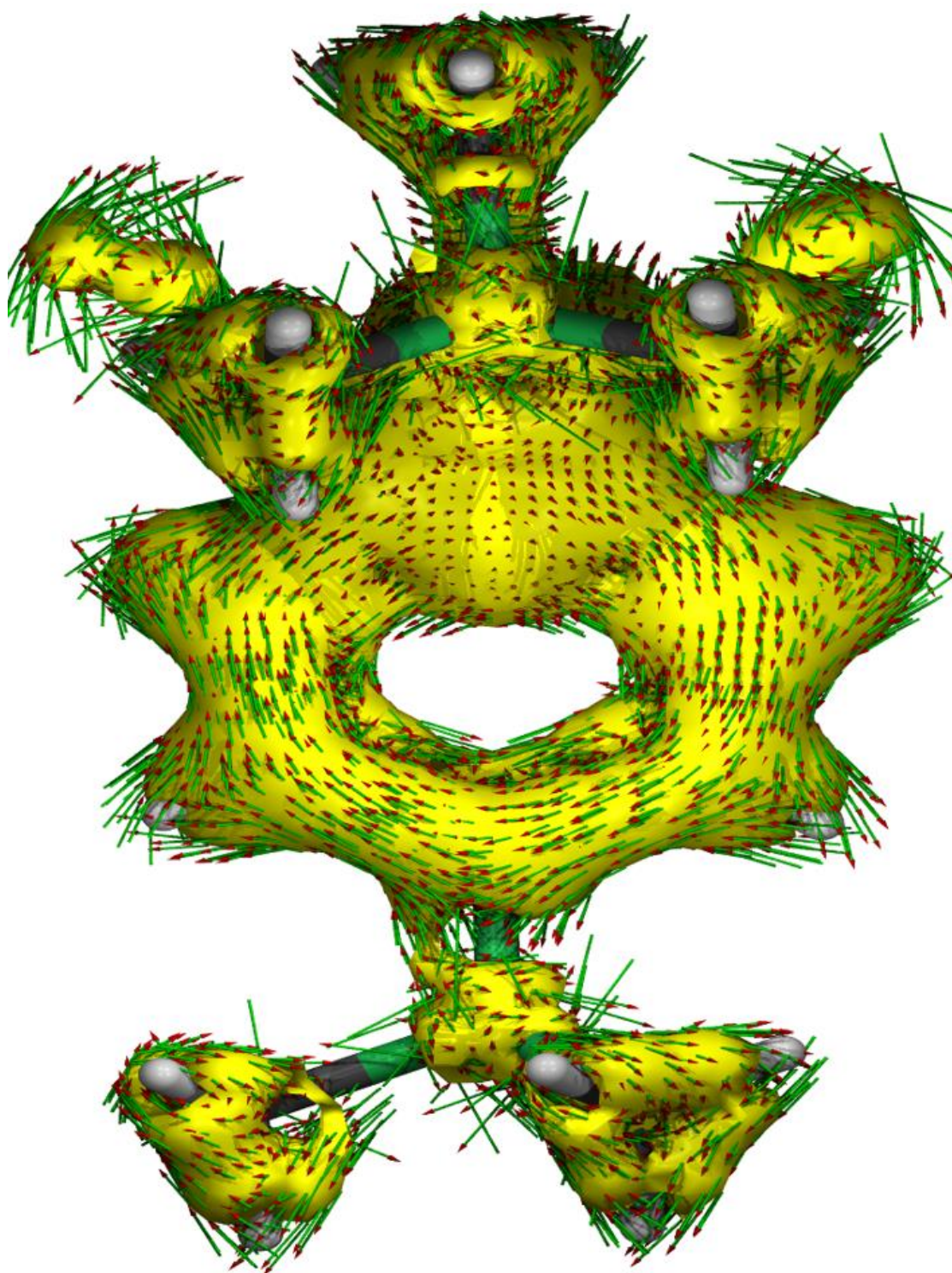


Fig. S33. ACID plot of **Re.Cl** in the singlet state. Isovalue for ACID is 0.035 a.u.

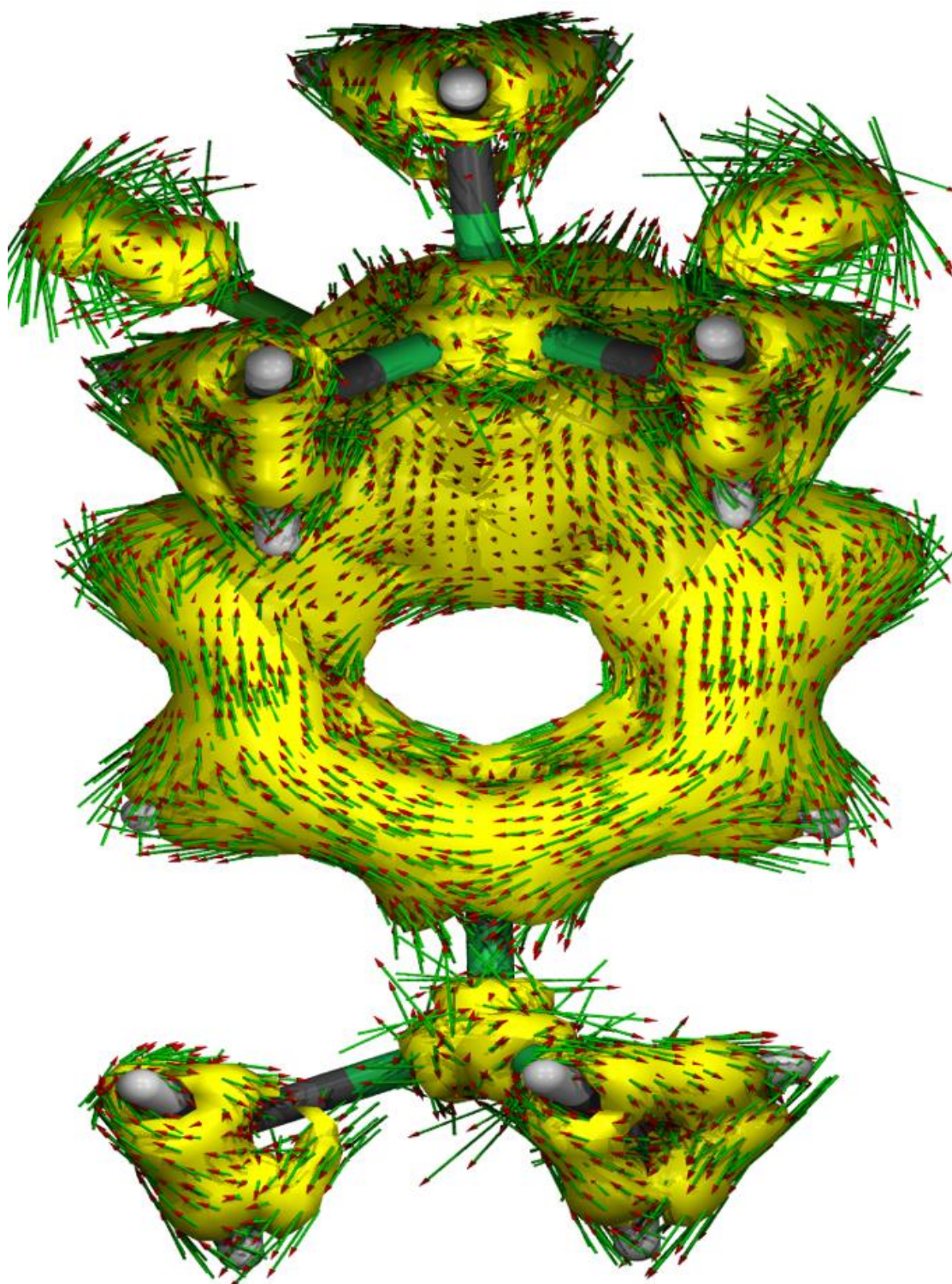


Fig. S34. ACID plot of **Os.Cl** in the singlet state. Isovalue for ACID is 0.035 a.u.

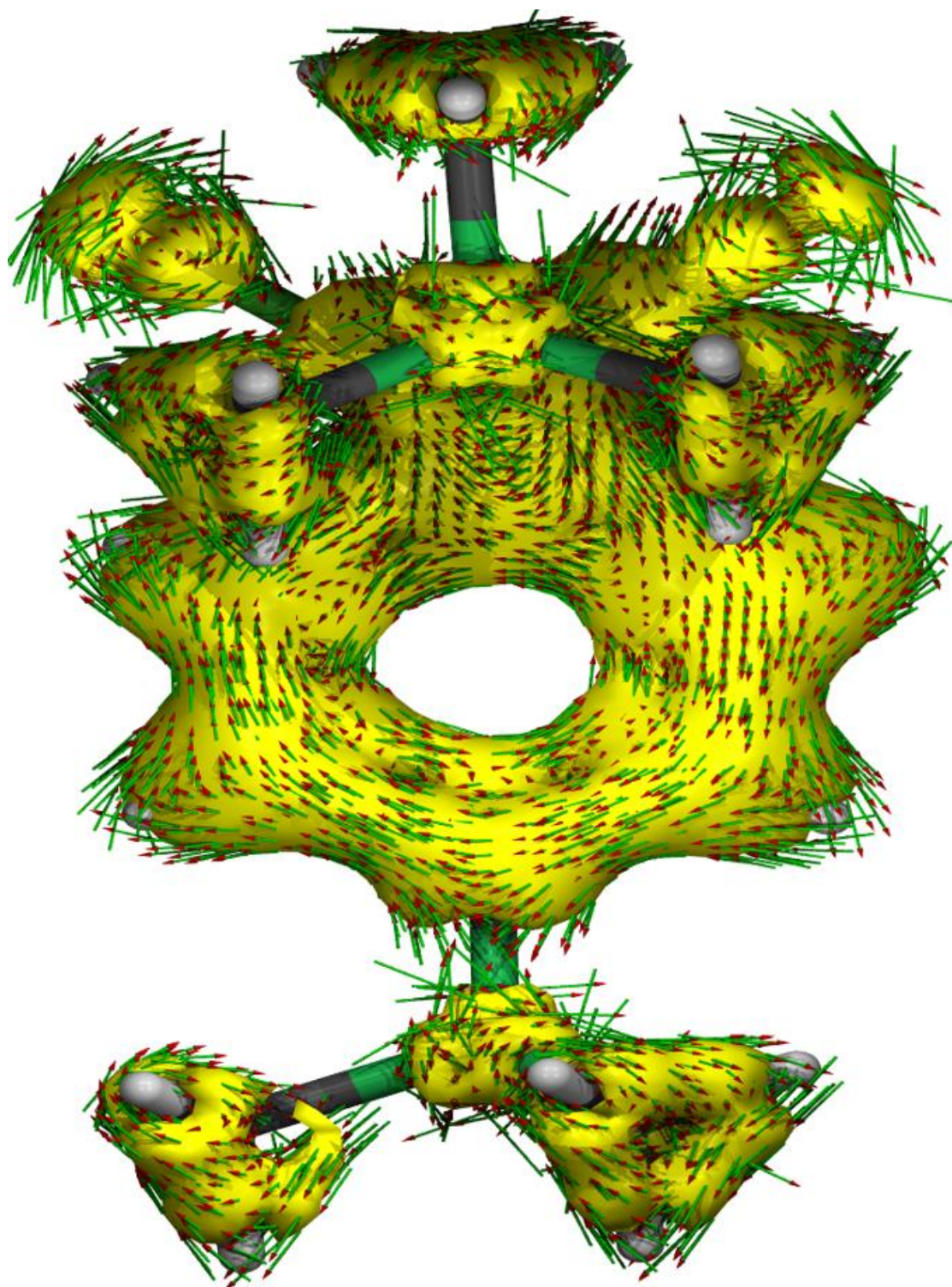


Fig. S35. ACID plot of **IrCl** in the singlet state. Isovalue for ACID is 0.035 a.u.

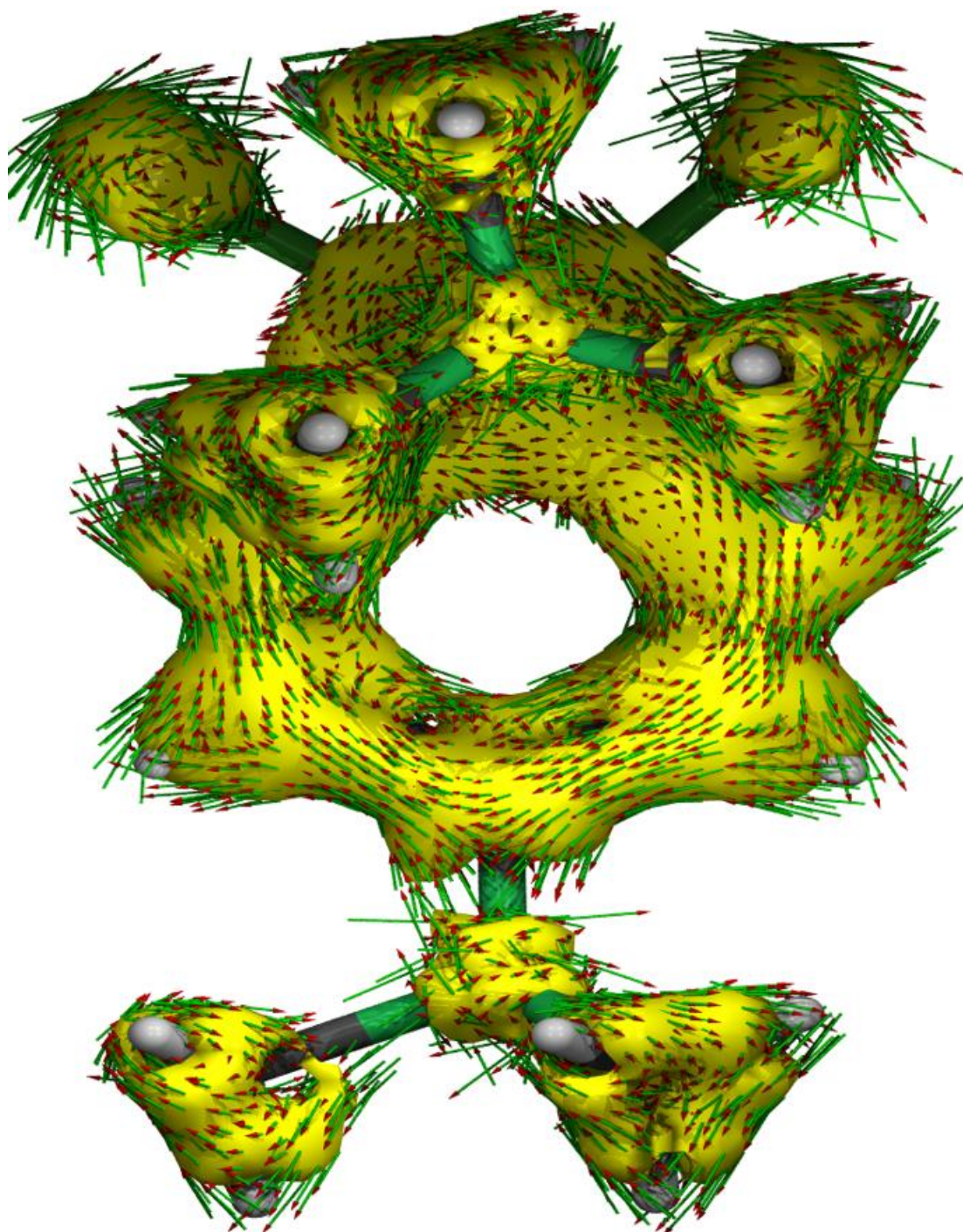


Fig. S36. ACID plot of **Re.Cl** in the triplet state. Isovalue for ACID is 0.035 a.u.

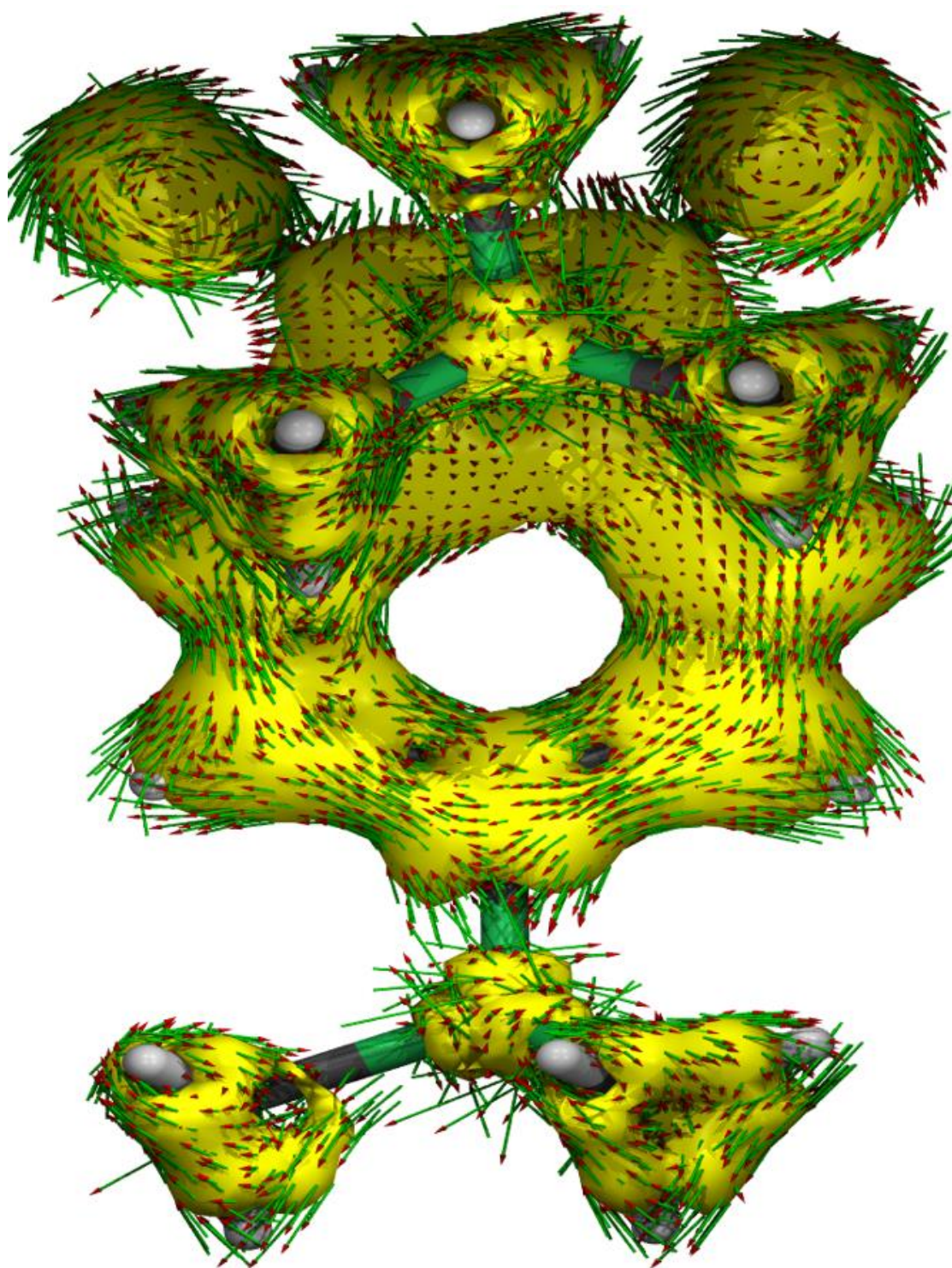


Fig. S37. ACID plot of **Os.Cl** in the triplet state. Isovalue for ACID is 0.035 a.u.

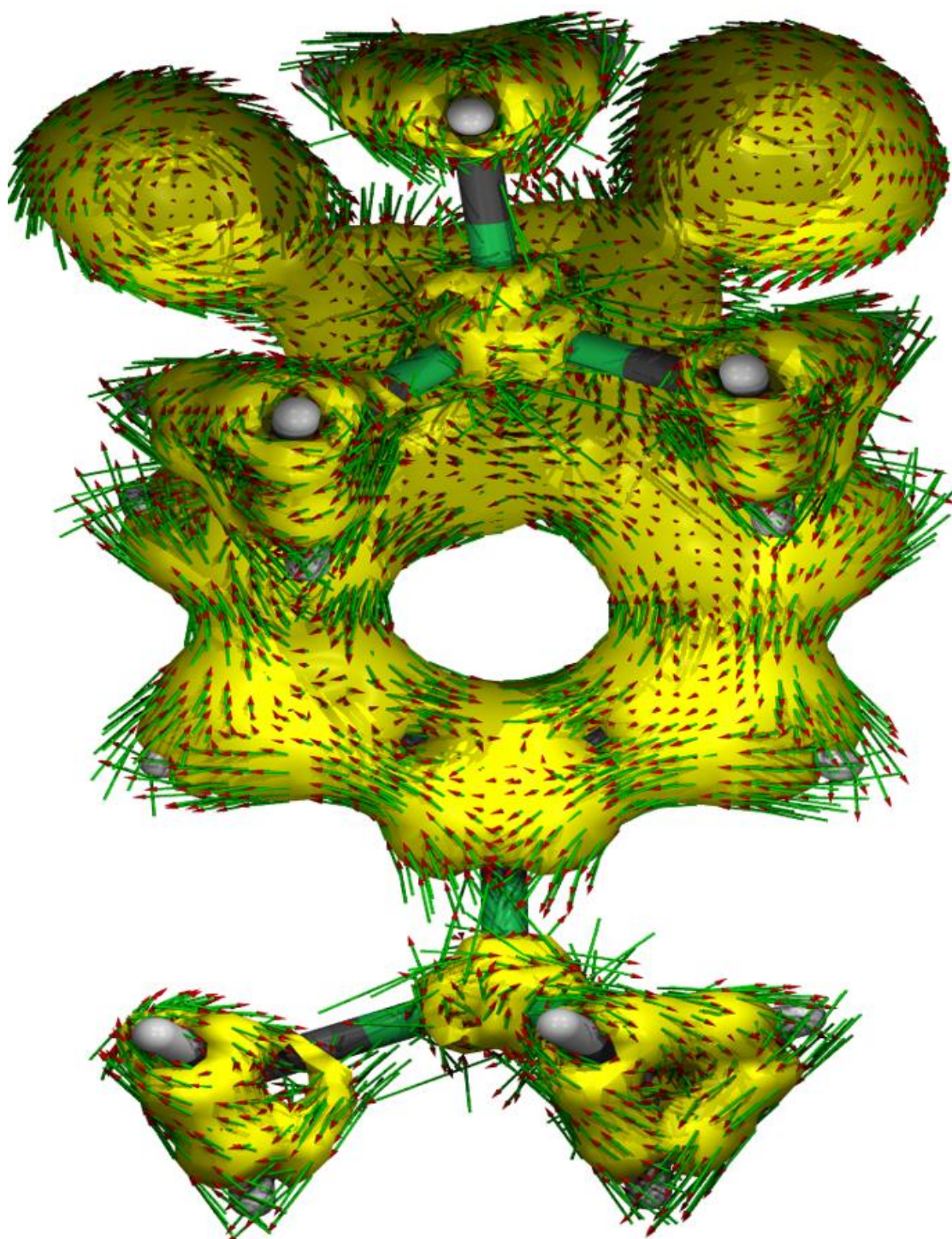


Fig. S38. ACID plot of IrCl in the triplet state. Isovalue for ACID is 0.035 a.u.

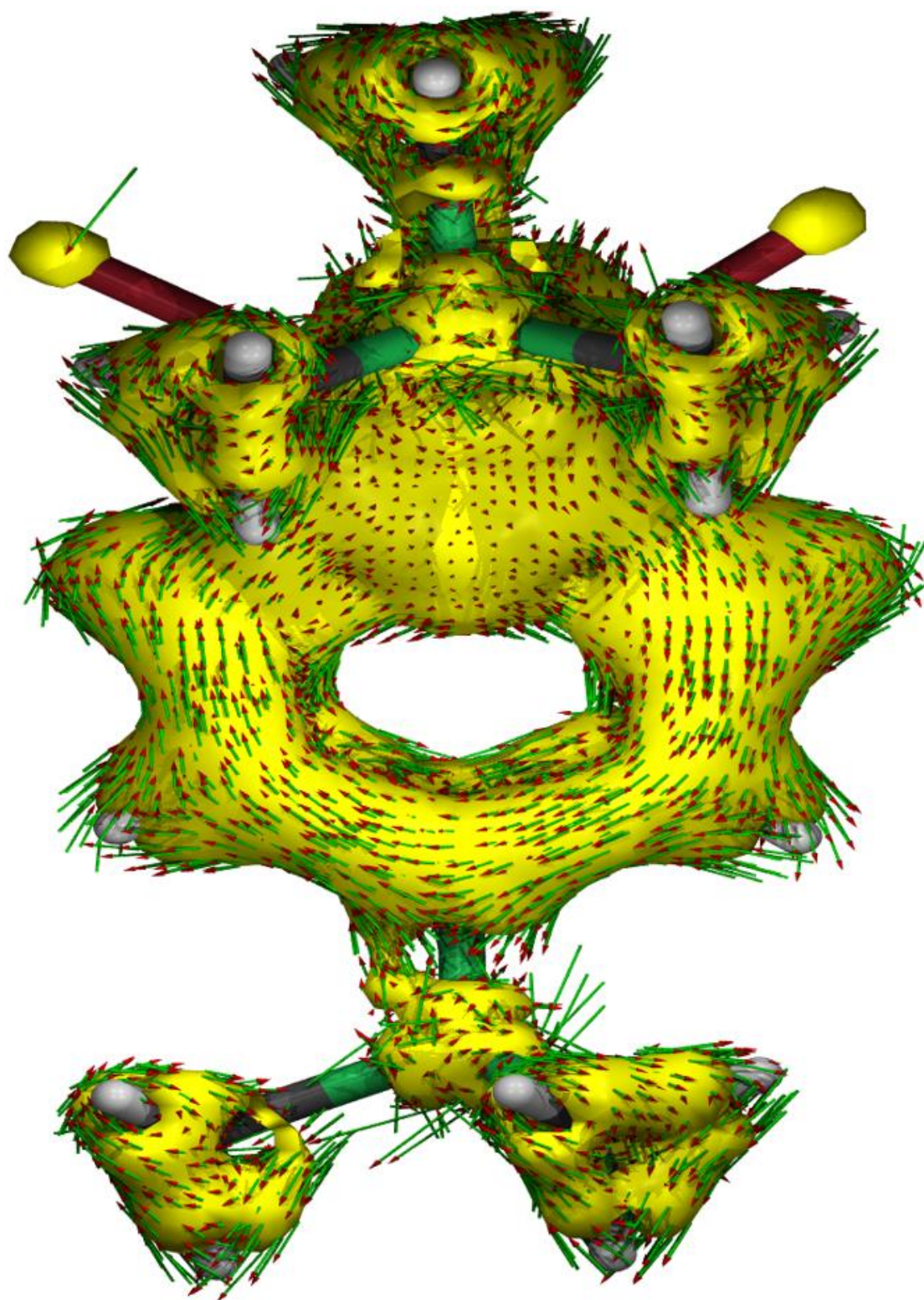


Fig. S39. ACID plot of **Re.Br** in the singlet state. Isovalue for ACID is 0.035 a.u.

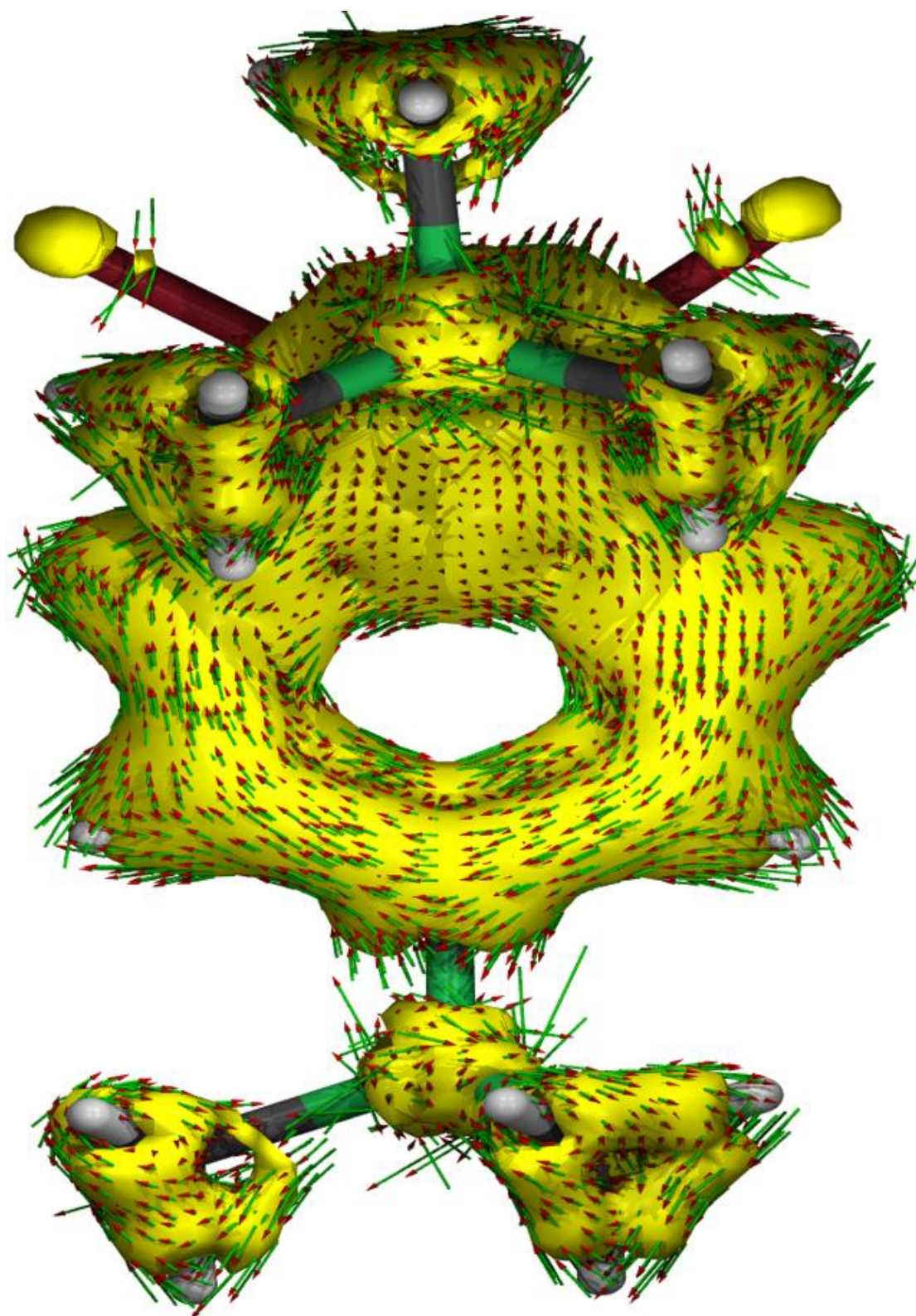


Fig. S40. ACID plot of **Os.Br** in the singlet state. Isovalue for ACID is 0.035 a.u.

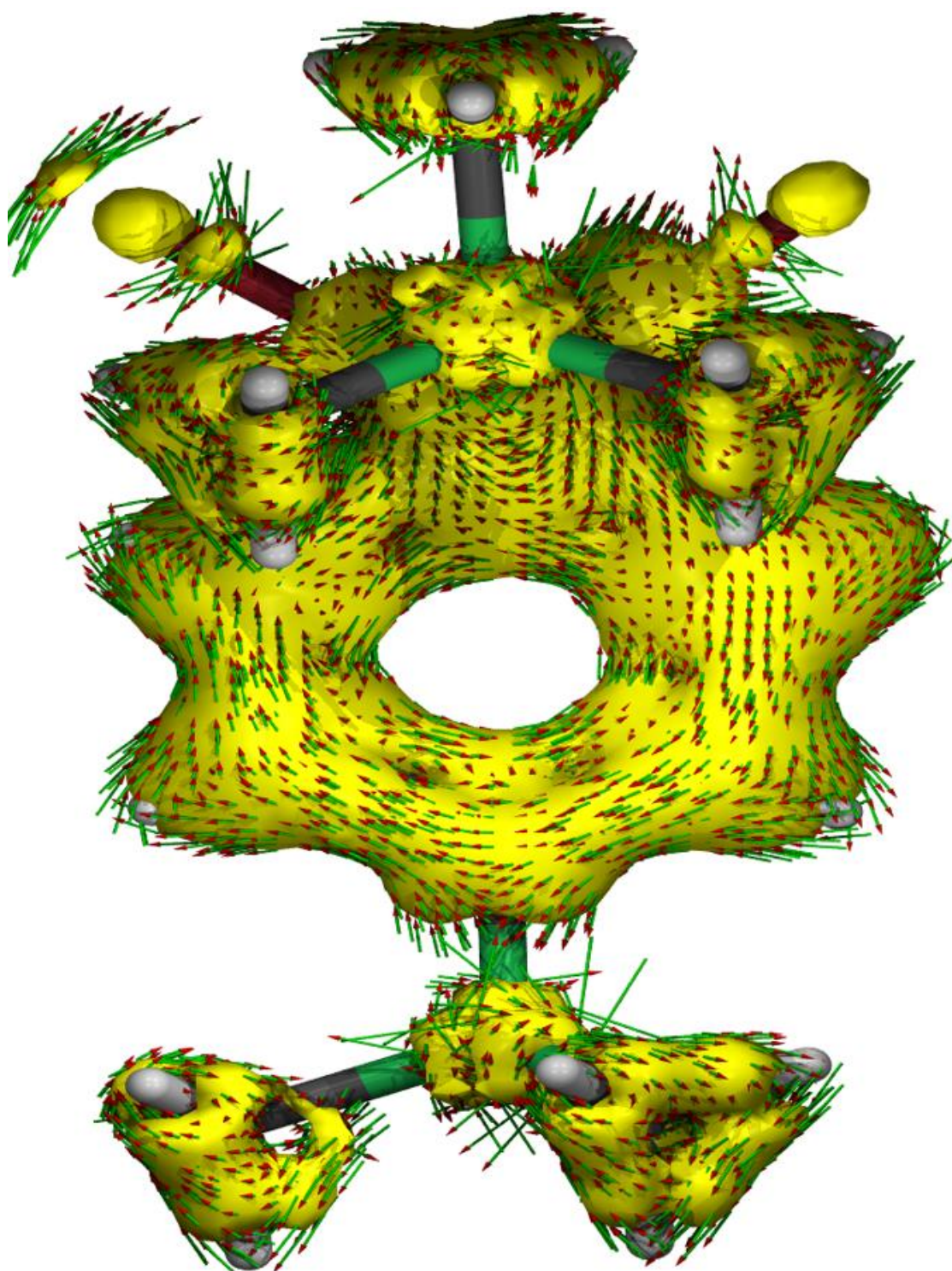


Fig. S41. ACID plot of **Ir.Br** in the singlet state. Isovalue for ACID is 0.035 a.u.

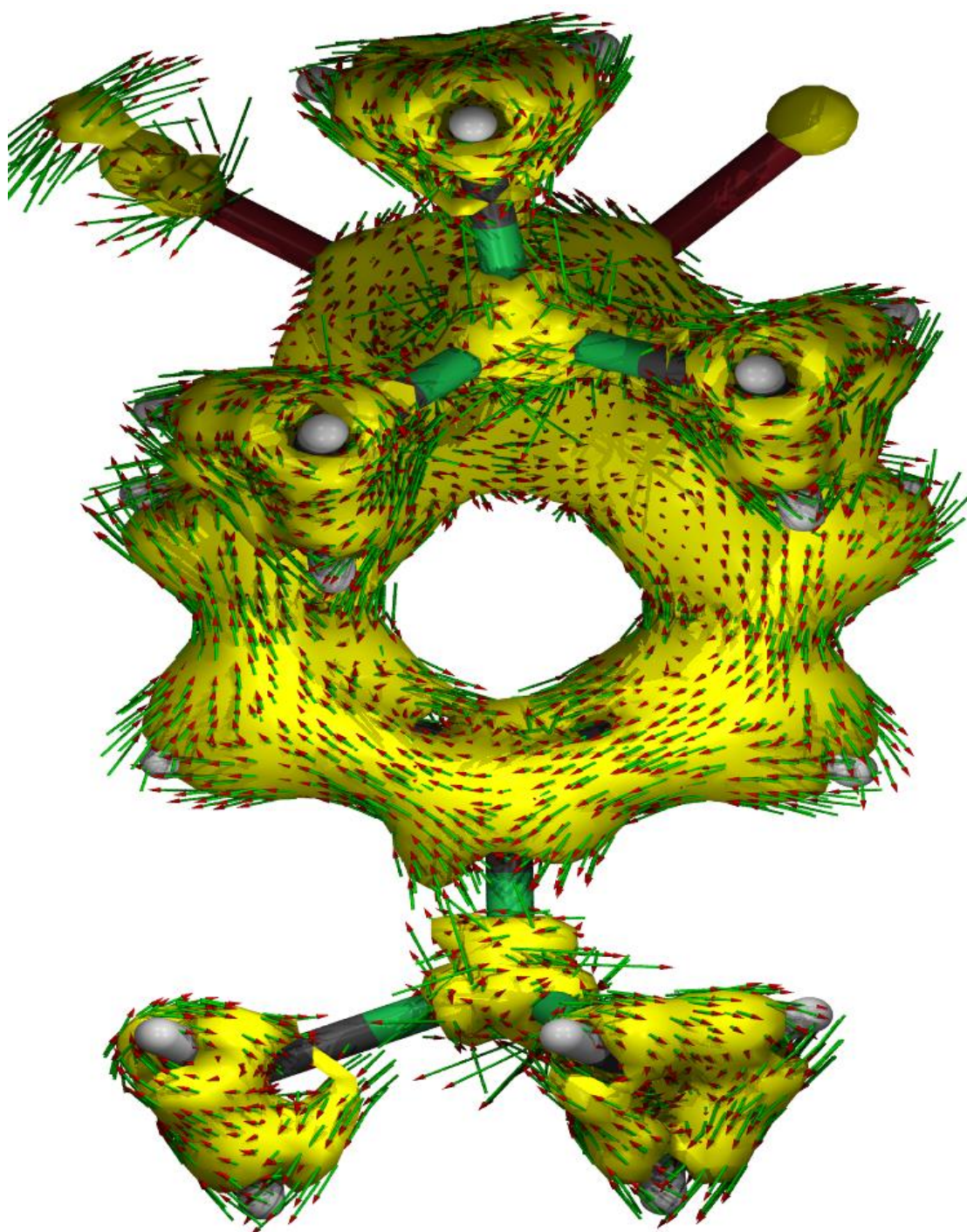


Fig. S42. ACID plot of **Re.Br** in the triplet state. Isovalue for ACID is 0.035 a.u.

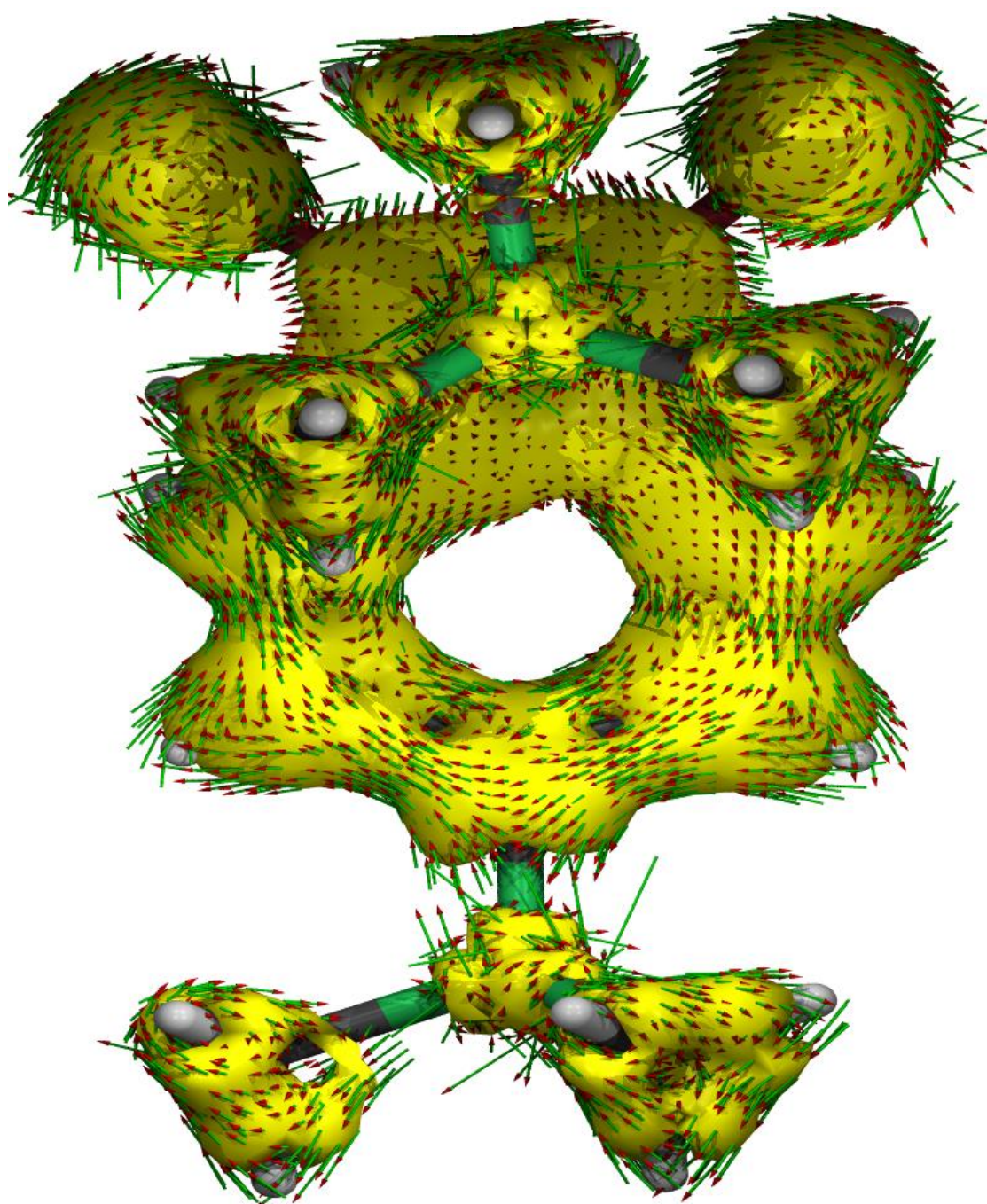


Fig. S43. ACID plot of **Os.Br** in the triplet state. Isovalue for ACID is 0.035 a.u.

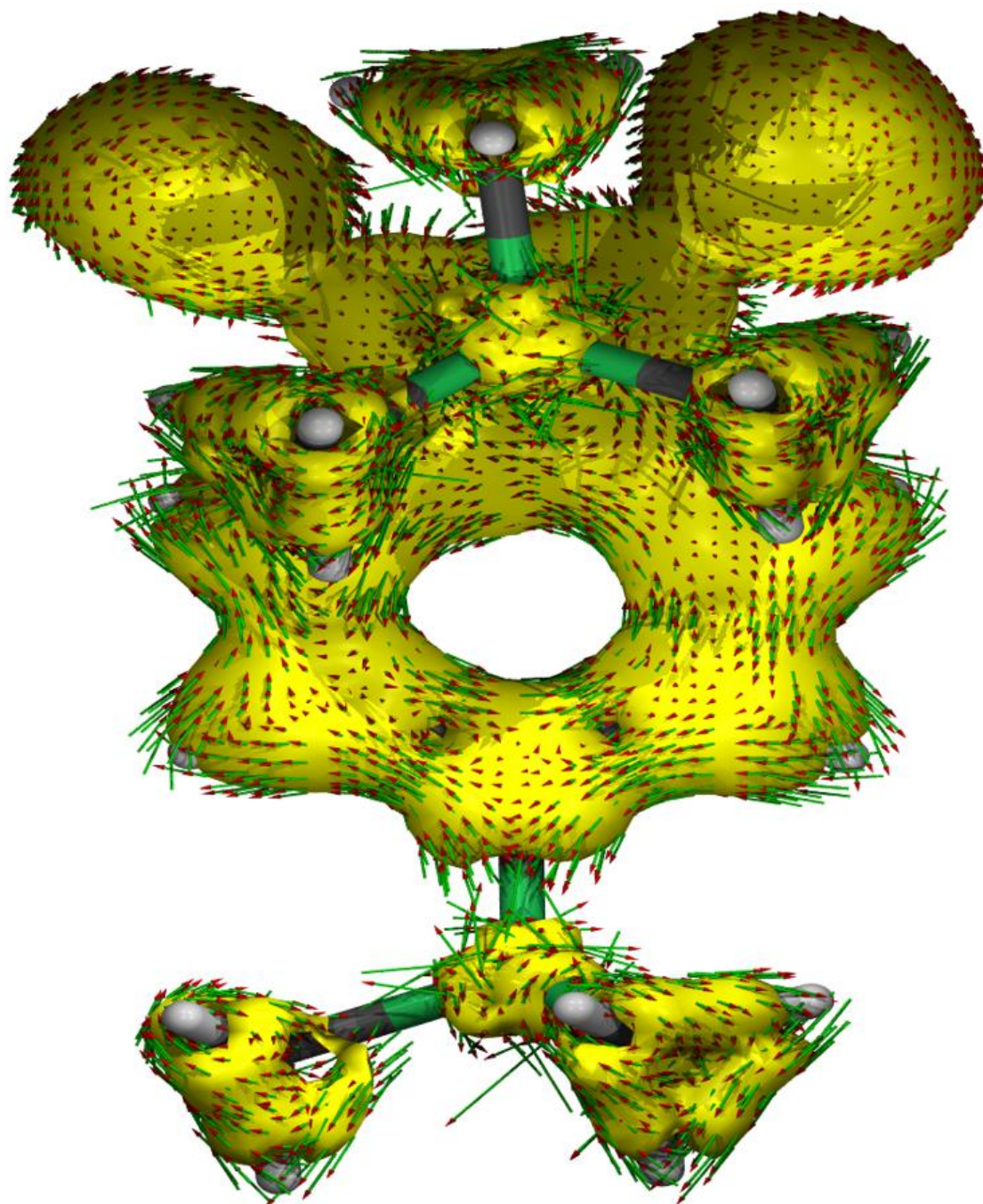


Fig. S44. ACID plot of **Ir.Br** in the triplet state. Isovalue for ACID is 0.035 a.u.

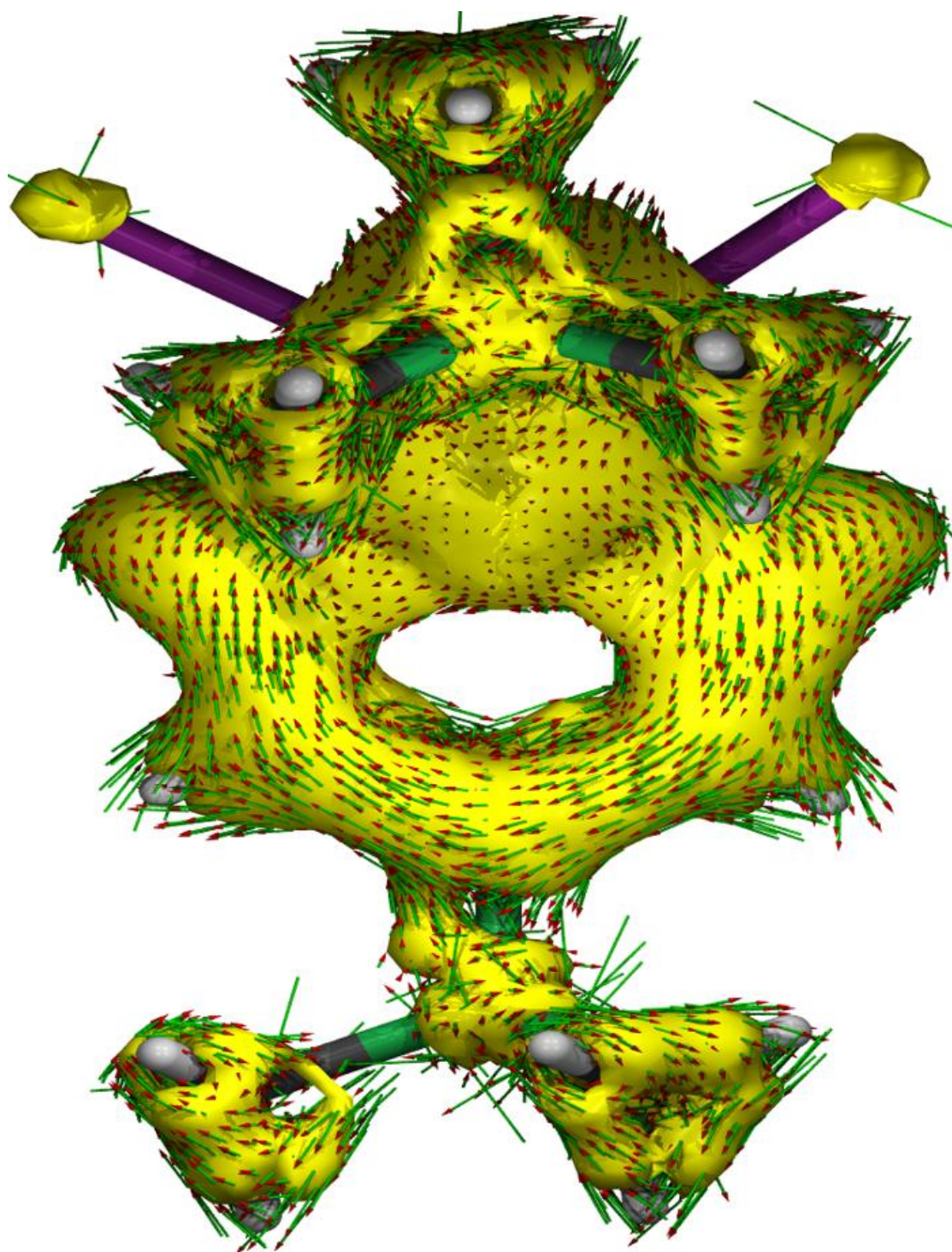


Fig. S45. ACID plot of **Re.I** in the singlet state. Isovalue for ACID is 0.035 a.u.

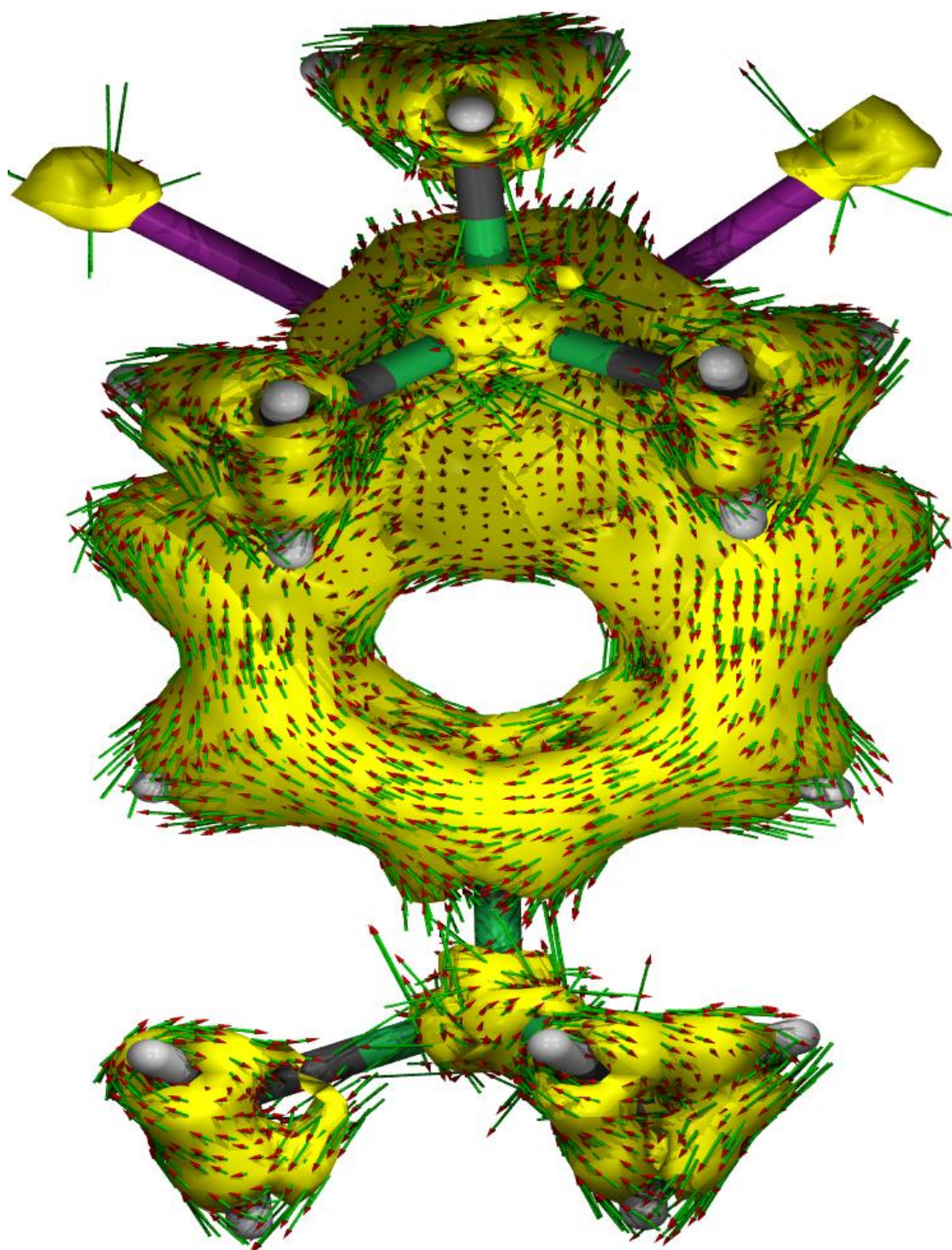


Fig. S46. ACID plot of **Os.I** in the singlet state. Isovalue for ACID is 0.035 a.u.

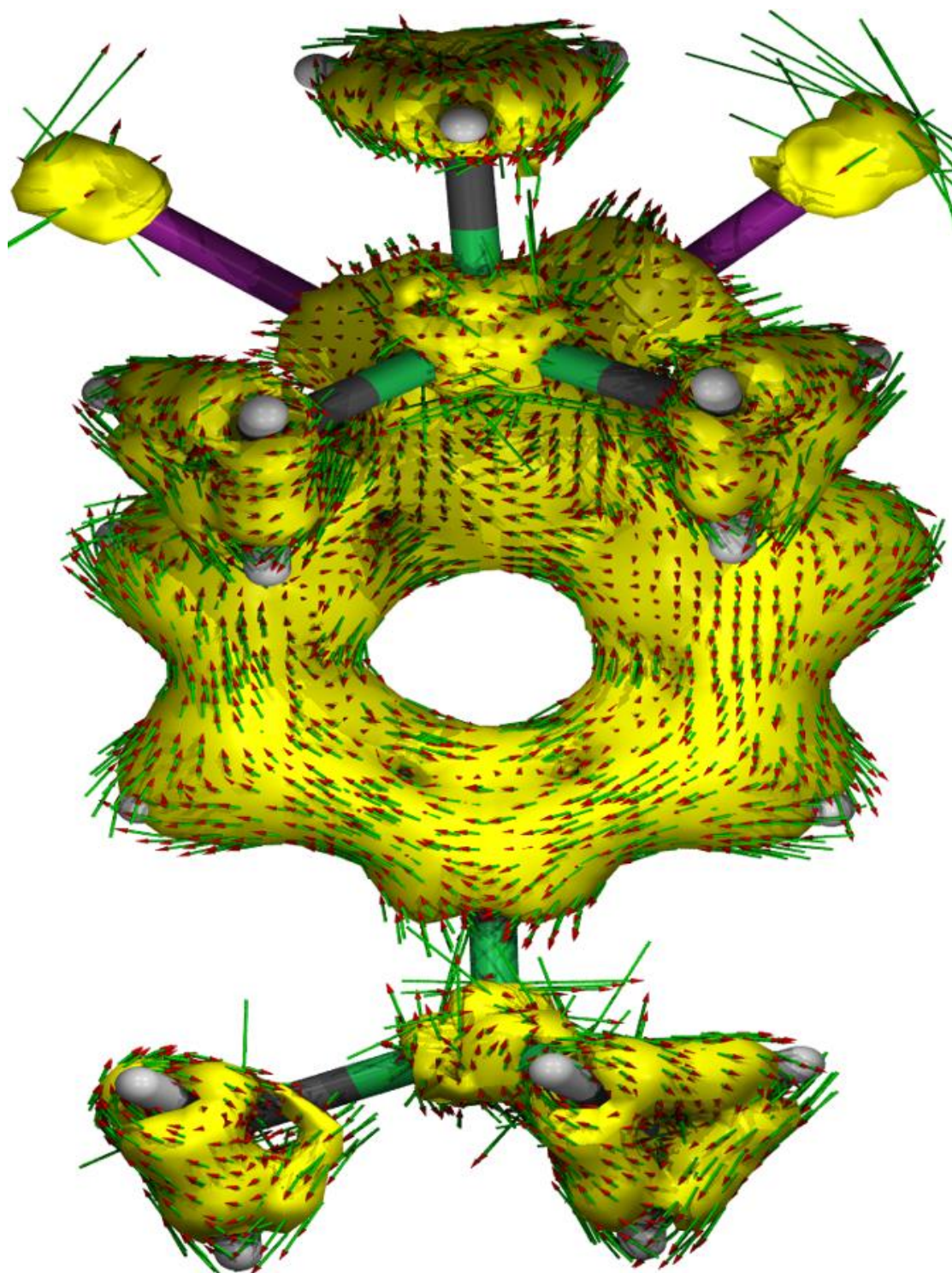


Fig. S47. ACID plot of **Ir.I** in the singlet state. Isovalue for ACID is 0.035 a.u.

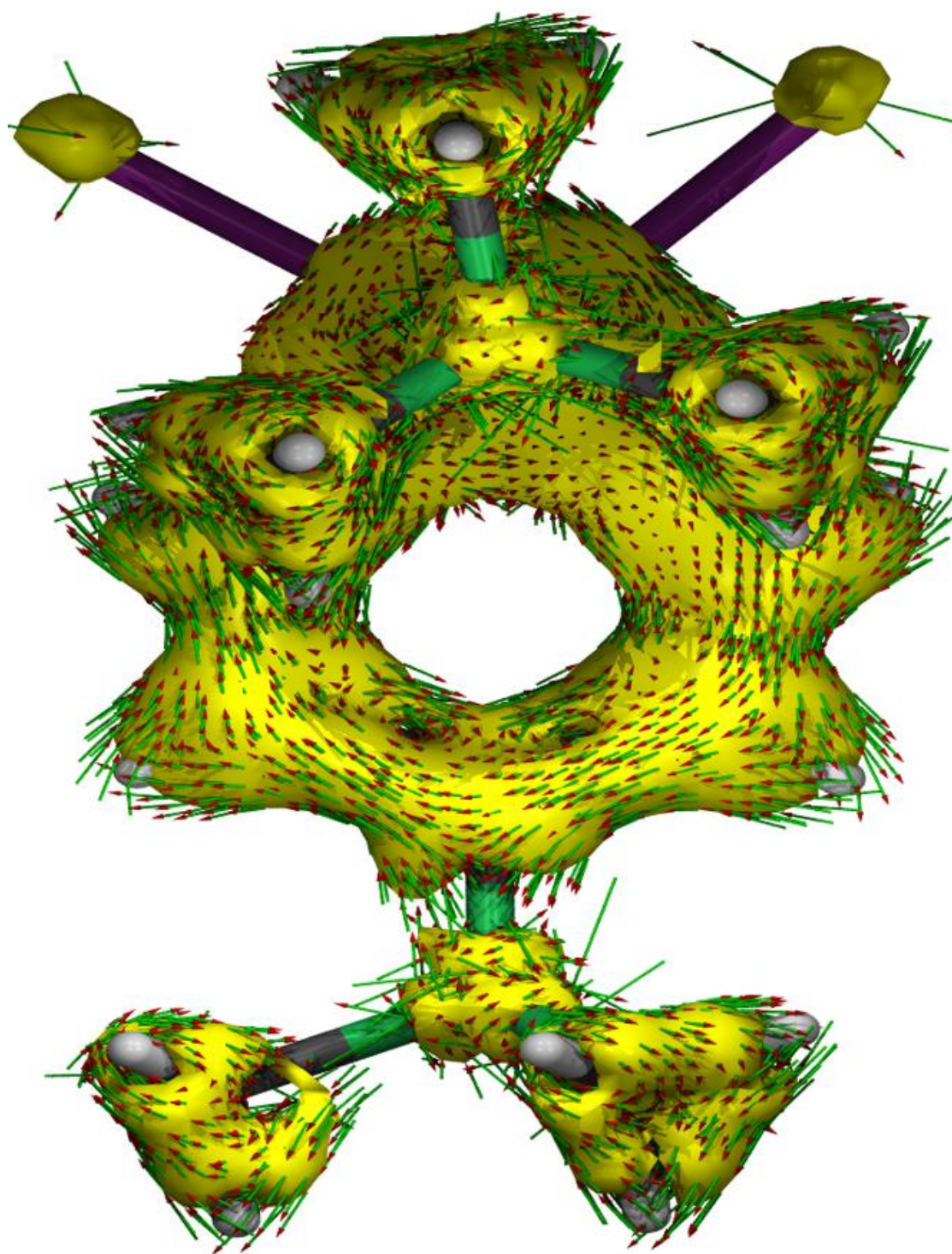


Fig. S48. ACID plot of **Re.I** in the triplet state. Isovalue for ACID is 0.035 a.u.

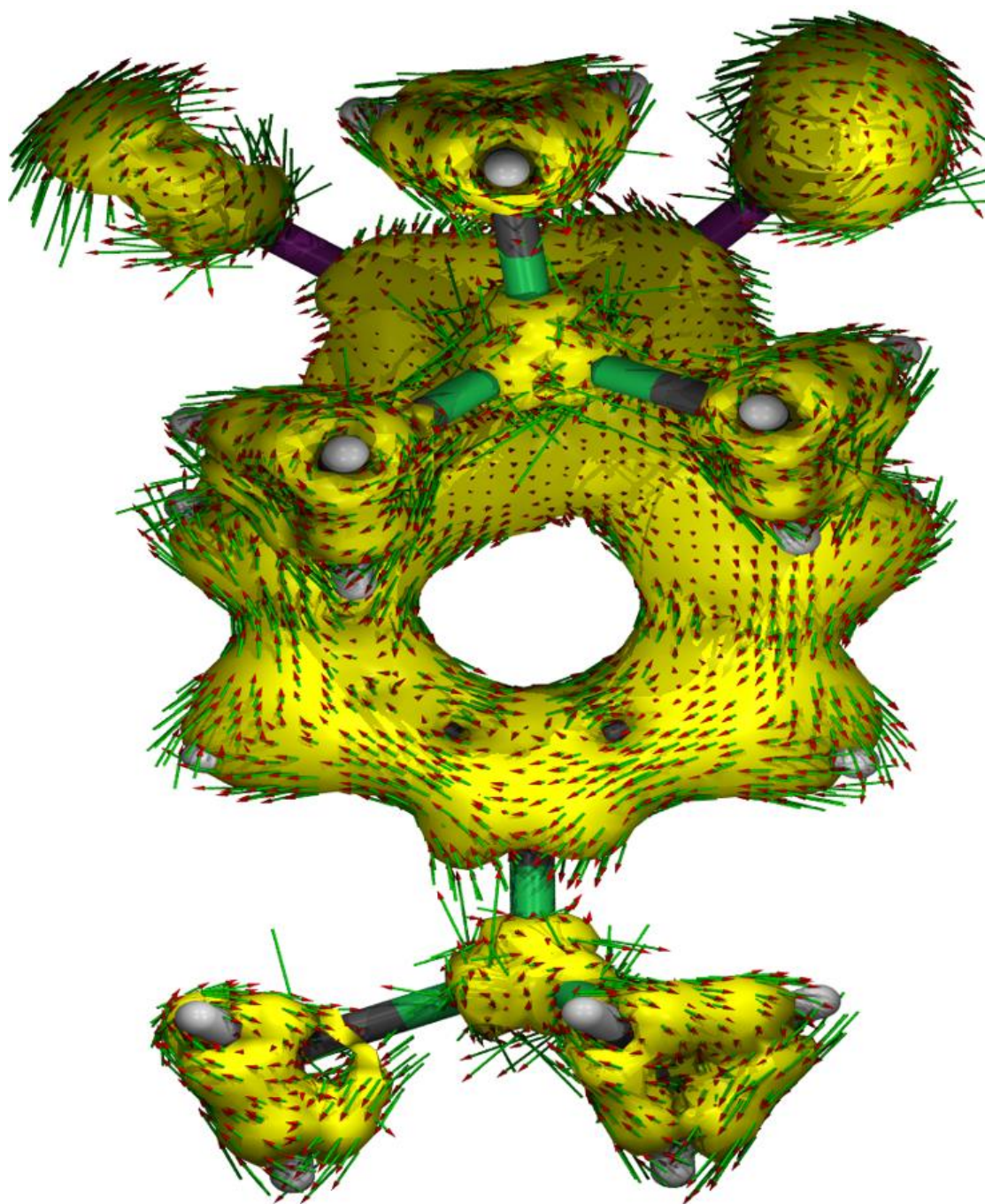


Fig. S49. ACID plot of **Os.I** in the triplet state. Isovalue for ACID is 0.035 a.u.

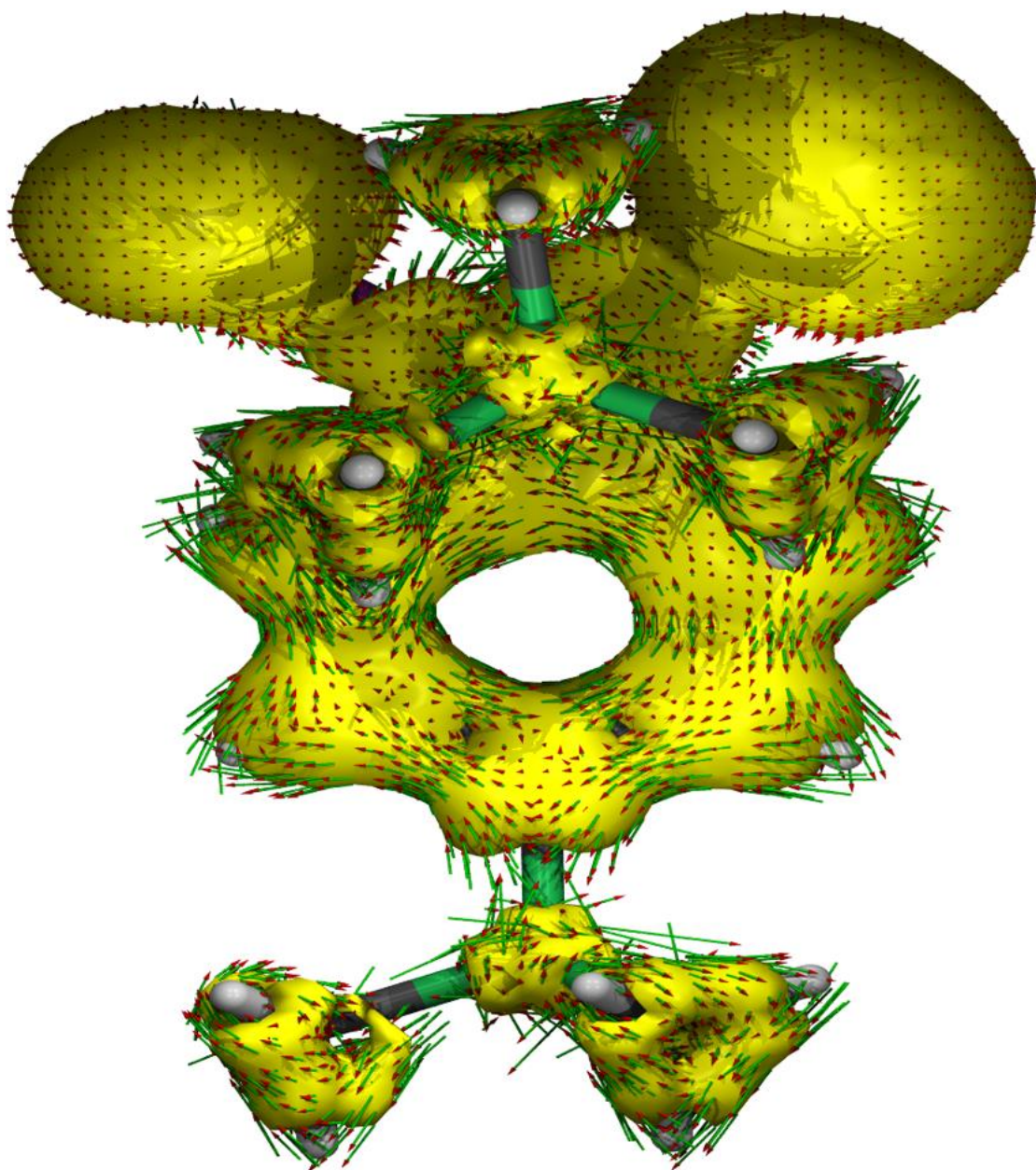


Fig. S50. ACID plot of **Ir.I** in the triplet state. Isovalue for ACID is 0.035 a.u.

15. Cartesian coordinates

Re.F (singlet)

P	-2.00555300	1.88787100	-0.00693900
N	0.80281700	-0.00008100	1.36612500
H	0.40066800	-0.00015100	2.30643500
P	-2.00560100	-1.88785000	-0.00702700
C	2.13854600	0.00004900	-1.25834200
C	2.13686000	-0.00007700	1.27015800
C	2.79411100	-0.00001800	0.02286400
C	0.76172000	0.00007500	-1.46467700
H	2.70534200	-0.00012800	2.19790000
H	0.45125300	0.00014100	-2.51569200
H	2.79821300	0.00008500	-2.13450500
P	4.54087000	-0.00001000	-0.00527500
Re	-0.61196600	0.00000000	-0.02239100
C	-1.78890000	-2.95814300	-1.49146100
H	-2.49375600	-3.79778200	-1.50874600
H	-1.94169400	-2.30793700	-2.35545700
H	-0.76416500	-3.34145700	-1.51651000
C	-3.83898900	-1.72227700	0.09308200
H	-4.18334900	-1.15635200	-0.77444400
H	-4.31822300	-2.70817200	0.10321300
H	-4.09316900	-1.18255800	1.00787400
C	-1.64298000	-2.98901500	1.42983800
H	-2.33998300	-3.83189300	1.50493500
H	-0.62029900	-3.37184100	1.34868000
H	-1.71197900	-2.35152800	2.31484300
C	-3.83898500	1.72229900	0.09234200
H	-4.09362200	1.18241200	1.00690800
H	-4.31822200	2.70819300	0.10242400
H	-4.18290700	1.15653000	-0.77545900
C	-1.64347400	2.98859300	1.43039800
H	-2.34052800	3.83142600	1.50551800
H	-1.71275800	2.35082700	2.31518100
H	-0.62077500	3.37147500	1.34971800
C	-1.78824400	2.95861000	-1.49096600
H	-2.49303100	3.79830700	-1.50824100
H	-0.76347100	3.34185300	-1.51553800
H	-1.94078800	2.30868600	-2.35521800
C	5.24100000	1.45578500	-0.87307700
H	6.33151900	1.39097300	-0.94973500
H	4.80956400	1.51620400	-1.87606900

H	4.96322200	2.36205200	-0.32705200
C	5.29564800	-0.00014600	1.65882800
H	4.98806600	0.88941800	2.21445000
H	4.98804000	-0.88978700	2.21431300
H	6.38549900	-0.00015400	1.56089300
C	5.24099500	-1.45566500	-0.87331300
H	4.80955800	-1.51592500	-1.87631400
H	6.33151400	-1.39084200	-0.94996400
H	4.96321800	-2.36201900	-0.32743200
F	-1.90700600	0.00011000	-1.82502900
F	-1.65574900	-0.00011300	1.97437200

Re.F (triplet)

P	-1.33110900	2.41722500	-0.04423500
N	0.45664000	0.00000200	1.39566200
H	0.10410200	0.00000400	2.35145400
P	-1.33108500	-2.41723000	-0.04423100
C	1.77178700	0.00000300	-1.26227000
C	1.77974700	0.00001000	1.28196200
C	2.44245800	0.00001200	0.03191600
C	0.40114100	-0.00000500	-1.42961400
H	2.36339500	0.00001500	2.20258500
H	0.08768700	-0.00000300	-2.48471800
H	2.42377900	0.00000600	-2.14346900
P	4.17762100	0.00001000	0.00426000
Re	-1.04243200	-0.00000400	0.00003200
C	0.05677400	3.49679100	0.52896600
H	0.94500100	3.27563900	-0.07117700
H	-0.18543800	4.56234800	0.44392100
H	0.28541400	3.26183500	1.57321600
C	-2.76220200	2.91737900	1.00726700
H	-2.69070500	2.35742500	1.94283100
H	-2.80992800	3.99735400	1.18601800
H	-3.67927300	2.58714600	0.50976700
C	-1.75290200	3.09264000	-1.70882100
H	-2.51903000	2.43361000	-2.12780600
H	-2.11874200	4.12504200	-1.67072200
H	-0.87082000	3.04018300	-2.35501200
C	0.05686700	-3.49679300	0.52880300
H	-0.18534300	-4.56235100	0.44376100
H	0.94503000	-3.27561900	-0.07142700
H	0.28561300	-3.26185700	1.57303600
C	-1.75303100	-3.09258900	-1.70880000
H	-2.11889200	-4.12498400	-1.67070600

H	-2.51917500	-2.43352300	-2.12769900
H	-0.87100100	-3.04012700	-2.35506100
C	-2.76207200	-2.91744400	1.00738600
H	-2.80980300	-3.99743500	1.18603900
H	-2.69047000	-2.35758900	1.94300100
H	-3.67918900	-2.58714200	0.51001600
C	4.89621100	1.44807600	-0.87266700
H	5.98364800	1.36280800	-0.97237400
H	4.44640900	1.51956800	-1.86700100
H	4.64782600	2.35858000	-0.31951600
C	4.94643100	0.00004700	1.66355300
H	6.03521500	0.00005200	1.55418800
H	4.64629700	0.88980900	2.22284000
H	4.64631000	-0.88969700	2.22287600
C	4.89621800	-1.44809300	-0.87260300
H	4.44641800	-1.51962700	-1.86693500
H	5.98365500	-1.36282600	-0.97231100
H	4.64783500	-2.35857300	-0.31941500
F	-2.29732900	-0.00000400	1.66109300
F	-2.61665800	-0.00000500	-1.23327200

Os.F (singlet)

Os	-0.67333400	-0.00000700	-0.03025100
P	-1.84767900	2.04856200	-0.00513000
N	0.69306400	-0.00003200	1.36166600
H	0.31093500	-0.00002700	2.31151200
P	-1.84779700	-2.04851600	-0.00513800
C	2.03106000	-0.00001800	-1.24505300
C	2.02451900	-0.00004300	1.26170300
C	2.68430000	-0.00003300	0.02047000
C	0.64791800	-0.00001200	-1.45672700
H	2.58585900	-0.00004700	2.19209300
H	0.33608100	0.00007000	-2.50702900
H	2.67554700	0.00000500	-2.12832700
P	4.46705100	-0.00003200	-0.00275500
C	-1.36296500	3.09641800	1.42060200
H	-0.30992300	3.38228000	1.34191300
H	-1.97847500	4.00080100	1.47450000
H	-1.50884000	2.49330000	2.32025600
C	-1.58433100	3.03339100	-1.52678500
H	-2.22882100	3.91894100	-1.53873100
H	-0.53828000	3.34408300	-1.59861900
H	-1.82461000	2.38331500	-2.37118700
C	-3.65290300	1.83281800	0.14749000

H	-4.14607500	2.80969000	0.18636300
H	-4.00157900	1.26801300	-0.71784500
H	-3.84412900	1.27277300	1.06379600
C	-1.58450100	-3.03335400	-1.52679700
H	-0.53846300	-3.34409000	-1.59863600
H	-2.22902700	-3.91887800	-1.53873800
H	-1.82475700	-2.38327200	-2.37120000
C	-1.36313500	-3.09640600	1.42058800
H	-1.97870500	-4.00074800	1.47449500
H	-0.31011400	-3.38233900	1.34188300
H	-1.50895800	-2.49327500	2.32024100
C	-3.65301000	-1.83267800	0.14748100
H	-4.00165100	-1.26783700	-0.71784400
H	-4.14622900	-2.80952700	0.18633100
H	-3.84421700	-1.27264700	1.06380000
C	5.18354900	-0.00003200	1.67303300
H	6.27474500	-0.00002800	1.58984400
H	4.87441700	0.89198800	2.22464100
H	4.87442400	-0.89205700	2.22463800
C	5.12029900	1.46921600	-0.86691600
H	6.21323800	1.43083700	-0.91390400
H	4.71993300	1.51111300	-1.88373400
H	4.81045000	2.37238000	-0.33307300
C	5.12029900	-1.46927800	-0.86691900
H	4.71993400	-1.51117000	-1.88373900
H	6.21323800	-1.43090000	-0.91390600
H	4.81044800	-2.37244200	-0.33308000
F	-2.06683800	0.00002600	-1.64760900
F	-1.88590300	0.00000700	1.80128000

Os.F (triplet)

Os	0.98491500	-0.00001000	-0.01162400
P	1.41158500	-2.39949000	-0.02744600
N	-0.50222800	0.00004100	1.36142700
H	-0.13370700	0.00007100	2.31124900
P	1.41166300	2.39946500	-0.02748200
C	-1.81179500	-0.00002800	-1.24433500
C	-1.82167600	0.00004200	1.25851400
C	-2.49466200	0.00001400	0.02187100
C	-0.43978800	-0.00004900	-1.39650700
H	-2.38566500	0.00007400	2.18876100
H	-0.08978200	-0.00005800	-2.43521500
H	-2.42973500	-0.00003700	-2.14438900
P	-4.26544100	0.00003300	-0.00739200

C	3.14992700	2.65194400	0.49532800
H	3.79627300	2.15618500	-0.23419300
H	3.40522500	3.71409500	0.56230900
H	3.28976800	2.15524000	1.45818400
C	0.40317500	3.45869100	1.08960400
H	0.71229400	4.50737600	1.02720400
H	-0.65469100	3.38161300	0.82056400
H	0.52785600	3.11361800	2.12037600
C	1.28532700	3.17333200	-1.68821800
H	0.24641200	3.15554900	-2.03095200
H	1.64698300	4.20678800	-1.67962900
H	1.89035500	2.58263900	-2.38235500
C	3.14964400	-2.65208800	0.49599300
H	3.40484600	-3.71425500	0.56306900
H	3.79628800	-2.15638600	-0.23330400
H	3.28918900	-2.15538200	1.45889100
C	0.40262900	-3.45881900	1.08912300
H	-0.65513100	-3.38164900	0.81969400
H	0.71171700	-4.50751100	1.02669100
H	0.52693400	-3.11390100	2.11999200
C	1.28586100	-3.17312900	-1.68833200
H	1.64761500	-4.20655100	-1.67978300
H	0.24705400	-3.15539400	-2.03140000
H	1.89105600	-2.58225500	-2.38216800
C	-4.92862800	1.46385000	-0.87801800
H	-6.02031800	1.41208700	-0.94004000
H	-4.63752100	2.37069200	-0.34004400
H	-4.51615700	1.51175000	-1.88987800
C	-4.99031100	0.00009900	1.66534100
H	-4.68525400	0.89220900	2.21903100
H	-6.08098400	0.00011100	1.57607800
H	-4.68527800	-0.89198100	2.21909200
C	-4.92866200	-1.46382800	-0.87791700
H	-4.63758100	-2.37064100	-0.33987800
H	-6.02035000	-1.41204200	-0.93994700
H	-4.51618700	-1.51181000	-1.88977200
F	2.48758600	-0.00008100	-1.28481900
F	2.16210000	0.00007400	1.65318700

Ir.F (singlet)

P	-1.75355600	2.17418800	0.01854000
N	0.63193200	-0.00000200	1.34085400
H	0.23490200	0.00001100	2.28469300
P	-1.75351800	-2.17420200	0.01852700

C	1.97713500	0.00002400	-1.22673800
C	1.94919000	-0.00001100	1.25549500
C	2.63370700	-0.00000300	0.01498900
C	0.58229000	0.00003300	-1.43494300
H	2.50004600	-0.00001400	2.19198800
H	0.25279400	0.00007500	-2.47717600
H	2.59781100	0.00005300	-2.12387800
P	4.45411600	0.00000800	0.00316500
Ir	-0.73765900	0.00000300	-0.05358600
C	-1.36365600	3.12627700	-1.48953900
H	-1.63917900	2.51633500	-2.35369400
H	-1.94592600	4.05484800	-1.49860700
H	-0.29852200	3.36763400	-1.53267200
C	-1.22241600	3.11223700	1.49218500
H	-0.15205200	3.33124300	1.45175000
H	-1.77839400	4.05524200	1.54609000
H	-1.44825000	2.50877900	2.37500000
C	-3.55879600	1.98277200	0.10458700
H	-3.80132400	1.41444500	1.00308900
H	-4.01876000	2.97652900	0.14390000
H	-3.89552800	1.44528900	-0.78263200
C	-3.55876000	-1.98282500	0.10463200
H	-4.01869600	-2.97659500	0.14391900
H	-3.80128100	-1.41454000	1.00316200
H	-3.89552900	-1.44531800	-0.78255800
C	-1.36364700	-3.12624900	-1.48958700
H	-0.29850800	-3.36757600	-1.53276300
H	-1.94589100	-4.05483700	-1.49865400
H	-1.63921800	-2.51629800	-2.35372000
C	-1.22231600	-3.11227400	1.49213500
H	-1.77828600	-4.05528300	1.54604500
H	-0.15195100	-3.33127300	1.45165100
H	-1.44811800	-2.50883100	2.37496800
C	5.06813900	1.48136100	-0.85956900
H	6.16291700	1.46222200	-0.88129300
H	4.69696400	1.50768500	-1.88826000
H	4.73619500	2.38316000	-0.33641000
C	5.12352500	-0.00000600	1.69454700
H	4.81248800	0.89526900	2.24096800
H	4.81250500	-0.89529900	2.24094700
H	6.21686500	0.00000600	1.62999700
C	5.06815900	-1.48131700	-0.85960100
H	4.69698700	-1.50762300	-1.88829300
H	6.16293700	-1.46216300	-0.88132300

H	4.73622700	-2.38313200	-0.33646400
F	-2.00831700	-0.00003900	1.65748000
F	-2.12156400	0.00000300	-1.56133200

Ir.F (triplet)

P	-1.43090900	2.41880300	-0.01553600
N	0.50838300	0.00004000	1.34560300
H	0.12466800	0.00004400	2.29067100
P	-1.43079500	-2.41884100	-0.01551900
C	1.81826300	0.00001400	-1.23055000
C	1.81783600	0.00005400	1.24754700
C	2.50954300	0.00003800	0.01258800
C	0.44682200	-0.00000200	-1.37830100
H	2.37166800	0.00006800	2.18357400
H	0.06065200	-0.00003900	-2.40141700
H	2.40923300	-0.00000200	-2.14601700
P	4.31899900	0.00004300	-0.01320300
Ir	-0.98855300	-0.00000900	-0.02538000
C	-1.19639700	3.19867800	-1.65482900
H	-1.75782400	2.62836800	-2.40067000
H	-1.56827400	4.22874100	-1.64106200
H	-0.13798800	3.20451200	-1.93050600
C	-0.49106900	3.40600600	1.20874900
H	0.58092200	3.36254300	0.99610000
H	-0.81553200	4.45163800	1.17418300
H	-0.67671400	3.01599800	2.21376400
C	-3.20050700	2.58810600	0.40628800
H	-3.38603600	2.10714200	1.36953100
H	-3.48163800	3.64534300	0.45190500
H	-3.79567800	2.08160300	-0.35826400
C	-3.20033000	-2.58823600	0.40653400
H	-3.48140200	-3.64548800	0.45217600
H	-3.38576300	-2.10728800	1.36980200
H	-3.79562300	-2.08175800	-0.35794000
C	-1.19646900	-3.19862600	-1.65488100
H	-0.13809200	-3.20443700	-1.93068100
H	-1.56833800	-4.22869100	-1.64112700
H	-1.75798700	-2.62827300	-2.40062100
C	-0.49074300	-3.40605700	1.20859300
H	-0.81515100	-4.45170600	1.17400900
H	0.58121700	-3.36252200	0.99580700
H	-0.67627800	-3.01611900	2.21365500
C	4.93427400	1.47796800	-0.88289800
H	6.02846100	1.45000700	-0.92001600

H	4.54960900	1.50808500	-1.90658500
H	4.61722900	2.38222100	-0.35495800
C	5.00160900	0.00006000	1.67312500
H	4.69544000	0.89533800	2.22227100
H	4.69544000	-0.89520600	2.22228900
H	6.09437900	0.00006000	1.60013600
C	4.93428300	-1.47789400	-0.88287200
H	4.54961700	-1.50803200	-1.90655800
H	6.02847000	-1.44992600	-0.91999200
H	4.61724400	-2.38213900	-0.35491400
F	-2.05765900	0.00000900	1.66761900
F	-2.40768600	-0.00005900	-1.33808600

Re.Cl (singlet)

P	1.65793500	-2.16515000	-0.01941200
Cl	2.22558800	-0.00003100	-2.17081400
Cl	1.99755400	0.00016800	2.36655000
N	-0.81443700	0.00025800	1.36468300
H	-0.47265500	0.00031200	2.33036300
P	1.65804000	2.16504100	-0.01955800
C	-2.15884500	0.00002200	-1.26006900
C	-2.15123800	0.00041400	1.25784900
C	-2.80959900	0.00031300	0.01435600
C	-0.77602200	-0.00009200	-1.47044000
H	-2.71906000	0.00065600	2.18617700
H	-0.49809300	-0.00030900	-2.53174700
H	-2.81384100	-0.00011400	-2.13977400
P	-4.56522300	0.00003700	-0.01128100
Re	0.58223800	-0.00002000	-0.03306500
C	1.29136700	3.21941400	-1.49192900
H	1.80561600	4.18523200	-1.42103100
H	1.61629200	2.68508400	-2.38697800
H	0.21175900	3.38786600	-1.55464200
C	3.49011000	2.23897100	0.12674600
H	3.92165200	1.71437700	-0.72808300
H	3.83087000	3.28094300	0.14420700
H	3.77749800	1.73029800	1.04941300
C	1.08143700	3.23875000	1.37367700
H	1.57460000	4.21766000	1.34724200
H	-0.00174700	3.38208000	1.30136100
H	1.30995200	2.73051300	2.31341100
C	3.48996200	-2.23917400	0.12727800
H	3.77719400	-1.73051200	1.04999700
H	3.83068200	-3.28117000	0.14486400

H	3.92174900	-1.71467300	-0.72748000
C	1.08090300	-3.23892200	1.37362000
H	1.57400500	-4.21785500	1.34731000
H	1.30901200	-2.73073200	2.31346700
H	-0.00227000	-3.38220500	1.30082300
C	1.29139500	-3.21955500	-1.49181100
H	1.80552000	-4.18542200	-1.42080700
H	0.21175600	-3.38790300	-1.55451900
H	1.61636300	-2.68531100	-2.38688400
C	-5.25223800	-1.45988500	-0.87767400
H	-6.34325700	-1.40223500	-0.95007600
H	-4.82458300	-1.51639100	-1.88251100
H	-4.96709700	-2.36452900	-0.33273300
C	-5.31269200	0.00147400	1.65487600
H	-5.00374600	-0.88790700	2.21017100
H	-5.00339400	0.89162300	2.20874500
H	-6.40284800	0.00159700	1.56052300
C	-5.25246700	1.45828500	-0.88027600
H	-4.82473000	1.51320900	-1.88516100
H	-6.34345800	1.40020000	-0.95270100
H	-4.96764400	2.36393600	-0.33684300

Re.Cl_(triplet)

P	1.13383600	2.44499900	0.04967100
Cl	2.71786500	0.00073200	1.72494100
Cl	2.37849000	-0.00006300	-2.11417700
N	-0.59903900	-0.00029600	-1.36199600
H	-0.24230000	-0.00033900	-2.31590400
P	1.13492400	-2.44479300	0.04990200
C	-1.92284000	-0.00031000	1.26638300
C	-1.92053700	-0.00044300	-1.25819100
C	-2.59786400	-0.00047500	-0.01983500
C	-0.55448400	-0.00005200	1.42925600
H	-2.48910900	-0.00054800	-2.18773900
H	-0.22426200	0.00006500	2.47453700
H	-2.56205100	-0.00041800	2.15536600
P	-4.33801700	-0.00043400	-0.00103100
Re	0.90010000	0.00008600	0.03061100
C	0.12941800	3.37276500	-1.19795600
H	-0.93245600	3.15220200	-1.05027800
H	0.28792700	4.45482200	-1.12594600
H	0.41721700	3.03171400	-2.19708100
C	2.84650500	3.03973200	-0.27502000
H	3.17110200	2.64872700	-1.24279200

H	2.90101300	4.13446400	-0.26537400
H	3.50374400	2.62470700	0.49392100
C	0.70001600	3.28315500	1.63828600
H	1.32714100	2.85703200	2.42711600
H	0.85717600	4.36692400	1.59034500
H	-0.34554800	3.07299000	1.88345800
C	0.13212300	-3.37280600	-1.19880100
H	0.29122100	-4.45479400	-1.12707200
H	-0.93001300	-3.15293600	-1.05196600
H	0.42059900	-3.03117000	-2.19753300
C	0.70019300	-3.28333300	1.63807200
H	0.85736100	-4.36709200	1.58993200
H	1.32696100	-2.85745800	2.42732600
H	-0.34547500	-3.07320900	1.88281800
C	2.84819700	-3.03862200	-0.27328800
H	2.90327600	-4.13332600	-0.26350700
H	3.17338600	-2.64754200	-1.24082900
H	3.50454700	-2.62317200	0.49617700
C	-5.05045200	1.45066000	0.87066100
H	-6.13931200	1.37213500	0.95749600
H	-4.61284600	1.51740000	1.87082000
H	-4.79005600	2.36048700	0.32204500
C	-5.08676000	-0.00084800	-1.66800800
H	-6.17663000	-0.00088400	-1.57063000
H	-4.78105100	0.88906500	-2.22414800
H	-4.78094500	-0.89099200	-2.22372200
C	-5.05046300	-1.45110600	0.87134100
H	-4.61267800	-1.51755800	1.87143800
H	-6.13929300	-1.37237100	0.95836400
H	-4.79033000	-2.36117000	0.32299600

Os.Cl (singlet)

Os	0.67203800	-0.00001400	-0.03655900
P	1.50111600	-2.27627700	-0.01425300
Cl	2.32773100	0.00021000	-1.96387800
Cl	2.12963100	0.00004400	2.15774800
N	-0.72573500	-0.00012800	1.34018200
H	-0.36537800	-0.00026200	2.30045000
P	1.50095000	2.27629700	-0.01418800
C	-2.06729600	0.00001200	-1.23797100
C	-2.05384800	-0.00011100	1.25023500
C	-2.72449600	0.00000100	0.01167300
C	-0.67280900	-0.00007400	-1.43621400
H	-2.60817100	-0.00017300	2.18501800

H	-0.37743100	0.00008500	-2.49076200
H	-2.69626800	0.00008700	-2.13191100
P	-4.51610700	-0.00004500	-0.00947400
C	0.80381400	-3.24027400	1.39016800
H	-0.28795900	-3.26566100	1.32462400
H	1.18731700	-4.26626100	1.37209300
H	1.09893100	-2.75607700	2.32435000
C	1.01911800	-3.21851300	-1.51715900
H	1.43572000	-4.23094000	-1.47794200
H	-0.07070200	-3.27776200	-1.58587100
H	1.40487000	-2.69585500	-2.39545600
C	3.31352400	-2.48693000	0.12563200
H	3.54706800	-3.55734000	0.13470400
H	3.79452200	-2.00447300	-0.72673100
H	3.65540400	-2.01731300	1.04944000
C	1.01882000	3.21855600	-1.51703500
H	-0.07100500	3.27775000	-1.58568500
H	1.43537200	4.23100500	-1.47781300
H	1.40454800	2.69594300	-2.39537000
C	0.80367600	3.24017400	1.39033300
H	1.18713000	4.26618000	1.37231200
H	-0.28810200	3.26551500	1.32484900
H	1.09886400	2.75592700	2.32446800
C	3.31335600	2.48702000	0.12557400
H	3.79430300	2.00488500	-0.72700200
H	3.54682800	3.55744200	0.13499100
H	3.65535800	2.01710900	1.04918900
C	-5.22149200	0.00091200	1.66996000
H	-6.31324400	0.00079000	1.59303000
H	-4.90956500	-0.89102600	2.22036800
H	-4.90965300	0.89355700	2.21927400
C	-5.15777800	-1.47283000	-0.87341200
H	-6.25114200	-1.44096200	-0.91558600
H	-4.76216600	-1.51002400	-1.89233600
H	-4.84121400	-2.37498100	-0.34174300
C	-5.15775200	1.47180700	-0.87501200
H	-4.76327100	1.50722300	-1.89443500
H	-6.25118100	1.44052800	-0.91594200
H	-4.84006300	2.37457000	-0.34506100
Os.Cl_(triplet)			
Os	-0.89349400	0.00002900	-0.04047400
P	-1.17802400	2.43678200	-0.02893600
Cl	-2.61701000	0.00030200	-1.71694300

Cl	-2.30697900	-0.00014300	2.02848800
N	0.61645200	-0.00017000	1.33660500
H	0.25793600	-0.00024600	2.28974200
P	-1.17836400	-2.43670100	-0.02909200
C	1.93397700	0.00004500	-1.24527000
C	1.93384800	-0.00018200	1.24103800
C	2.62084800	-0.00005400	0.01294200
C	0.56250900	0.00006800	-1.39708200
H	2.48723400	-0.00026400	2.17797400
H	0.21533900	0.00023800	-2.43317600
H	2.54190600	0.00012800	-2.15176400
P	4.39534500	-0.00013700	-0.00884100
C	-2.91928300	-2.96704100	0.20410600
H	-3.52719300	-2.56385800	-0.60942000
H	-2.98556500	-4.06016800	0.20958200
H	-3.29315500	-2.56421200	1.14825900
C	-0.25647900	-3.30847200	1.30586500
H	-0.43967500	-4.38728600	1.26639000
H	0.81696700	-3.12356600	1.20360400
H	-0.59075800	-2.92521200	2.27440900
C	-0.65438000	-3.26955700	-1.58395700
H	0.41092800	-3.09429900	-1.75982900
H	-0.84240200	-4.34721900	-1.53576600
H	-1.21986300	-2.84285900	-2.41743600
C	-2.91871200	2.96735500	0.20541200
H	-2.98496500	4.06048700	0.21010800
H	-3.52733700	2.56356500	-0.60728200
H	-3.29178600	2.56523900	1.15018300
C	-0.25509100	3.30857100	1.30529100
H	0.81825200	3.12346100	1.20232500
H	-0.43812400	4.38741300	1.26579400
H	-0.58876900	2.92552200	2.27412700
C	-0.65498500	3.26940500	-1.58423600
H	-0.84318300	4.34704100	-1.53617300
H	0.41027000	3.09431200	-1.76059300
H	-1.22080700	2.84241300	-2.41733100
C	5.05536700	-1.46592400	-0.87650100
H	6.14761700	-1.41777800	-0.93125200
H	4.75817400	-2.37234400	-0.34113500
H	4.65022100	-1.51111800	-1.89152000
C	5.10495600	0.00013800	1.66963900
H	4.79591500	-0.89213700	2.22099300
H	6.19639200	0.00013300	1.58937900
H	4.79588800	0.89258900	2.22069300

C	5.05544200	1.46530900	-0.87701000
H	4.75842200	2.37192400	-0.34187600
H	6.14767900	1.41700800	-0.93186000
H	4.65020300	1.51026200	-1.89200000

Ir.Cl_(singlet)

P	-1.45360600	2.33096700	0.01161400
Cl	-2.33590600	0.00026300	-1.88646700
Cl	-2.19727700	-0.00010700	2.01874100
N	0.70501100	-0.00029900	1.33374800
H	0.32257600	-0.00043200	2.28523000
P	-1.45395700	-2.33087000	0.01142400
C	2.04500400	0.00025200	-1.21878000
C	2.01584600	-0.00029000	1.25204700
C	2.70816500	-0.00000100	0.00874700
C	0.64040600	0.00027700	-1.41867200
H	2.56681200	-0.00046400	2.18918800
H	0.33250700	0.00054700	-2.46653200
H	2.65272800	0.00043900	-2.12476700
P	4.53507400	-0.00013800	-0.00498800
Ir	-0.71013900	0.00001100	-0.05616400
C	-0.88654800	3.22382200	-1.48513300
H	-1.26770500	4.25095400	-1.45319700
H	0.20549800	3.24718900	-1.52647900
H	-1.27784500	2.72292900	-2.37388600
C	-3.25949500	2.56934500	0.10378400
H	-3.44722900	3.64958300	0.12441300
H	-3.73748000	2.12751500	-0.77166900
H	-3.65014400	2.10605400	1.01076900
C	-0.73418200	3.20254700	1.45387600
H	0.35809300	3.19284000	1.40617700
H	-1.08002600	4.24258700	1.44790300
H	-1.07154900	2.71839200	2.37346500
C	-3.25987600	-2.56908500	0.10347600
H	-3.44772100	-3.64931700	0.12343400
H	-3.65045400	-2.10630800	1.01075500
H	-3.73783100	-2.12666500	-0.77169500
C	-0.88693000	-3.22357300	-1.48543400
H	0.20511400	-3.24701100	-1.52678100
H	-1.26815700	-4.25068400	-1.45363100
H	-1.27818700	-2.72253500	-2.37412200
C	-0.73473200	-3.20276600	1.45359700
H	-1.08086000	-4.24271100	1.44752900
H	0.35754400	-3.19335100	1.40589600

H	-1.07198200	-2.71861700	2.37323300
C	5.14042600	1.48250300	-0.87065300
H	6.23536800	1.46526800	-0.89343900
H	4.76871900	1.50619100	-1.89927300
H	4.80852800	2.38448300	-0.34769500
C	5.19979000	0.00096800	1.68772800
H	4.88829400	0.89676400	2.23325500
H	4.88885000	-0.89442200	2.23423800
H	6.29341400	0.00125700	1.62490700
C	5.14020300	-1.48400700	-0.86871500
H	4.76852500	-1.50886400	-1.89732200
H	6.23515100	-1.46707000	-0.89144300
H	4.80804100	-2.38525500	-0.34466300

Ir.Cl (triplet)

P	-1.17972200	2.45766600	-0.02529800
Cl	-2.56857300	0.00020900	-1.69462700
Cl	-2.26246700	0.00003100	1.99178100
N	0.61827300	-0.00030400	1.33925700
H	0.26599300	-0.00045800	2.29509400
P	-1.17985300	-2.45764000	-0.02542600
C	1.93125300	0.00008900	-1.22906100
C	1.92630800	-0.00028300	1.23897300
C	2.62538300	-0.00008200	0.00825500
C	0.55983800	0.00012000	-1.38622600
H	2.47816500	-0.00045600	2.17690800
H	0.20418400	0.00021500	-2.41634200
H	2.51964000	0.00019300	-2.14677900
P	4.43640900	-0.00004600	-0.01431700
Ir	-0.91125200	0.00000500	-0.04235300
C	-0.62375100	3.25874600	-1.57923800
H	-1.17596600	2.83723700	-2.42406300
H	-0.81708700	4.33572300	-1.53363500
H	0.44612600	3.09397000	-1.73392800
C	-0.26604900	3.28094100	1.33648800
H	0.80907800	3.10595800	1.24016700
H	-0.45231500	4.35977800	1.30763700
H	-0.61282100	2.89118100	2.29780200
C	-2.92905000	2.95194700	0.18571700
H	-3.31876600	2.55367200	1.12516100
H	-2.99282000	4.04556100	0.19689300
H	-3.52817300	2.56388800	-0.64132900
C	-2.92928100	-2.95179500	0.18516900
H	-2.99308900	-4.04540100	0.19669200

H	-3.31928100	-2.55319600	1.12436200
H	-3.52813800	-2.56397900	-0.64218300
C	-0.62364000	-3.25875700	-1.57926100
H	0.44624100	-3.09395500	-1.73387800
H	-0.81697200	-4.33573400	-1.53366100
H	-1.17579600	-2.83727100	-2.42414200
C	-0.26670500	-3.28105700	1.33663000
H	-0.45322900	-4.35984900	1.30774900
H	0.80849500	-3.10634400	1.24068300
H	-0.61373200	-2.89120200	2.29781800
C	5.05108400	1.47856700	-0.88295100
H	6.14537500	1.45072200	-0.91858200
H	4.66813200	1.50850700	-1.90731600
H	4.73369300	2.38278100	-0.35511300
C	5.11357100	-0.00045900	1.67404300
H	4.80608200	0.89477300	2.22259700
H	4.80605100	-0.89594100	2.22216900
H	6.20660400	-0.00046000	1.60418000
C	5.05113900	-1.47820200	-0.88368800
H	4.66825600	-1.50761500	-1.90809300
H	6.14543200	-1.45033100	-0.91923600
H	4.73372100	-2.38269200	-0.35634000

Re.Br (singlet)

P	1.31683100	-2.23175700	-0.03382800
N	-1.05267400	-0.00012700	1.34526800
H	-0.71874800	-0.00030600	2.31457800
P	1.31700900	2.23168800	-0.03335900
C	-2.39083500	0.00057600	-1.27809000
C	-2.38966000	0.00007500	1.23662900
C	-3.04522800	0.00049300	-0.00795800
C	-1.00464400	0.00034800	-1.47971600
H	-2.95894800	-0.00000300	2.16413600
H	-0.72760000	0.00050000	-2.54199600
H	-3.04101200	0.00083000	-2.16139800
P	-4.80258700	0.00004400	-0.03742900
Re	0.35354600	0.00000700	-0.04306100
C	0.89701500	3.25581100	-1.51374300
H	1.34678500	4.25318500	-1.44347700
H	1.26595400	2.73848600	-2.40210400
H	-0.19056700	3.35144500	-1.58912500
C	3.13919900	2.42828200	0.12702200
H	3.61193100	1.92160400	-0.71682800
H	3.40742300	3.49126500	0.13300700

H	3.45341500	1.95062200	1.05749500
C	0.66203100	3.27005200	1.35302100
H	1.09126000	4.27855100	1.32852000
H	-0.42771300	3.34179100	1.27449700
H	0.91751800	2.77774400	2.29470400
C	3.13897800	-2.42860100	0.12658700
H	3.45324900	-1.95108900	1.05712000
H	3.40708300	-3.49162000	0.13248000
H	3.61180900	-1.92191100	-0.71720200
C	0.66157100	-3.27045300	1.35218000
H	1.09093800	-4.27888500	1.32770700
H	0.91654700	-2.77824200	2.29404200
H	-0.42813600	-3.34234500	1.27312400
C	0.89669300	-3.25546200	-1.51448000
H	1.34637400	-4.25289500	-1.44455000
H	-0.19091900	-3.35098800	-1.58969300
H	1.26550900	-2.73793100	-2.40276400
C	-5.48483600	-1.46080800	-0.90504000
H	-6.57585000	-1.40517800	-0.97853600
H	-5.05597100	-1.51603900	-1.90942900
H	-5.19870200	-2.36506100	-0.35997400
C	-5.55247700	0.00186900	1.62743100
H	-5.24448300	-0.88748000	2.18332800
H	-5.24367300	0.89198900	2.18164300
H	-6.64249700	0.00224000	1.53156300
C	-5.48515700	1.45873900	-0.90835600
H	-5.05582600	1.51225400	-1.91263000
H	-6.57609600	1.40228800	-0.98231000
H	-5.19987300	2.36424800	-0.36493500
Br	1.84659500	-0.00036400	2.45766300
Br	2.10823000	0.00025400	-2.25600500

Re.Br (triplet)

P	-0.81001000	2.44871300	-0.07298500
N	0.90949300	-0.00026600	1.33626400
H	0.55050900	-0.00028100	2.28933300
P	-0.81064200	-2.44867300	-0.07315600
C	2.23990200	-0.00037000	-1.28368300
C	2.23064700	-0.00039000	1.23728000
C	2.91322700	-0.00048400	0.00254300
C	0.87254000	-0.00016600	-1.45048500
H	2.79504600	-0.00046100	2.16943900
H	0.54662500	-0.00009400	-2.49630400
H	2.87953000	-0.00049700	-2.17225300

P	4.65376700	-0.00019600	-0.01137800
Re	-0.59298900	-0.00000300	-0.06103100
C	0.17427200	3.34750300	1.21163000
H	1.23610200	3.10997700	1.09300800
H	0.03606100	4.43266200	1.14539800
H	-0.14922800	3.00120100	2.19794100
C	-2.51693400	3.08352700	0.20716100
H	-2.87742800	2.69632300	1.16374300
H	-2.54179100	4.17934000	0.20340300
H	-3.16294000	2.69044400	-0.58242000
C	-0.31359100	3.29153500	-1.64132600
H	-0.92713200	2.88609900	-2.45149700
H	-0.44893600	4.37788400	-1.58713200
H	0.73363500	3.06073400	-1.85928800
C	0.17308300	-3.34771700	1.21168200
H	0.03455300	-4.43284000	1.14549600
H	1.23501700	-3.11053200	1.09332100
H	-0.15057000	-3.00124600	2.19788600
C	-0.31431700	-3.29161200	-1.64146300
H	-0.44967000	-4.37795500	-1.58716000
H	-0.92801700	-2.88624900	-2.45155600
H	0.73286400	-3.06083400	-1.85963900
C	-2.51782900	-3.08296800	0.20663000
H	-2.54304000	-4.17877200	0.20273100
H	-2.87838400	-2.69576000	1.16318500
H	-3.16354500	-2.68957700	-0.58303500
C	5.36725500	1.45143800	-0.88070400
H	6.45650700	1.37407700	-0.96332300
H	4.93353700	1.51745000	-1.88262400
H	5.10371700	2.36111000	-0.33334100
C	5.39609200	-0.00077200	1.65827100
H	6.48631700	-0.00079000	1.56499200
H	5.08833400	0.88910300	2.21336200
H	5.08823600	-0.89100100	2.21273900
C	5.36756700	-1.45100500	-0.88180200
H	4.93351600	-1.51666500	-1.88359800
H	6.45675100	-1.37307300	-0.96478800
H	5.10467700	-2.36110500	-0.33484200
Br	-2.14244000	0.00004100	2.21423600
Br	-2.48702600	0.00037700	-1.87741700

Os.Br (singlet)

Os	0.41825900	0.00001600	-0.04999200
P	1.18155800	-2.30705000	-0.02566000

N	-0.98981900	0.00012800	1.32394900
H	-0.63011600	0.00018300	2.28499600
P	1.18174700	2.30702800	-0.02593500
C	-2.32921000	0.00003500	-1.24964000
C	-2.31666800	0.00015500	1.23564600
C	-2.98835500	0.00011100	-0.00318800
C	-0.93278300	0.00000700	-1.44547400
H	-2.87078300	0.00023000	2.17068100
H	-0.64094000	-0.00012600	-2.50081100
H	-2.95542000	-0.00000900	-2.14551800
P	-4.78102200	0.00003600	-0.02537400
C	0.44060800	-3.24735700	1.37463400
H	-0.65105000	-3.22759400	1.30517100
H	0.78211300	-4.28791600	1.35380500
H	0.75133100	-2.77836800	2.31153300
C	0.66011500	-3.23421000	-1.52699200
H	1.03503400	-4.26259900	-1.48528600
H	-0.43133800	-3.24827100	-1.59437700
H	1.06566200	-2.72979700	-2.40707800
C	2.98174300	-2.61343000	0.11570000
H	3.15812000	-3.69472600	0.11706100
H	3.48935400	-2.15007800	-0.73182400
H	3.34708700	-2.16897800	1.04297500
C	0.66028200	3.23415200	-1.52728500
H	-0.43117600	3.24836300	-1.59456500
H	1.03534800	4.26249200	-1.48568200
H	1.06567600	2.72962200	-2.40737100
C	0.44097400	3.24746800	1.37436100
H	0.78257200	4.28799500	1.35347500
H	-0.65068900	3.22780100	1.30496100
H	0.75170600	2.77848600	2.31126200
C	2.98196500	2.61325800	0.11531800
H	3.48947300	2.14989000	-0.73225900
H	3.15842800	3.69453900	0.11670300
H	3.34735000	2.16874800	1.04255200
C	-5.48567600	0.00087000	1.65418700
H	-6.57748100	0.00084300	1.57775000
H	-5.17366100	-0.89116300	2.20442200
H	-5.17362200	0.89344100	2.20352900
C	-5.42052500	-1.47313500	-0.88982200
H	-6.51388700	-1.44198700	-0.93258900
H	-5.02440200	-1.50983900	-1.90857400
H	-5.10379400	-2.37516200	-0.35804600
C	-5.42057500	1.47233500	-0.89126600

H	-5.02506900	1.50770200	-1.91030300
H	-6.51396900	1.44143600	-0.93334600
H	-5.10327800	2.37491600	-0.36077000
Br	1.94882700	0.00014300	2.26158700
Br	2.16508200	-0.00025600	-2.07710800

Os.Br (triplet)

Os	-0.60287000	-0.00000800	-0.06434700
P	-0.85710200	2.44191600	-0.04992300
N	0.91734900	0.00000900	1.31766000
H	0.56004000	0.00003700	2.27098700
P	-0.85716000	-2.44192400	-0.04985700
C	2.23565600	-0.00005100	-1.26028200
C	2.23397100	0.00000800	1.22351800
C	2.92331400	-0.00000400	-0.00323700
C	0.86459500	-0.00006600	-1.41526000
H	2.78646200	0.00004100	2.16122700
H	0.52493000	-0.00004100	-2.45297600
H	2.84355300	-0.00005500	-2.16695700
P	4.69749400	-0.00001500	-0.02403600
C	-2.58211500	-3.03116800	0.16943500
H	-3.19813400	-2.64659000	-0.64682900
H	-2.61023900	-4.12594500	0.17097300
H	-2.97590500	-2.64530400	1.11250400
C	0.07522100	-3.29088100	1.29341400
H	-0.08418300	-4.37345200	1.25464900
H	1.14495200	-3.08257900	1.19789400
H	-0.27368700	-2.91248000	2.25864500
C	-0.29823600	-3.26917000	-1.59669300
H	0.76348800	-3.06648600	-1.76455900
H	-0.45825300	-4.35108600	-1.54398800
H	-0.86701100	-2.86179200	-2.43752800
C	-2.58205200	3.03119900	0.16930300
H	-2.61016900	4.12597700	0.17067400
H	-3.19808400	2.64650000	-0.64689400
H	-2.97583400	2.64548300	1.11243700
C	0.07525300	3.29088500	1.29335800
H	1.14499600	3.08266100	1.19780000
H	-0.08422500	4.37344800	1.25463400
H	-0.27360500	2.91242900	2.25858500
C	-0.29810300	3.26909700	-1.59676800
H	-0.45806500	4.35102400	-1.54409600
H	0.76361400	3.06635300	-1.76460400
H	-0.86687900	2.86172700	-2.43760600

C	5.35839500	-1.46577700	-0.89114700
H	6.45070600	-1.41773200	-0.94467200
H	5.06043200	-2.37220700	-0.35621500
H	4.95435900	-1.51086100	-1.90662400
C	5.40545200	0.00029400	1.65515800
H	5.09571600	-0.89196000	2.20616200
H	6.49695900	0.00033400	1.57611800
H	5.09562000	0.89269900	2.20586300
C	5.35837200	1.46544200	-0.89167400
H	5.06044500	2.37205600	-0.35703300
H	6.45068000	1.41736200	-0.94522700
H	4.95430100	1.51019500	-1.90715000
Br	-2.40878800	-0.00001700	-1.84489100
Br	-2.08227400	0.00008200	2.13183600

Ir.Br (singlet)

P	-1.14205400	2.35220200	0.00417100
N	0.97967800	-0.00133600	1.32598600
H	0.59644200	-0.00220800	2.27782900
P	-1.14279300	-2.35204900	0.00261600
C	2.31585000	0.00136700	-1.22523900
C	2.28859200	-0.00120100	1.24467600
C	2.98071500	0.00008000	-0.00068900
C	0.90908800	0.00161400	-1.42522600
H	2.84156300	-0.00213400	2.18088900
H	0.60810600	0.00301800	-2.47487000
H	2.92205400	0.00225900	-2.13236800
P	4.80832100	-0.00029100	-0.01662400
Ir	-0.44917300	0.00002200	-0.06655500
C	-0.54616700	3.23361300	-1.49078800
H	-0.89029700	4.27334400	-1.45313400
H	0.54603800	3.21774300	-1.53336800
H	-0.95501600	2.75094800	-2.38156200
C	-2.93587200	2.67913000	0.10087300
H	-3.07117300	3.76719400	0.11121400
H	-3.43876400	2.25152600	-0.76751400
H	-3.34536600	2.24395100	1.01335500
C	-0.38643900	3.20880100	1.43918800
H	0.70462700	3.16320400	1.38452000
H	-0.69862600	4.25923700	1.42964100
H	-0.73208700	2.73958000	2.36326700
C	-2.93671100	-2.67876400	0.09841500
H	-3.07221600	-3.76681400	0.10715700
H	-3.34633000	-2.24479800	1.01142000

H	-3.43930300	-2.24982300	-0.76948900
C	-0.54657300	-3.23216400	-1.49300900
H	0.54563600	-3.21623600	-1.53539800
H	-0.89068200	-4.27194000	-1.45627800
H	-0.95528000	-2.74874500	-2.38343700
C	-0.38782200	-3.21030700	1.43699500
H	-0.70048100	-4.26059400	1.42633200
H	0.70327400	-3.16516300	1.38261900
H	-0.73349300	-2.74189000	2.36147000
C	5.41223300	1.48255200	-0.88287800
H	6.50715400	1.46532300	-0.90694100
H	5.03927700	1.50631400	-1.91104200
H	5.08101200	2.38444000	-0.35932900
C	5.47426200	0.00071100	1.67558800
H	5.16305700	0.89642600	2.22143200
H	5.16375300	-0.89472500	2.22228200
H	6.56785100	0.00107400	1.61200400
C	5.41162000	-1.48446600	-0.88104200
H	5.03872300	-1.50913100	-1.90921300
H	6.50655500	-1.46791700	-0.90497000
H	5.07977700	-2.38556900	-0.35653400
Br	-2.00478800	-0.00088700	2.13336100
Br	-2.16052600	0.00106000	-2.00366900

Ir.Br (triplet)

P	-0.85783600	2.46021300	-0.04536800
N	0.91041800	-0.00018800	1.32726400
H	0.56205200	-0.00029700	2.28416500
P	-0.85796200	-2.46022600	-0.04544900
C	2.22446400	0.00008300	-1.24234000
C	2.21770800	-0.00021000	1.22642100
C	2.91691000	-0.00006900	-0.00476900
C	0.85290200	0.00011700	-1.40884500
H	2.77139600	-0.00034400	2.16353900
H	0.51477300	0.00019800	-2.44369900
H	2.81690000	0.00016900	-2.15775500
P	4.72720700	-0.00003200	-0.02699800
Ir	-0.62623600	-0.00000900	-0.06526000
C	-0.26202000	3.25796400	-1.58790000
H	-0.81658600	2.86007700	-2.44249400
H	-0.42313400	4.33981100	-1.53554700
H	0.80383800	3.06167500	-1.73315700
C	0.06321300	3.26297600	1.32521400
H	1.13462000	3.06244500	1.23845300

H	-0.09726600	4.34578600	1.29450900
H	-0.30023000	2.88123000	2.28347600
C	-2.58981000	3.02438300	0.14727300
H	-3.00499500	2.64251500	1.08244900
H	-2.60982400	4.11955400	0.15805400
H	-3.19590100	2.66090300	-0.68562500
C	-2.59002100	-3.02428000	0.14683400
H	-2.61005200	-4.11944600	0.15811700
H	-3.00553500	-2.64198100	1.08168700
H	-3.19581200	-2.66118400	-0.68644700
C	-0.26189000	-3.25791200	-1.58791700
H	0.80398200	-3.06156100	-1.73298400
H	-0.42297200	-4.33976700	-1.53565900
H	-0.81633200	-2.85998600	-2.44257600
C	0.06274600	-3.26314000	1.32527800
H	-0.09810300	-4.34589700	1.29466000
H	1.13422600	-3.06298200	1.23855800
H	-0.30063900	-2.88119400	2.28348200
C	5.34341700	1.47837700	-0.89515200
H	6.43768300	1.45019800	-0.93048500
H	4.96060500	1.50864700	-1.91954200
H	5.02604100	2.38259200	-0.36732300
C	5.40520400	-0.00069800	1.66111400
H	5.09773400	0.89437800	2.20989100
H	5.09755800	-0.89610500	2.20925200
H	6.49819300	-0.00077700	1.59101900
C	5.34346500	-1.47772800	-0.89632300
H	4.96079600	-1.50714000	-1.92079000
H	6.43773600	-1.44953500	-0.93149100
H	5.02600700	-2.38237900	-0.36929200
Br	-2.36634100	0.00008800	-1.81931700
Br	-2.05847000	0.00002400	2.09107800

Re.I (singlet)

P	0.89202200	-0.06662900	2.34535900
N	-1.24887600	1.31690200	-0.00021000
H	-0.93080500	2.29230200	-0.00039500
P	0.89190200	-0.06757700	-2.34539300
C	-2.58751200	-1.30115400	0.00026200
C	-2.58766800	1.20850000	-0.00016400
C	-3.24209200	-0.03627100	0.00005600
C	-1.19497700	-1.49393000	0.00028700
H	-3.15594100	2.13642200	-0.00031400
H	-0.92305900	-2.55855300	0.00047000

H	-3.23141200	-2.18869400	0.00040700
P	-5.00449400	-0.06584000	0.00006300
Re	0.15812700	-0.06357800	0.00000200
C	0.38257900	-1.56325900	-3.30639600
H	0.68579700	-1.47465600	-4.35620200
H	0.84765300	-2.44475400	-2.85890300
H	-0.70423300	-1.67494600	-3.24793300
C	2.66836500	0.12973500	-2.78100200
H	3.23087700	-0.70392900	-2.35568400
H	2.78190300	0.14447900	-3.87134400
H	3.03462400	1.06360200	-2.34936600
C	0.08261200	1.29119100	-3.31086300
H	0.36005100	1.23797100	-4.37003200
H	-1.00498800	1.20880600	-3.21892600
H	0.39949300	2.25088000	-2.89413900
C	2.66849100	0.13104900	2.78077500
H	3.03463800	1.06475700	2.34869400
H	2.78209200	0.14629900	3.87110300
H	3.23105500	-0.70275300	2.35580100
C	0.08267600	1.29241600	3.31038800
H	0.36021800	1.23962200	4.36955200
H	0.39941100	2.25198800	2.89327900
H	-1.00492300	1.20987400	3.21858300
C	0.38290500	-1.56201500	3.30694000
H	0.68615000	-1.47298400	4.35670200
H	-0.70389700	-1.67385100	3.24856100
H	0.84806100	-2.44362700	2.85976400
C	-5.67951400	-0.93516000	1.46178900
H	-6.77072000	-1.00688700	1.40946900
H	-5.25217900	-1.94035100	1.51369500
H	-5.39026100	-0.39163100	2.36596500
C	-5.75113200	1.59985100	-0.00023700
H	-5.44204700	2.15461900	0.88947800
H	-5.44202100	2.15430600	-0.89013700
H	-6.84128900	1.50561200	-0.00023500
C	-5.67950200	-0.93567300	-1.46136300
H	-5.25217300	-1.94088500	-1.51291400
H	-6.77070900	-1.00737700	-1.40902700
H	-5.39024100	-0.39246200	-2.36572700
I	1.81994600	2.64253300	-0.00045600
I	2.13191500	-2.38676300	0.00041500

Re.I (triplet)

P	-0.47978000	2.46260200	-0.09636500
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N	1.18248900	-0.00039300	1.31367500
H	0.83299300	-0.00068600	2.26999300
P	-0.47982000	-2.46252500	-0.09780300
C	2.51590300	0.00037800	-1.29969900
C	2.50409100	-0.00037400	1.21538000
C	3.18988000	-0.00001200	-0.01583300
C	1.14887200	0.00043600	-1.46592200
H	3.06463600	-0.00065800	2.14962600
H	0.82289800	0.00075400	-2.51065400
H	3.15164100	0.00063900	-2.19056400
P	4.93290500	-0.00001000	-0.02705100
Re	-0.32163600	0.00003900	-0.08501500
C	0.53666800	3.31177800	1.19843600
H	1.58675700	3.02433700	1.08804200
H	0.44994800	4.40178900	1.12611900
H	0.18945000	2.98643000	2.18368600
C	-2.14380700	3.21466200	0.15934400
H	-2.54404700	2.87500000	1.11792800
H	-2.08218300	4.30895700	0.14180900
H	-2.81336300	2.86739600	-0.63172700
C	0.09134100	3.28674100	-1.65067600
H	-0.53410700	2.93750400	-2.47754600
H	0.02594500	4.37846500	-1.57927200
H	1.12467600	2.99151200	-1.85576700
C	0.53691400	-3.31248400	1.19625700
H	0.45013600	-4.40245100	1.12334100
H	1.58698500	-3.02501800	1.08576200
H	0.18995300	-2.98767800	2.18177600
C	0.09091300	-3.28573700	-1.65275200
H	0.02557900	-4.37750500	-1.58197200
H	-0.53477500	-2.93604400	-2.47924800
H	1.12417900	-2.99034400	-1.85795600
C	-2.14379100	-3.21470600	0.15789400
H	-2.08217500	-4.30899200	0.13979700
H	-2.54381400	-2.87553000	1.11674400
H	-2.81352300	-2.86703400	-0.63284800
C	5.64349900	1.45266100	-0.89499600
H	6.73319200	1.37769100	-0.97282500
H	5.21433400	1.51656600	-1.89901200
H	5.37568800	2.36213600	-0.34943400
C	5.66866100	-0.00057700	1.64496600
H	6.75916600	-0.00056000	1.55531700
H	5.35921000	0.88945600	2.19890100
H	5.35918600	-0.89097200	2.19830600

C	5.64347200	-1.45210900	-0.89597000
H	5.21431900	-1.51533200	-1.90003300
H	6.73316700	-1.37710800	-0.97373800
H	5.37563800	-2.36194600	-0.35102200
I	-2.03410200	-0.00081600	2.40001600
I	-2.38574000	0.00070400	-2.08140200

Os.I (singlet)

Os	0.20257100	-0.00885100	-0.06309400
P	0.81434500	-2.36009900	0.23825000
N	-1.21735500	0.15315900	1.29833700
H	-0.87077200	0.26819200	2.25742900
P	0.80511300	2.34949300	-0.32788600
C	-2.55646200	-0.15437000	-1.25076900
C	-2.54300900	0.14219700	1.21238200
C	-3.21658700	-0.00592600	-0.01847900
C	-1.15481700	-0.17715600	-1.44029300
H	-3.09687200	0.25329700	2.14098100
H	-0.87268400	-0.30459400	-2.49061800
H	-3.17788000	-0.26208800	-2.14337400
P	-5.01314400	-0.00708700	-0.04063300
C	-0.02343300	-3.07906900	1.71624400
H	-1.10692500	-2.95457000	1.63039900
H	0.20894500	-4.14646100	1.79625100
H	0.32796900	-2.56339700	2.61342100
C	0.21658700	-3.41918500	-1.14625200
H	0.48207600	-4.46525000	-0.95899600
H	-0.86975100	-3.33101700	-1.23594600
H	0.67811900	-3.08798700	-2.07942400
C	2.57065600	-2.84311300	0.44848300
H	2.61868600	-3.93095300	0.57039200
H	3.14110700	-2.54203500	-0.43172000
H	2.98327400	-2.34885800	1.32959000
C	0.20244700	3.04983600	-1.92232200
H	-0.88362100	2.93948300	-1.98710500
H	0.46430300	4.11144900	-1.98745100
H	0.66459400	2.50954400	-2.75178800
C	-0.03571400	3.39308500	0.93986100
H	0.19133600	4.45036400	0.76574500
H	-1.11856200	3.24646200	0.88708600
H	0.31815200	3.10506800	1.93292200
C	2.55923700	2.87621700	-0.23993900
H	3.13051300	2.38040900	-1.02649900
H	2.60187500	3.96264000	-0.37580700

H	2.97506900	2.60369700	0.73148000
C	-5.71470300	0.18864700	1.62848100
H	-6.80664500	0.18093800	1.55387400
H	-5.40298300	-0.63429400	2.27775800
H	-5.40142300	1.13851200	2.07070000
C	-5.64889500	-1.57105000	-0.72946200
H	-6.74227400	-1.54581800	-0.77561000
H	-5.25282800	-1.72462100	-1.73729300
H	-5.33209200	-2.40537600	-0.09674800
C	-5.64606100	1.35718100	-1.07165900
H	-5.24897700	1.27405000	-2.08734200
H	-6.73945900	1.32366900	-1.11184900
H	-5.32826700	2.31427000	-0.64763100
I	2.13020200	-0.26202800	-2.20214200
I	1.89700300	0.29047000	2.39592200

Os.I (triplet)

Os	-0.34608400	-0.00002100	-0.08630700
P	-0.52128500	2.45581600	-0.07787000
N	1.18465600	0.00017500	1.29941100
H	0.84231700	0.00028600	2.25759000
P	-0.52114500	-2.45588400	-0.07740300
C	2.50283000	-0.00009000	-1.27690500
C	2.50115400	0.00018000	1.20320700
C	3.19231100	0.00004900	-0.02204700
C	1.13153100	-0.00011300	-1.43086600
H	3.05344300	0.00029200	2.14122100
H	0.79866400	-0.00026100	-2.47014100
H	3.10815800	-0.00018700	-2.18536700
P	4.96740600	0.00005300	-0.04240800
C	-2.19322400	-3.18599700	0.14478300
H	-2.84918800	-2.85283600	-0.66265800
H	-2.12245400	-4.27892900	0.13199000
H	-2.61577600	-2.85380000	1.09562200
C	0.47332200	-3.26218200	1.24996300
H	0.37471700	-4.35139900	1.19716800
H	1.52812200	-2.99287900	1.14403100
H	0.11659200	-2.91921800	2.22539200
C	0.08950100	-3.25288500	-1.62303600
H	1.13297600	-2.97476100	-1.79604900
H	0.00943500	-4.34287800	-1.55586400
H	-0.50886400	-2.90148200	-2.46840100
C	-2.19342300	3.18582700	0.14419800
H	-2.12273300	4.27876200	0.13128500

H	-2.84934600	2.85252400	-0.66321800
H	-2.61597100	2.85370400	1.09506900
C	0.47310300	3.26242400	1.24936800
H	1.52792600	2.99318900	1.14348800
H	0.37441000	4.35162400	1.19638500
H	0.11640000	2.91959600	2.22485600
C	0.08930000	3.25257200	-1.62366100
H	0.00916200	4.34257200	-1.55669100
H	1.13279000	2.97448600	-1.79663500
H	-0.50904800	2.90097600	-2.46896000
C	5.62719400	-1.46596800	-0.90954200
H	6.71960100	-1.41855900	-0.96177100
H	5.32825200	-2.37251600	-0.37534000
H	5.22460300	-1.51025300	-1.92565000
C	5.67342500	0.00028600	1.63742000
H	5.36337700	-0.89204300	2.18817300
H	6.76501100	0.00029300	1.55921800
H	5.36334600	0.89275100	2.18793600
C	5.62717300	1.46585000	-0.90993700
H	5.32821600	2.37253800	-0.37598100
H	6.71958100	1.41844300	-0.96215000
H	5.22458700	1.50985600	-1.92605900
I	-2.33735200	-0.00023800	-1.99626100
I	-1.97959700	0.00025800	2.29178000

Ir.I (singlet)

P	-0.78965118	2.39953751	-0.01450559
N	1.22402407	0.00408961	1.32470909
H	0.85506833	0.00702552	2.28215853
P	-0.78929089	-2.39968236	-0.00361109
C	2.55475597	-0.00450115	-1.22843132
C	2.53002930	0.00352781	1.24116213
C	3.22128239	-0.00048198	-0.00914371
C	1.14209123	-0.00549994	-1.42601041
H	3.08841628	0.00630843	2.17456711
H	0.85670446	-0.01004432	-2.48014708
H	3.15797890	-0.00729232	-2.13773606
P	5.05180849	0.00018974	-0.02869890
Ir	-0.22661368	-0.00020738	-0.07359267
C	-0.12052367	3.24329143	-1.50463354
H	-0.36934248	4.30901139	-1.45142060
H	0.96594481	3.13025185	-1.54825887
H	-0.56808158	2.81702701	-2.40542338
C	-2.54125446	2.91631073	0.08157753

H	-2.55309689	4.01275163	0.09151233
H	-3.09297102	2.55193132	-0.78599135
H	-3.00187327	2.53483619	0.99373026
C	0.04055556	3.22111085	1.40378877
H	1.12243493	3.07084557	1.35414579
H	-0.17000799	4.29557708	1.36074715
H	-0.34518752	2.82072991	2.34419010
C	-2.54089563	-2.91584339	0.09558235
H	-2.55275412	-4.01220955	0.11190940
H	-3.00150570	-2.52904060	1.00549265
H	-3.09262262	-2.55653279	-0.77408842
C	-0.12071524	-3.25094088	-1.48968271
H	0.96582833	-3.13882399	-1.53388803
H	-0.37021864	-4.31623808	-1.43152177
H	-0.56804725	-2.82863371	-2.39244988
C	0.04125796	-3.21380647	1.41873704
H	-0.16958299	-4.28844018	1.38161425
H	1.12315420	-3.06406645	1.36794644
H	-0.34409399	-2.80817420	2.35704677
I	-2.10668816	-0.00509743	-2.14834180
I	-1.94690635	0.00547002	2.27847241
C	5.65059626	1.48493459	-0.89500159
H	6.74563428	1.47028415	-0.91847836
H	5.27821326	1.50741429	-1.92342203
H	5.31741970	2.38613891	-0.37147835
C	5.71970474	-0.00017431	1.66265224
H	5.41062469	0.89562961	2.20963622
H	5.40964201	-0.89572198	2.20950882
H	6.81324725	-0.00070798	1.59707044
C	5.65176410	-1.48355899	-0.89585639
H	5.27928548	-1.50609590	-1.92423042
H	6.74677952	-1.46769841	-0.91960076
H	5.31971596	-2.38533201	-0.37259960

Ir.I (triplet)

P	-0.51396100	2.46643700	-0.07627300
N	1.16591400	0.00023000	1.31343000
H	0.83253600	0.00033500	2.27539700
P	-0.51359800	-2.46632300	-0.07667800
C	2.48730400	0.00004600	-1.25877300
C	2.47343000	0.00019600	1.21137600
C	3.17468300	0.00007700	-0.01887800
C	1.11489700	0.00008600	-1.43488800
H	3.02796800	0.00027200	2.14820200

H	0.79798500	0.00002200	-2.47597800
H	3.08539700	-0.00001500	-2.17087000
P	4.98472400	0.00004200	-0.03557500
Ir	-0.36553800	0.00010200	-0.09164500
C	0.13206000	3.23600300	-1.61613600
H	0.05288000	4.32598900	-1.54836500
H	1.17944100	2.96196900	-1.76842200
H	-0.45204000	2.89506500	-2.47553400
C	-2.19130200	3.18360600	0.11897600
H	-2.10616900	4.27575600	0.11920800
H	-2.83590500	2.87695000	-0.70757800
H	-2.63842200	2.85599800	1.05976600
C	0.46616000	3.23264700	1.27736300
H	1.52283300	2.96864000	1.18317800
H	0.36897000	4.32223700	1.22897600
H	0.09324400	2.89122600	2.24702800
C	-2.19085000	-3.18367900	0.11861000
H	-2.10560500	-4.27582000	0.11872000
H	-2.63794800	-2.85620900	1.05946000
H	-2.83553200	-2.87699700	-0.70787600
C	0.13235400	-3.23565600	-1.61669100
H	1.17970200	-2.96154900	-1.76905000
H	0.05324600	-4.32565300	-1.54901900
H	-0.45185000	-2.89467300	-2.47600400
C	0.46672700	-3.23257000	1.27679000
H	0.36968300	-4.32216700	1.22826600
H	1.52335600	-2.96840200	1.18256900
H	0.09383600	-2.89131500	2.24652400
I	-2.30539000	0.00006800	-1.96232800
I	-1.97717700	-0.00042500	2.25075000
C	5.60511100	1.47759200	-0.90249700
H	6.69946900	1.44894600	-0.93384400
H	5.22603100	1.50737400	-1.92826700
H	5.28625000	2.38231500	-0.37645900
C	5.65924300	0.00014800	1.65404200
H	5.35059200	0.89540600	2.20181900
H	5.35030400	-0.89486600	2.20205300
H	6.75235200	-0.00004100	1.58619200
C	5.60507700	-1.47763600	-0.90230000
H	5.22536000	-1.50795600	-1.92781800
H	6.69940500	-1.44864200	-0.93434000
H	5.28684500	-2.38225800	-0.37570300

Re.SnCl₃ (singlet)

P	-0.19198400	0.00200000	2.44841800
N	1.73786600	-1.34131600	0.00081500
H	1.44223900	-2.32459100	0.00164000
P	-0.19062400	0.00207700	-2.44909200
C	3.10230700	1.22227400	-0.00034200
C	3.06448600	-1.26132400	0.00087300
C	3.75318500	-0.03358800	0.00021900
C	1.71349200	1.43206200	-0.00041300
H	3.61313500	-2.20182400	0.00153200
H	1.50988300	2.50882600	-0.00037200
H	3.74497500	2.10921300	-0.00049700
P	5.52811000	-0.02941400	0.00048600
C	0.26308300	-1.59574400	3.26602000
H	1.25318900	-1.91183600	2.92565400
H	0.27963700	-1.46110200	4.35358800
H	-0.46010500	-2.37708600	3.02152800
C	0.92852500	1.17644400	3.33459700
H	0.78687900	1.07737700	4.41707800
H	1.96694800	0.94859600	3.07938600
H	0.69824700	2.19896000	3.02788700
C	-1.84111100	0.38275300	3.17505600
H	-1.79760800	0.21120400	4.25638500
H	-2.09853800	1.42923700	2.99466600
H	-2.60693500	-0.26557600	2.74457000
C	0.92545100	1.18084100	-3.33506100
H	1.96471900	0.95783800	-3.07908100
H	0.78484400	1.08090400	-4.41759400
H	0.69024500	2.20243200	-3.02881000
C	0.27020300	-1.59423500	-3.26623900
H	0.28648300	-1.45990900	-4.35385200
H	1.26138000	-1.90663000	-2.92556000
H	-0.45026500	-2.37806200	-3.02163500
C	-1.84096300	0.37713200	-3.17597700
H	-2.10242400	1.42241000	-2.99445600
H	-1.79633800	0.20712300	-4.25750900
H	-2.60437000	-0.27482800	-2.74671900
C	6.22926000	-1.71242000	0.00117400
H	7.32139100	-1.64404100	0.00120500
H	5.90896300	-2.25977200	0.89178100
H	5.90905000	-2.26046100	-0.88904100
C	6.19823700	0.83070600	1.46647500
H	7.29110700	0.87596000	1.42328100
H	5.79745600	1.84734700	1.51075100
H	5.88996000	0.29714100	2.37031600

C	6.19863900	0.82967300	-1.46592300
H	5.79789700	1.84629300	-1.51101400
H	7.29149900	0.87493600	-1.42246200
H	5.89060000	0.29548000	-2.36947300
Sn	-1.48699300	-2.16645700	-0.00037600
Sn	-1.42054700	2.20426300	-0.00040700
Cl	-2.91006800	-2.89605400	-1.81386900
Cl	-2.91669100	-2.89029100	1.80999300
Cl	0.06004200	-4.13841500	0.00450000
Cl	-3.81760500	2.10212100	0.00952700
Cl	-1.09006000	3.82311200	1.79162900
Cl	-1.10455900	3.81882000	-1.79872800
Re	0.25358000	0.05170700	-0.00028700

Re.SnCl₃ (triplet)

P	0.10519600	-0.04364000	-2.48702800
N	1.75837600	1.31313000	-0.00013200
H	1.45680200	2.29156400	-0.00014100
P	0.10550900	-0.04358800	2.48694100
C	3.07138800	-1.30404400	-0.00024600
C	3.07550200	1.19826900	-0.00021000
C	3.75507400	-0.03447000	-0.00029900
C	1.70418700	-1.47154300	-0.00015500
H	3.64126000	2.12950100	-0.00023100
H	1.41028500	-2.52614100	-0.00012200
H	3.69597100	-2.20164600	-0.00028600
P	5.51033500	-0.05637100	-0.00003000
C	0.72731200	1.52667600	-3.24492700
H	1.72926800	1.74800000	-2.86644200
H	0.76436600	1.43712100	-4.33623100
H	0.06766500	2.35896600	-2.98296100
C	1.15737600	-1.31543900	-3.31763900
H	1.12850400	-1.18530300	-4.40521900
H	2.18772300	-1.22734100	-2.96290400
H	0.78165500	-2.31012800	-3.06275500
C	-1.51538400	-0.26933500	-3.34053800
H	-1.37924900	-0.14518000	-4.42071200
H	-1.90018100	-1.27466100	-3.14998800
H	-2.23947100	0.46994600	-2.98922000
C	1.15769300	-1.31544900	3.31745800
H	2.18801300	-1.22740700	2.96263300
H	1.12892200	-1.18532200	4.40504200
H	0.78189500	-2.31011500	3.06259500
C	0.72783300	1.52668700	3.24476000

H	0.76499100	1.43713600	4.33606100
H	1.72976800	1.74792100	2.86616900
H	0.06823200	2.35903500	2.98285700
C	-1.51498800	-0.26916600	3.34064300
H	-1.89984300	-1.27448600	3.15016800
H	-1.37872900	-0.14498100	4.42079800
H	-2.23908800	0.47012800	2.98938100
C	6.23870700	1.61661700	-0.00126000
H	7.32935800	1.52844900	-0.00145900
H	5.92956500	2.16959000	-0.89218400
H	5.93001900	2.17075100	0.88910000
C	6.19797900	-0.92704400	-1.45709900
H	7.28890100	-0.99478700	-1.39445700
H	5.77909400	-1.93603300	-1.51121900
H	5.91638600	-0.38727700	-2.36588900
C	6.19783100	-0.92482200	1.45845600
H	5.77897200	-1.93375100	1.51396600
H	7.28877100	-0.99259600	1.39613100
H	5.91603000	-0.38374100	2.36640000
Sn	-1.53292600	2.21914100	0.00006900
Sn	-1.61877400	-2.17502900	0.00006700
Cl	-2.90377100	2.92296100	1.84220200
Cl	-2.90394300	2.92281300	-1.84200700
Cl	0.05055300	4.12894600	-0.00012700
Cl	-3.97598900	-1.82483700	0.00005500
Cl	-1.38297800	-3.76451300	-1.80850200
Cl	-1.38297400	-3.76440800	1.80872900
Re	0.21888700	-0.08931700	-0.00003500

Re.SiCl₃ (singlet)

P	-0.47866000	0.12077100	-2.44154800
N	1.37962600	1.37618000	-0.03172700
H	1.05937300	2.34750800	-0.08278000
P	-0.50292300	-0.09434000	2.47596900
C	2.77391000	-1.17060800	0.11056200
C	2.70390500	1.31394300	-0.04461800
C	3.40836200	0.09422300	0.02122400
C	1.39148000	-1.40121200	0.13202600
H	3.24901500	2.25561900	-0.10812000
H	1.20446400	-2.47425000	0.25045400
H	3.43628300	-2.04310000	0.15992700
P	5.17770800	0.10586900	-0.00372700
C	0.83649100	-0.88230900	-3.27747300
H	0.71637000	-1.93157300	-3.00386000

H	0.75710500	-0.76890800	-4.36527400
H	1.81930300	-0.53577200	-2.94599100
C	-0.13317100	1.77818200	-3.19545000
H	0.82315300	2.15531000	-2.82214400
H	-0.08085900	1.68050600	-4.28599800
H	-0.91502200	2.49424500	-2.93873600
C	-2.00906000	-0.40842400	-3.31962400
H	-2.87419900	0.10861000	-2.90376800
H	-1.90924200	-0.15849600	-4.38196200
H	-2.14411900	-1.48528900	-3.21024800
C	-2.12187100	-0.51946300	3.24669500
H	-2.05751800	-0.34529800	4.32677200
H	-2.91617500	0.09754800	2.82759000
H	-2.34228200	-1.57213200	3.06132600
C	0.64662500	-1.26305000	3.34082400
H	1.67983100	-0.98694600	3.11372200
H	0.48371500	-1.20791000	4.42364600
H	0.46370300	-2.28120600	2.99499200
C	-0.01233300	1.47977600	3.32344600
H	-0.02545700	1.33789300	4.41042000
H	1.00032500	1.74919600	3.00816500
H	-0.69109400	2.29212800	3.06114800
C	5.84248600	-0.85393500	-1.41046800
H	6.93594500	-0.89167200	-1.37457100
H	5.44540000	-1.87243200	-1.37858800
H	5.52261500	-0.38812800	-2.34710800
C	5.86868400	1.78859300	-0.13963600
H	5.53006300	2.26656000	-1.06273200
H	5.55861700	2.39918800	0.71257600
H	6.96112200	1.72679600	-0.15237500
C	5.88747700	-0.63581300	1.50928500
H	5.49447500	-1.64832400	1.63785800
H	6.97970700	-0.67770000	1.44797600
H	5.59205700	-0.03766300	2.37623200
Si	-1.76761800	1.94287200	0.07755100
Si	-1.56221600	-2.05283600	-0.08959100
Cl	-1.13059600	-3.45071900	-1.70637100
Cl	-3.68832200	-1.93538500	-0.23910600
Cl	-1.37104300	-3.53381000	1.49608600
Cl	-3.22422200	2.32809300	-1.46477900
Cl	-3.02389300	2.49034800	1.74419500
Cl	-0.64113700	3.85680100	-0.06563700
Re	-0.11852700	-0.04590100	0.02275100

Re.SiCl (triplet)

P	0.24572700	-0.00377600	2.49020200
N	-1.35674500	1.37576900	-0.00306300
H	-1.02763200	2.34117000	-0.00613800
P	0.25312000	-0.00893000	-2.48667400
C	-2.72471700	-1.20261700	0.00162500
C	-2.67374200	1.29932900	-0.00402900
C	-3.38415600	0.08266800	-0.00130700
C	-1.36365300	-1.40299800	0.00245100
H	-3.22281700	2.24188700	-0.00736700
H	-1.11708100	-2.46938400	0.00370000
H	-3.37539900	-2.08296900	0.00285800
P	-5.13303800	0.09582000	-0.00352000
C	-0.96609900	-1.14811700	3.29449000
H	-0.70790200	-2.17855600	3.03842300
H	-0.94534100	-1.02608500	4.38334400
H	-1.97093700	-0.93782900	2.91905100
C	-0.26069200	1.62042600	3.22374100
H	-1.22291200	1.92721300	2.80427900
H	-0.35032500	1.54013000	4.31288200
H	0.48169000	2.38626400	2.98455700
C	1.78888000	-0.37959900	3.43204800
H	2.59922600	0.26923700	3.09676800
H	1.61365300	-0.21677700	4.50163500
H	2.07420300	-1.42049300	3.26930000
C	1.79482000	-0.40354700	-3.42294500
H	1.62468000	-0.24121000	-4.49325200
H	2.61096600	0.23769800	-3.08592400
H	2.06902500	-1.44693300	-3.25674800
C	-0.96911600	-1.14287000	-3.28964300
H	-1.97265000	-0.91913200	-2.91861900
H	-0.94333500	-1.02587800	-4.37906700
H	-0.72387900	-2.17517600	-3.02815800
C	-0.23484700	1.61763200	-3.22768800
H	-0.32461800	1.53303100	-4.31658100
H	-1.19411600	1.93713300	-2.81072100
H	0.51534200	2.37654200	-2.99168900
C	-5.84913000	-0.75922700	1.45159300
H	-6.94069100	-0.81017100	1.38268400
H	-5.44554900	-1.77426000	1.51081300
H	-5.56374900	-0.22190000	2.36104200
C	-5.83491200	1.78134500	-0.00523100
H	-5.51725500	2.32991600	0.88529000
H	-5.51502800	2.32893200	-0.89547900

H	-6.92709100	1.71209300	-0.00664600
C	-5.84643200	-0.76148800	-1.45848000
H	-5.44168500	-1.77599400	-1.51594700
H	-6.93791800	-0.81357600	-1.39100700
H	-5.56054700	-0.22501900	-2.36762700
Si	1.85086400	2.02051400	0.00002900
Si	1.68322100	-2.10815100	0.00259600
Cl	1.44500200	-3.49969900	1.62827500
Cl	3.77506500	-1.77822600	-0.02367200
Cl	1.40584700	-3.51540600	-1.60325500
Cl	3.16371400	2.42862600	1.63873900
Cl	3.18460500	2.40235500	-1.62751200
Cl	0.70932600	3.88880900	-0.02012200
Re	0.20553100	-0.06674000	0.00196600

Re.CO (singlet)

P	-1.00689700	2.41713500	-0.07115200
N	0.54988200	-0.00000100	1.49145400
H	0.30448000	-0.00001300	2.47597500
P	-1.00692200	-2.41712400	-0.07116400
C	1.81643700	0.00000100	-1.24887500
C	1.85285000	0.00000000	1.31009800
C	2.50615000	0.00000200	0.05798600
C	0.47248000	0.00000500	-1.44073400
H	2.47737200	-0.00001200	2.20854600
H	0.20987500	-0.00000300	-2.50589600
H	2.48634400	-0.00001300	-2.12066600
P	4.23610700	-0.00001400	0.01418800
C	0.45928700	3.24615800	0.70718300
H	1.37126600	2.82644800	0.27302500
H	0.44134400	4.33085000	0.54962100
H	0.46711600	3.03888000	1.78162800
C	-0.94397900	3.11174800	-1.78628200
H	-0.88515600	4.20649300	-1.78609700
H	-0.07154600	2.69560500	-2.29829900
H	-1.83878800	2.79732800	-2.33250800
C	-2.40796500	3.38770800	0.65821000
H	-2.27114700	4.46878700	0.53604300
H	-3.33993300	3.08604000	0.16999600
H	-2.49887000	3.15237500	1.72325300
C	-0.94401900	-3.11173500	-1.78629600
H	-0.07158500	-2.69559900	-2.29831700
H	-0.88520600	-4.20648100	-1.78611200
H	-1.83882800	-2.79730600	-2.33251700

C	0.45926800	-3.24614400	0.70716200
H	0.44132900	-4.33083800	0.54960800
H	1.37124000	-2.82643200	0.27299200
H	0.46710700	-3.03885700	1.78160500
C	-2.40798900	-3.38769600	0.65820000
H	-3.33995600	-3.08604100	0.16997500
H	-2.27116100	-4.46877500	0.53604300
H	-2.49890500	-3.15235500	1.72324100
C	5.02934800	-0.00003200	1.66297800
H	6.11597400	-0.00002800	1.53349500
H	4.74146300	0.89010500	2.22801700
H	4.74146900	-0.89018200	2.22799700
C	4.95689100	1.44485900	-0.87095700
H	6.04219400	1.35031400	-0.98497900
H	4.49696200	1.52171600	-1.86037200
H	4.72375300	2.35718900	-0.31410500
C	4.95688300	-1.44488000	-0.87098000
H	4.49695600	-1.52171300	-1.86039800
H	6.04218800	-1.35034700	-0.98499700
H	4.72373200	-2.35721800	-0.31414600
C	-2.40559000	-0.00000900	1.51564500
C	-2.51339600	0.00001900	-1.26228400
O	-3.14132400	-0.00005800	2.43215700
O	-3.34646900	0.00001900	-2.09465900
Re	-1.13269500	0.00000600	0.05005100

Re.CO (triplet)

P	-1.05155900	-2.43605000	0.05138400
N	0.48336000	0.04682100	-1.45503000
H	0.23278200	0.06904100	-2.44052800
P	-1.17608500	2.43834500	0.06451300
C	1.80535000	0.10690100	1.19186900
C	1.80637200	0.02161800	-1.29247900
C	2.47174700	0.05217700	-0.05847100
C	0.43160900	0.06645500	1.39866300
H	2.40457300	-0.00175600	-2.20543300
H	0.18650300	0.12900000	2.46709200
H	2.45989000	0.20849400	2.06535600
P	4.48386600	0.26852900	0.06430200
C	0.27772200	-3.26493500	-0.93488200
H	1.25011000	-2.86522200	-0.63354800
H	0.26676100	-4.35083800	-0.78814300
H	0.13474500	-3.04491300	-1.99725600
C	-0.78183300	-3.15301800	1.73461300

H	-0.75534600	-4.24838900	1.71046900
H	0.16163400	-2.77173300	2.13543400
H	-1.58887700	-2.82649500	2.39781600
C	-2.56631800	-3.34337300	-0.50217600
H	-2.44387600	-4.42931200	-0.41855800
H	-3.41585500	-3.02972300	0.11241800
H	-2.78972100	-3.08387900	-1.54148900
C	-1.06718500	3.15710600	1.76482100
H	-0.13570900	2.82532300	2.23227700
H	-1.09453000	4.25238500	1.74295900
H	-1.90191300	2.78734100	2.36833700
C	0.19440400	3.31978500	-0.81112400
H	0.13416500	4.40349400	-0.66013200
H	1.15288700	2.95064700	-0.43523100
H	0.14292100	3.10304600	-1.88240500
C	-2.67949000	3.28637600	-0.60256300
H	-3.56068400	2.93495100	-0.05680100
H	-2.60803000	4.37580200	-0.50628800
H	-2.81132800	3.02501500	-1.65693900
C	4.81012100	-1.18855500	1.17643000
H	5.79484900	-1.61472100	0.95646900
H	4.80445700	-0.87017500	2.22373900
H	4.04523100	-1.95758900	1.04540700
C	6.23381200	1.14328300	0.37265000
H	7.08030400	0.45534700	0.23478900
H	6.32809200	1.98214100	-0.32449100
H	6.24393500	1.53624500	1.39420500
C	-2.43590200	-0.02977000	-1.50990300
C	-2.48663000	-0.04417000	1.34157300
O	-3.16359700	-0.04598600	-2.42672100
O	-3.27285800	-0.06925200	2.21223500
Re	-1.14848700	-0.00095300	-0.03213900
C	4.92303500	-0.41234200	-1.61220900
H	4.81440400	0.35864500	-2.38272900
H	5.96523800	-0.74529800	-1.61345900
H	4.28285700	-1.25880900	-1.87570000

Re.PF₃ (singlet)

P	0.44260300	-2.42524400	-0.10064600
N	-1.02436800	0.01061500	1.44213000
H	-0.74746600	0.02588700	2.41762600
P	0.41252500	2.42955300	-0.13773600
C	-2.31399800	-0.02256000	-1.26090500
C	-2.32934900	0.00617500	1.28578500

C	-2.99998100	-0.00649900	0.04493700
C	-0.97165800	-0.02235400	-1.45781700
H	-2.93269500	0.01563900	2.19761500
H	-0.70320300	-0.05231300	-2.51856400
H	-2.97916600	-0.04423700	-2.13436700
P	-4.73147600	-0.01150400	0.01773600
C	-0.83084700	-3.23449100	0.97968500
H	-1.81658100	-2.82537700	0.74084600
H	-0.84200800	-4.32083700	0.83491700
H	-0.61415100	-3.01606100	2.02990700
C	-0.01112800	-3.11117200	-1.76025800
H	-0.05468500	-4.20617000	-1.74510500
H	-0.98090800	-2.70407100	-2.05780900
H	0.72823900	-2.78434600	-2.49669000
C	1.94561500	-3.43595600	0.28690400
H	1.76872400	-4.50118800	0.09914100
H	2.77485900	-3.08723400	-0.33464600
H	2.23327600	-3.28979800	1.33021500
C	0.05510200	3.09931900	-1.82726000
H	-0.84403700	2.61612300	-2.21832100
H	-0.08454000	4.18633700	-1.80734900
H	0.89313500	2.85746100	-2.48734700
C	-0.94999700	3.20791300	0.85102600
H	-0.97830900	4.29324400	0.70127100
H	-1.90610200	2.77223800	0.54782800
H	-0.79857600	2.99683700	1.91393800
C	1.85855300	3.48378700	0.34052500
H	2.72116600	3.18690200	-0.26176000
H	1.64679100	4.54616500	0.17282100
H	2.11161000	3.32251100	1.39081400
C	-5.50096200	0.00976000	1.67686100
H	-6.58928500	0.00694100	1.56309900
H	-5.20401800	-0.87245000	2.24965200
H	-5.20596400	0.90775400	2.22563300
C	-5.45414500	-1.47090500	-0.83937300
H	-6.54118600	-1.38287400	-0.94046900
H	-5.00718200	-1.55852000	-1.83388300
H	-5.20960500	-2.37493900	-0.27399800
C	-5.45925100	1.42052800	-0.87974500
H	-5.01092000	1.48297600	-1.87553600
H	-6.54571500	1.32488000	-0.98003700
H	-5.21957400	2.34070500	-0.33885700
P	2.04816200	0.02465800	1.74508300
P	2.22026000	-0.01456200	-1.52547000

F	1.40321200	0.13574500	3.24123800
F	3.16197500	1.16987900	1.99646500
F	3.05309500	-1.18090100	2.14007400
F	3.58554800	-0.86005900	-1.34181600
F	2.98078600	1.32669500	-2.03740600
F	1.92901200	-0.55739600	-3.02544800
Re	0.61302900	0.00230700	0.00546400

Re.PF₃ (triplet)

P	-0.57249600	2.45746500	-0.09237100
N	0.95711600	0.02527800	1.41772100
H	0.68198300	0.02938000	2.39643800
P	-0.47327900	-2.44118500	-0.10697600
C	2.29546600	0.09591400	-1.19651500
C	2.28132400	-0.00208500	1.27676500
C	2.96224800	0.03601600	0.05207800
C	0.92309400	0.06924500	-1.40448000
H	2.86024700	-0.03772800	2.20095700
H	0.67274000	0.15194600	-2.46791500
H	2.94547100	0.19895500	-2.07252200
P	4.97674600	0.25594800	-0.06653700
C	0.59046300	3.27795500	1.09003500
H	1.59946000	2.88665100	0.93469700
H	0.59569100	4.36419600	0.94670900
H	0.28842200	3.05456300	2.11794200
C	-0.01617800	3.15782300	-1.71220700
H	-0.04081800	4.25301200	-1.69801600
H	1.00092400	2.81722100	-1.92222600
H	-0.66857300	2.78913100	-2.50862700
C	-2.13538400	3.40735900	0.18347600
H	-1.97344900	4.47771500	0.01496600
H	-2.90412800	3.04226800	-0.50237800
H	-2.49489000	3.24784300	1.20171900
C	0.01066700	-3.11654200	-1.76041500
H	0.95164200	-2.65836600	-2.07577700
H	0.12367300	-4.20596500	-1.72574000
H	-0.76200000	-2.86099400	-2.49114700
C	0.79776700	-3.20854100	0.99784600
H	0.83962400	-4.29372900	0.85259900
H	1.77759200	-2.77449800	0.78214600
H	0.55152000	-2.99663400	2.04276800
C	-1.96353700	-3.47121000	0.26836000
H	-2.78016400	-3.17208800	-0.39336300
H	-1.74589300	-4.53442600	0.11701000

H	-2.28490900	-3.30832300	1.29904500
C	5.40467400	-0.36573900	1.63453800
H	6.45353800	-0.67531600	1.66157400
H	5.26650700	0.42483800	2.38006200
H	4.77988400	-1.21875000	1.91364000
C	6.71935800	1.12881900	-0.39810200
H	7.56811500	0.44998400	-0.23313800
H	6.73184200	1.48645100	-1.43245600
H	6.80651700	1.99151900	0.27015000
C	5.30556200	-1.23673300	-1.12869000
H	5.27299800	-0.95879200	-2.18699100
H	6.30116200	-1.63900600	-0.91346100
H	4.55632200	-2.01233800	-0.95277200
P	-2.09764200	-0.02765500	1.75779700
P	-2.20850300	-0.00336800	-1.59758600
F	-1.44704300	-0.13126400	3.24424400
F	-3.19453700	-1.18396000	1.99925200
F	-3.10429400	1.17337400	2.14075300
F	-3.57810300	0.83719400	-1.47236000
F	-2.92782700	-1.35269400	-2.12683100
F	-1.84470200	0.53679700	-3.07659200
Re	-0.64303800	0.00450100	0.00417100

Re.H (singlet)

P	-2.11137000	1.83091400	0.06045200
N	0.83766400	-0.33429400	1.34399000
H	0.54768300	-0.53460200	2.29273100
P	-2.29416000	-1.75071600	-0.07588700
C	2.14947900	0.26369700	-1.20918500
C	2.16187000	-0.32146000	1.23222700
C	2.82923000	-0.03221500	0.03191200
C	0.78548200	0.29162900	-1.39096200
H	2.74386600	-0.54007200	2.12996900
H	0.54349700	0.51776300	-2.43249300
H	2.80511200	0.46914800	-2.06778600
P	4.56908000	-0.04213100	-0.00392800
C	-1.11451700	3.40835000	0.12896400
H	-0.45849400	3.44921800	-0.74556200
H	-1.75318100	4.30070900	0.15078800
H	-0.48585900	3.39424200	1.02510300
C	-3.25244200	2.25079200	-1.35100100
H	-3.75865100	3.21289800	-1.20328500
H	-2.67010000	2.28191300	-2.27651700
H	-4.00536300	1.46281200	-1.45521500

C	-3.26606200	2.13779500	1.49052900
H	-3.75608200	3.11716500	1.42048600
H	-4.03077400	1.35572800	1.51655000
H	-2.69521500	2.07995500	2.42169600
C	-2.57447200	-2.55638100	-1.72910900
H	-1.60446600	-2.83738000	-2.15046300
H	-3.21401000	-3.44487500	-1.65610500
H	-3.03429800	-1.83130300	-2.40701000
C	-1.81168500	-3.24671800	0.92857300
H	-2.52282700	-4.07373500	0.80872300
H	-0.81724400	-3.58080500	0.61538900
H	-1.76030900	-2.96388400	1.98421700
C	-4.06395400	-1.57346400	0.48336300
H	-4.55911800	-0.80469200	-0.11912700
H	-4.62352100	-2.51267100	0.38860100
H	-4.07400300	-1.24943500	1.52825300
C	5.33509000	-0.43170900	1.60971900
H	6.42415600	-0.41779100	1.50380200
H	5.04127400	0.30841000	2.35839000
H	5.02388300	-1.42305800	1.94879800
C	5.28646800	1.56635100	-0.52023600
H	6.37485700	1.50628800	-0.62635900
H	4.84512200	1.86294100	-1.47589300
H	5.02943400	2.32543300	0.22428400
C	5.26035900	-1.26096700	-1.18984600
H	4.81697600	-1.08975800	-2.17480400
H	6.35008400	-1.17950700	-1.26291800
H	4.98662800	-2.26858900	-0.86363200
H	-1.50558600	0.06048900	-1.50808400
H	-1.52704000	-0.19550300	1.56203300
Re	-0.76456500	-0.02616800	0.00451000

Re.H (triplet)

P	-1.64040300	2.34058500	-0.01246900
N	0.44335000	0.00003000	1.42460800
H	0.14671600	0.00003600	2.39423100
P	-1.64027700	-2.34063500	-0.01246700
C	1.72905700	0.00003200	-1.24701400
C	1.75597300	0.00004600	1.28999300
C	2.41656800	0.00004000	0.03899300
C	0.36379600	0.00002200	-1.40547600
H	2.35841900	0.00006400	2.20198800
H	0.06678100	-0.00004300	-2.46271900
H	2.37772000	0.00002900	-2.13348000

P	4.14974800	0.00005000	-0.00288200
C	-0.77590500	3.42713600	1.22595000
H	0.30615600	3.33939100	1.08504300
H	-1.06788000	4.48020100	1.13122500
H	-1.01736600	3.07427600	2.23329200
C	-1.31690300	3.28203400	-1.58087800
H	-1.58551800	4.34249800	-1.49807100
H	-0.25621000	3.19237300	-1.83529700
H	-1.89506300	2.82175800	-2.38779900
C	-3.41256700	2.77034700	0.30375200
H	-3.58366100	3.85302400	0.26178800
H	-4.03251200	2.27116000	-0.44610000
H	-3.69759800	2.38666400	1.28688600
C	-1.31674400	-3.28207700	-1.58087300
H	-0.25605900	-3.19236400	-1.83530600
H	-1.58530200	-4.34255500	-1.49805000
H	-1.89493800	-2.82184200	-2.38779300
C	-0.77569900	-3.42713200	1.22594600
H	-1.06761700	-4.48021300	1.13123100
H	0.30635400	-3.33932700	1.08502200
H	-1.01716500	-3.07428000	2.23329000
C	-3.41241100	-2.77050000	0.30377700
H	-4.03239500	-2.27135300	-0.44607000
H	-3.58344200	-3.85318700	0.26181900
H	-3.69745600	-2.38683000	1.28691200
C	4.93347800	0.00007000	1.64981100
H	6.02117200	0.00007500	1.52959500
H	4.63933000	0.88986100	2.21218000
H	4.63933800	-0.88971300	2.21219700
C	4.86426400	1.44744500	-0.88565900
H	5.95090200	1.36067600	-0.99296200
H	4.40813000	1.51899500	-1.87715400
H	4.62033900	2.35851500	-0.33149000
C	4.86427900	-1.44735100	-0.88563500
H	4.40814400	-1.51892500	-1.87712800
H	5.95091600	-1.36057200	-0.99294100
H	4.62036500	-2.35841400	-0.33144900
H	-2.42917700	-0.00004300	-1.20178800
H	-2.12447000	-0.00003100	1.51677300
Re	-1.16852700	-0.00001100	0.00268000
Os.SnCl₃ (singlet)			
Os	0.26174400	0.07145700	-0.00008100
P	-0.14349000	-0.01983600	2.43758900

N	1.71047100	-1.37290300	0.00024600
H	1.36411300	-2.34394900	0.00053000
P	-0.14313000	-0.02075200	-2.43776900
C	3.12399200	1.13968500	-0.00018000
C	3.02360000	-1.32901700	0.00028500
C	3.74899600	-0.10700500	0.00007600
C	1.72219700	1.38362400	-0.00026700
H	3.55273200	-2.28027200	0.00052100
H	1.53729500	2.46216600	-0.00039800
H	3.76703900	2.02312700	-0.00028300
P	5.55598600	-0.14163200	0.00018800
C	0.27017300	-1.65147100	3.19295400
H	1.24597900	-1.99412000	2.83912500
H	0.30424400	-1.53385300	4.28168800
H	-0.48247800	-2.40500300	2.95197400
C	1.03414800	1.10820200	3.30092800
H	0.88395900	1.01964100	4.38263900
H	2.06148200	0.82772500	3.05421000
H	0.84921600	2.13985900	2.99472900
C	-1.76977200	0.42012000	3.16979200
H	-1.73259500	0.18452500	4.23915900
H	-1.95781600	1.48978500	3.05331400
H	-2.57820100	-0.15379700	2.71419900
C	1.03390000	1.10754900	-3.30159500
H	2.06139000	0.82765100	-3.05488400
H	0.88360900	1.01861300	-4.38326100
H	0.84851500	2.13922700	-2.99573400
C	0.27169200	-1.65245000	-3.19233400
H	0.30397700	-1.53579900	-4.28122300
H	1.24859300	-1.99317600	-2.83963700
H	-0.47936800	-2.40694000	-2.94948500
C	-1.76966400	0.41807600	-3.17008600
H	-1.95815500	1.48769500	-3.05392800
H	-1.73245600	0.18213000	-4.23937400
H	-2.57780400	-0.15607800	-2.71429100
C	6.19077300	-1.84741900	0.00085000
H	7.28494700	-1.81231300	0.00096000
H	5.85978400	-2.38521200	0.89393500
H	5.85999000	-2.38584300	-0.89193000
C	6.20597300	0.70513800	1.47713400
H	7.30049100	0.70713500	1.45300700
H	5.84974500	1.73891400	1.50736600
H	5.86613000	0.18736000	2.37900400
C	6.20615800	0.70409200	-1.47727700

H	5.84986800	1.73782400	-1.50829800
H	7.30067200	0.70616800	-1.45299700
H	5.86647100	0.18564800	-2.37882400
Sn	-1.60034700	-2.07574100	0.00010700
Sn	-1.39096100	2.19847000	-0.00024900
Cl	-3.01187500	-2.69030500	-1.81140800
Cl	-3.01387300	-2.68804400	1.81075800
Cl	-0.08431100	-4.02265500	0.00175800
Cl	-3.73668400	1.94452400	0.00183300
Cl	-1.00288500	3.74969400	1.78477900
Cl	-1.00597500	3.74813400	-1.78725800

Os.SnCl₃ (triplet)

P	0.19465600	-0.19533400	-2.51599500
N	1.83364400	1.16331800	-0.04547700
H	1.57058400	2.14977300	-0.13238800
P	0.22514300	-0.27475500	2.44815500
C	3.09060500	-1.46883700	-0.03814600
C	3.13995600	1.01176500	-0.03463400
C	3.80495500	-0.23606800	-0.01481500
C	1.71331400	-1.56036800	-0.05774300
H	3.72656900	1.92934900	-0.06021500
H	1.31403900	-2.58398400	-0.06288600
H	3.66271200	-2.39777000	-0.03860600
P	5.59090800	-0.29420500	0.01629500
C	1.45457800	0.95202900	-3.22190400
H	2.45463300	0.67032100	-2.88179900
H	1.42254100	0.90117700	-4.31522400
H	1.24769900	1.97883700	-2.90675200
C	0.64894900	-1.81792900	-3.26427800
H	0.71521000	-1.71670100	-4.35271600
H	1.61397200	-2.15137400	-2.87298000
H	-0.11220300	-2.56626500	-3.02863500
C	-1.32489100	0.27900200	-3.43674100
H	-1.11964800	0.19749000	-4.50971400
H	-2.15400900	-0.38720200	-3.18898300
H	-1.61851400	1.30567500	-3.20810600
C	1.12765300	-1.72320300	3.14723000
H	2.16258700	-1.72708800	2.79628700
H	1.11595000	-1.66741100	4.24081900
H	0.63900900	-2.64887400	2.83244400
C	1.11135200	1.15698300	3.20076700
H	1.16950700	1.01875500	4.28554700
H	2.12333300	1.22947700	2.79444900

H	0.57361600	2.08626800	2.99619400
C	-1.36284400	-0.32751100	3.37698100
H	-1.87370200	-1.27793300	3.20388100
H	-1.14066000	-0.24245600	4.44628800
H	-2.02037400	0.49449000	3.08852600
C	6.32350200	1.37284600	0.02272200
H	7.41334800	1.27395100	0.04678400
H	6.04429400	1.92448100	-0.87938200
H	6.00559800	1.93434200	0.90570500
C	6.24410900	-1.18238000	-1.43797900
H	7.33510500	-1.25012200	-1.37799200
H	5.82873700	-2.19346600	-1.47969200
H	5.96480600	-0.64906000	-2.35135300
C	6.19038400	-1.16940200	1.50120900
H	5.77369200	-2.18027000	1.53569500
H	7.28289200	-1.23711000	1.48257400
H	5.87712000	-0.62843500	2.39894900
Sn	-1.28456800	2.16542200	0.03855500
Sn	-2.01206900	-1.77332500	-0.01067100
Cl	-1.92531900	3.12044200	2.11414200
Cl	-3.15995600	2.60553300	-1.31655600
Cl	0.27108500	3.88922300	-0.71729000
Cl	-3.99990000	-0.89624500	0.88033900
Cl	-2.74238400	-2.82547100	-2.00084300
Cl	-1.53449800	-3.68915700	1.33290500
Os	0.24229000	-0.22457400	-0.04133200

Os.SiCl₃ (singlet)

P	-0.44444300	0.24230100	-2.44082600
N	1.36943700	1.39319000	-0.03505400
H	1.02151000	2.35651100	-0.08482500
P	-0.43433800	-0.15927100	2.45051800
C	2.75954200	-1.12751900	0.13209000
C	2.67878300	1.34189200	-0.02167900
C	3.39586200	0.11273000	0.03600700
C	1.36336100	-1.36272000	0.21208700
H	3.22460000	2.28358700	-0.06857500
H	1.17221800	-2.41069900	0.46077200
H	3.39836600	-2.01502500	0.14478300
P	5.19574600	0.12378400	-0.00844900
C	0.92589200	-0.70024200	-3.24889800
H	0.82462600	-1.76138000	-3.01609900
H	0.87266000	-0.55416900	-4.33367200
H	1.88949500	-0.33595600	-2.88264900

C	-0.13461500	1.94500500	-3.08453600
H	0.79883700	2.34165100	-2.67739300
H	-0.05364000	1.89509000	-4.17585600
H	-0.94954700	2.62138300	-2.82349100
C	-1.93443900	-0.30019600	-3.37180200
H	-1.83592200	0.06020600	-4.40156700
H	-1.99873500	-1.38834000	-3.37308600
H	-2.83937500	0.11627800	-2.93054900
C	-2.04233000	-0.62809900	3.21719500
H	-2.05963400	-0.24441000	4.24279700
H	-2.88818100	-0.21574100	2.67058400
H	-2.12040600	-1.71610600	3.23382100
C	0.73009600	-1.31609000	3.30173300
H	1.76304900	-1.01630400	3.10576600
H	0.54288900	-1.27360300	4.38033300
H	0.57258800	-2.33788500	2.95388000
C	0.05978600	1.42852700	3.25606200
H	0.04790700	1.29444400	4.34329700
H	1.07386500	1.69018200	2.94045700
H	-0.61591500	2.24300600	2.99522600
C	5.80599200	-0.88203800	-1.40111900
H	6.90053200	-0.90038600	-1.39612500
H	5.43421200	-1.90742000	-1.31976100
H	5.45586500	-0.45439200	-2.34517900
C	5.85286500	1.81015800	-0.20737500
H	5.49471300	2.25819000	-1.13858500
H	5.56217500	2.44303300	0.63594200
H	6.94569200	1.75787400	-0.24226900
C	5.88833700	-0.56669400	1.53045700
H	5.52490200	-1.58768800	1.67922900
H	6.98168700	-0.58187300	1.47655700
H	5.57700200	0.04589000	2.38181000
Si	-1.84823600	1.87253700	0.15533700
Si	-1.57596700	-2.02723900	-0.15753200
Cl	-1.13531700	-3.30962800	-1.81028500
Cl	-3.65297000	-1.76531300	-0.26704900
Cl	-1.34316600	-3.49496300	1.37852700
Cl	-3.28967100	2.17436000	-1.36246300
Cl	-3.05787300	2.26723200	1.84466500
Cl	-0.74866800	3.74825800	0.05263400
Os	-0.12295000	-0.07186900	0.00668600

Os.SiCl₃ (triplet)

P	-0.27971100	-0.12231100	-2.48245900
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N	1.46317600	1.26499500	-0.01088000
H	1.25443600	2.25993100	-0.03447500
P	-0.22178200	-0.24051500	2.46963500
C	2.61920400	-1.39421300	-0.03623900
C	2.76358800	1.07826300	-0.01381200
C	3.38393300	-0.19223700	-0.01822900
C	1.23988500	-1.44809000	-0.03859400
H	3.38889600	1.97095200	-0.01933700
H	0.82922000	-2.46326600	-0.05913300
H	3.16107000	-2.34218200	-0.05248700
P	5.16142000	-0.32174900	-0.01818900
C	-0.19496900	-1.82218900	-3.19581600
H	-1.11630600	-2.37204600	-2.99265100
H	-0.05568100	-1.75764900	-4.28027000
H	0.64293400	-2.37037600	-2.75681200
C	1.23321900	0.66104000	-3.19344300
H	2.12748000	0.17549500	-2.79391400
H	1.22342000	0.55469900	-4.28333400
H	1.25481200	1.72330800	-2.93974200
C	-1.61714900	0.67510300	-3.46811000
H	-1.58100100	1.75809300	-3.34223200
H	-1.46193000	0.43174500	-4.52486400
H	-2.59632700	0.31016300	-3.15837800
C	-1.54585000	0.47318000	3.53472900
H	-1.36077600	0.16425700	4.56932500
H	-1.52793900	1.56203100	3.47811700
H	-2.52724500	0.11390900	3.22603100
C	-0.08953200	-1.97344900	3.09029300
H	0.75199900	-2.48000500	2.61043800
H	0.06485200	-1.96435500	4.17453800
H	-1.00292900	-2.53052800	2.87063500
C	1.29342300	0.53863500	3.17992200
H	1.31395300	0.38201400	4.26360600
H	2.18639900	0.09133600	2.73568200
H	1.28733600	1.61174500	2.97507100
C	5.76094400	-1.21310400	-1.49450500
H	6.84878400	-1.32770000	-1.45118100
H	5.30183300	-2.20464200	-1.54568600
H	5.49116600	-0.65445500	-2.39550400
C	5.96436400	1.31317900	-0.00055100
H	5.69237400	1.88915800	-0.88948000
H	5.68419400	1.87370600	0.89568300
H	7.04939300	1.16951300	0.00301700
C	5.75661600	-1.24259400	1.44159200

H	5.29544900	-2.23403800	1.47241800
H	6.84432500	-1.35838600	1.39820800
H	5.48606000	-0.70107000	2.35275900
Si	-1.35337500	2.18509900	0.06194700
Si	-2.21350700	-1.64847200	-0.02057700
Cl	-3.56810100	-1.57962600	-1.62432600
Cl	-3.52980600	-1.67066800	1.61592200
Cl	-1.51135900	-3.64947500	-0.08402000
Cl	-3.43032400	2.20402300	-0.00374500
Cl	-0.80440200	3.39789900	1.71429600
Cl	-0.70061600	3.48444300	-1.49283400
Os	-0.25398400	-0.09570700	-0.00522700

Os.OH (singlet)

Os	-0.68514700	0.00059600	-0.00936700
P	-1.88107500	2.03588800	-0.00500900
N	0.73503900	-0.03487800	1.37508200
H	0.44100300	-0.07090600	2.35253200
P	-1.86088400	-2.04571300	-0.01983600
C	2.06687400	0.02880800	-1.23576600
C	2.07040700	-0.03472300	1.26046300
C	2.72980400	0.00040000	0.02459100
C	0.68445600	0.02221900	-1.42462600
H	2.63796300	-0.06475800	2.18706000
H	0.41318100	0.03831600	-2.49109900
H	2.70343800	0.05473100	-2.12439200
P	4.50976500	0.00781800	-0.00368100
C	-1.44292200	3.10783300	1.42758700
H	-0.37378500	3.34068100	1.41383500
H	-2.01117500	4.04400900	1.39751200
H	-1.68564600	2.56698200	2.34438800
C	-1.52849000	3.08848100	-1.47147600
H	-2.11680000	4.01182300	-1.43093700
H	-0.46501200	3.34148400	-1.50746100
H	-1.79664800	2.52658200	-2.36784700
C	-3.69911900	1.88279200	0.05589300
H	-4.14922500	2.88118300	0.07577100
H	-4.02498200	1.33843900	-0.83091900
H	-3.95892100	1.32850000	0.95835600
C	-1.50654600	-3.07887600	-1.49867100
H	-0.44148200	-3.32405800	-1.54102000
H	-2.08856100	-4.00653300	-1.46682800
H	-1.78150600	-2.50797300	-2.38732200
C	-1.41065700	-3.11980300	1.40592200

H	-1.97920400	-4.05592500	1.38132100
H	-0.34154200	-3.35200700	1.38343700
H	-1.64673200	-2.57391100	2.32160400
C	-3.67902000	-1.90022400	0.05080400
H	-4.01189100	-1.35258400	-0.83137200
H	-4.12549500	-2.90026800	0.06871100
H	-3.93591400	-1.35169000	0.95780500
C	5.23439900	-0.04204400	1.66809100
H	6.32516700	-0.03573500	1.57992100
H	4.92507400	0.83122300	2.24876800
H	4.93078700	-0.95201900	2.19274600
C	5.15599900	1.50523600	-0.82436600
H	6.24867400	1.47098500	-0.87995100
H	4.74846600	1.57845800	-1.83658000
H	4.84755600	2.39029500	-0.26025600
C	5.16731200	-1.43027500	-0.91621900
H	4.76147900	-1.44287100	-1.93163600
H	6.25974100	-1.38451100	-0.96797900
H	4.86495400	-2.35126300	-0.40923400
O	-2.08945500	-0.01239300	1.72394500
H	-1.56699300	0.06785200	2.53842800
O	-2.11994500	0.00643200	-1.63820800
H	-1.57696600	0.01318500	-2.44238300

Os.OH (triplet)

Os	-1.07392100	0.02168500	-0.03317400
P	-1.21177500	2.45421700	0.02921500
N	0.43579500	-0.15179500	1.35501500
H	0.06549100	-0.24625600	2.29938800
P	-1.39291400	-2.40593800	-0.06398700
C	1.75711900	0.08929000	-1.24153700
C	1.75229400	-0.15827100	1.25474200
C	2.43225500	-0.04352400	0.02450100
C	0.38763800	0.13179600	-1.41120100
H	2.31884100	-0.26235100	2.17890600
H	0.06503300	0.23981700	-2.45248300
H	2.38969600	0.15901200	-2.13017000
P	4.19971700	-0.07788000	-0.00003200
C	0.18669500	3.34568500	0.83168400
H	1.12014400	3.07393700	0.32991700
H	0.05121800	4.43090400	0.77696200
H	0.25834200	3.04714200	1.88191100
C	-1.34522100	3.19111800	-1.64685700
H	-1.56993400	4.26159800	-1.60044200

H	-0.40543600	3.03976200	-2.18610400
H	-2.13889200	2.66109600	-2.17975800
C	-2.70410300	3.07946300	0.90934500
H	-2.76478900	4.17145200	0.85721100
H	-3.59430000	2.65067900	0.43933100
H	-2.67615100	2.77941000	1.96172000
C	-0.32162000	-3.40061900	-1.18534400
H	0.72882900	-3.22246000	-0.93720800
H	-0.53619600	-4.47111400	-1.10019500
H	-0.48433300	-3.08245900	-2.21954800
C	-1.18222500	-3.16461400	1.59643600
H	-1.49459600	-4.21381000	1.60222100
H	-0.13288000	-3.10179500	1.90054700
H	-1.78904500	-2.58536900	2.29769300
C	-3.10473000	-2.89001500	-0.54357700
H	-3.30528000	-2.61294300	-1.58393000
H	-3.24819500	-3.97070400	-0.44269600
H	-3.81122100	-2.37307300	0.11263700
C	4.92157400	-0.24884500	1.66586400
H	6.01223700	-0.25952800	1.57742300
H	4.63057200	0.59162500	2.30170900
H	4.59985800	-1.18372500	2.13264500
C	4.90209900	1.44513400	-0.72886100
H	5.99212700	1.37230300	-0.79864700
H	4.49051200	1.59948600	-1.73041800
H	4.63425000	2.30369100	-0.10620600
C	4.84475100	-1.46552900	-1.00149000
H	4.43373000	-1.41348400	-2.01374200
H	5.93729000	-1.42572800	-1.05762700
H	4.53820800	-2.41345600	-0.54979700
O	-2.28116500	-0.23025900	1.63850500
H	-2.91056400	0.49505500	1.76362300
O	-2.56007200	0.32544000	-1.33087200
H	-3.19182000	-0.40809600	-1.36999900

Os.CO (singlet)

Os	-1.11057000	0.00003300	0.04208600
P	-0.98723800	2.43526900	-0.06107300
N	0.50077400	-0.00003400	1.47412000
H	0.25188100	-0.00001000	2.45645800
P	-0.98757300	-2.43521600	-0.06105200
C	1.77060400	-0.00010000	-1.24113700
C	1.81260800	-0.00007200	1.28882400
C	2.46857700	-0.00009500	0.05282300

C	0.43131400	-0.00006700	-1.43877100
H	2.41829000	-0.00008100	2.19643100
H	0.14404800	-0.00006200	-2.49283800
H	2.41823100	-0.00012900	-2.12408600
P	4.22220200	-0.00012800	0.01056000
C	0.49176800	3.19647800	0.72812900
H	1.39512100	2.77713700	0.27810500
H	0.48212600	4.28276500	0.59074500
H	0.49919400	2.97020900	1.79775600
C	-0.94859700	3.10302000	-1.77629000
H	-0.87262500	4.19527200	-1.76903500
H	-0.09163700	2.68030300	-2.30726600
H	-1.86060200	2.81407300	-2.30757900
C	-2.39687000	3.34287100	0.70784700
H	-2.27658400	4.42563600	0.59618700
H	-3.33387700	3.04007700	0.23034100
H	-2.46286300	3.10056500	1.77294600
C	-0.94908000	-3.10299100	-1.77626400
H	-0.09208100	-2.68039500	-2.30727300
H	-0.87325300	-4.19525300	-1.76899800
H	-1.86106500	-2.81393000	-2.30752600
C	0.49135100	-3.19662800	0.72810700
H	0.48155300	-4.28291400	0.59072500
H	1.39474700	-2.77741200	0.27805500
H	0.49884000	-2.97036000	1.79773300
C	-2.39730100	-3.34262400	0.70792100
H	-3.33428400	-3.03970700	0.23044400
H	-2.27716500	-4.42540500	0.59626400
H	-2.46322600	-3.10030200	1.77302000
C	4.98046900	-0.00011600	1.67080200
H	6.06889600	-0.00013700	1.55817400
H	4.68808600	0.89169900	2.23136500
H	4.68805400	-0.89190300	2.23139200
C	4.90855300	1.45440300	-0.86728400
H	5.99762600	1.38122700	-0.95126700
H	4.47902100	1.51590500	-1.87139900
H	4.64675400	2.36550100	-0.32138200
C	4.90849800	-1.45471400	-0.86723700
H	4.47896600	-1.51623000	-1.87135100
H	5.99757300	-1.38158200	-0.95122000
H	4.64666400	-2.36578400	-0.32130700
C	-2.40061200	0.00015200	1.50431200
C	-2.44585800	0.00016300	-1.30553900
O	-3.14177000	0.00017800	2.39242500

O	-3.23846900	0.00007100	-2.15179400
Os.CO (triplet)			
Os	-1.09804500	-0.01306900	0.00061000
P	-1.15775500	2.41976300	0.00716100
N	0.50682300	0.10615700	1.42716900
H	0.24818900	0.00453600	2.40289600
P	-0.84711700	-2.43977600	-0.05859600
C	1.81828500	0.18098600	-1.27471700
C	1.82246500	-0.22260200	1.23218100
C	2.46652900	-0.01971900	-0.05820100
C	0.40515400	0.21742500	-1.45971500
H	2.43004300	-0.40153400	2.11612000
H	0.12884600	0.38995900	-2.50250800
H	2.43735600	0.33682900	-2.15810600
P	4.24018500	0.11282000	-0.01865400
C	0.42513600	3.23466100	0.46813700
H	1.20324000	2.92501700	-0.23432500
H	0.31716100	4.32402500	0.44351400
H	0.71942500	2.91444400	1.47000000
C	-1.58435400	3.17771800	-1.61622600
H	-1.57317900	4.27062500	-1.54950600
H	-0.86154800	2.85601900	-2.37112500
H	-2.58037500	2.85218500	-1.93073500
C	-2.38019300	3.18177100	1.15803100
H	-2.34965700	4.27468600	1.09438600
H	-3.38884100	2.83995600	0.90671000
H	-2.16206100	2.87995900	2.18693800
C	0.12646500	-3.11469400	-1.46797400
H	1.13992900	-2.70716900	-1.44080600
H	0.16678900	-4.20814100	-1.42074200
H	-0.33789400	-2.81240100	-2.41115600
C	-0.04192300	-3.17755300	1.42258000
H	0.05274600	-4.26263000	1.31020400
H	0.94859900	-2.73038000	1.55071100
H	-0.64052700	-2.96392300	2.31351300
C	-2.44469700	-3.35141600	-0.17702300
H	-2.97682900	-3.05581200	-1.08632000
H	-2.27578400	-4.43310500	-0.20021200
H	-3.07558900	-3.10893800	0.68346500
C	4.81996100	1.60761900	0.86692000
H	5.90451000	1.57524500	1.01191700
H	4.55686300	2.49968400	0.29159700
H	4.32695900	1.66046100	1.84144800

C	5.00559200	0.11497000	-1.67482900
H	6.09376000	0.08765800	-1.56087700
H	4.68561300	-0.76400900	-2.24022000
H	4.73239700	1.01662200	-2.22841000
C	4.96415400	-1.31176400	0.87658600
H	4.70915700	-2.23819600	0.35384900
H	6.05304000	-1.21418800	0.92745500
H	4.56642100	-1.36383900	1.89338200
C	-2.37601200	-0.18585500	1.46927700
C	-2.41950600	-0.10895500	-1.36466400
O	-3.10648800	-0.29751500	2.36040300
O	-3.20190000	-0.19262600	-2.21670500

Os.PF₃ (singlet)

Os	0.59217400	0.00453700	-0.01578600
P	0.49457600	-2.44399000	-0.02016400
N	-0.98787600	-0.00292900	1.42612000
H	-0.72015100	0.04371100	2.40193000
P	0.39731100	2.44378500	-0.08268200
C	-2.28585600	-0.02918200	-1.25973600
C	-2.30273200	-0.00974100	1.26204600
C	-2.97432300	-0.01974100	0.03685200
C	-0.95013300	-0.02672400	-1.46983300
H	-2.89080900	0.00258100	2.18090200
H	-0.67567900	-0.05656400	-2.52564100
H	-2.93571100	-0.05621700	-2.14005600
P	-4.72832500	-0.03548900	0.01309900
C	-0.15406200	-3.18643700	1.53842700
H	-1.15090100	-2.79273100	1.74995900
H	-0.20524500	-4.27662500	1.45097800
H	0.50842200	-2.93050800	2.37056400
C	-0.54747500	-3.20948200	-1.33015200
H	-0.51822200	-4.30104000	-1.24817600
H	-1.57663300	-2.85655200	-1.24042500
H	-0.17029200	-2.91081100	-2.31215100
C	2.10340700	-3.32181900	-0.24231600
H	1.95927100	-4.40428700	-0.16179100
H	2.52236000	-3.09869100	-1.22757600
H	2.81635500	-2.99884100	0.51972700
C	-0.17279600	3.14877100	-1.68599500
H	-1.12413800	2.69151900	-1.96653100
H	-0.29055200	4.23438000	-1.60558400
H	0.56209800	2.92694400	-2.46435100
C	-0.78701800	3.15702200	1.13612200

H	-0.78915900	4.24962200	1.06470600
H	-1.79284900	2.77899100	0.93785600
H	-0.49718700	2.86597400	2.14958500
C	1.93806400	3.40661800	0.24396900
H	2.71495600	3.11251400	-0.46660300
H	1.74679200	4.47930500	0.13560500
H	2.30631500	3.21382000	1.25488300
C	-5.46649600	-0.01103100	1.68197700
H	-6.55619800	-0.01734100	1.58272000
H	-5.16375100	-0.89210100	2.25393700
H	-5.17103500	0.89125300	2.22391100
C	-5.41156300	-1.51110100	-0.83074300
H	-6.50248800	-1.45077900	-0.89988500
H	-4.99641400	-1.58413600	-1.84019400
H	-5.13200200	-2.41033400	-0.27409600
C	-5.43081400	1.39860300	-0.88395500
H	-5.01124900	1.44431800	-1.89312000
H	-6.52013700	1.31749200	-0.95618400
H	-5.16911100	2.32093900	-0.35728500
P	2.08645200	0.05572900	1.70260200
P	2.12977500	-0.01573500	-1.62349400
F	1.53668100	0.64480000	3.08834700
F	3.43142600	0.90128400	1.62665200
F	2.73538300	-1.27012700	2.31867000
F	3.59350900	-0.56628300	-1.33868600
F	2.57192400	1.32056600	-2.37744900
F	1.82965700	-0.87903200	-2.92876600

Os.PF₃ (triplet)

Os	0.59120300	-0.00735700	-0.02823100
P	0.59466500	-2.44816100	0.08503500
N	-1.01698200	-0.08958500	1.39928600
H	-0.73570800	0.07114800	2.36093600
P	0.35584400	2.43018600	-0.09040000
C	-2.32584700	-0.13020900	-1.28406900
C	-2.31053000	0.31572300	1.20203600
C	-2.97696900	0.08751400	-0.07308300
C	-0.91935200	-0.17299900	-1.47195600
H	-2.88259400	0.62772000	2.07178800
H	-0.65521800	-0.37783400	-2.51103800
H	-2.94147200	-0.31266300	-2.16494700
P	-4.74584500	-0.09092300	-0.01332200
C	0.07698700	-3.11879700	1.72030500
H	-0.89454400	-2.69813000	1.98880900

H	0.01491800	-4.21137100	1.68520800
H	0.80685000	-2.83122100	2.48246600
C	-0.52068700	-3.30440300	-1.10255700
H	-0.46105100	-4.38946300	-0.96614100
H	-1.54957000	-2.97050900	-0.94731700
H	-0.22544500	-3.05360500	-2.12492800
C	2.21263500	-3.28180400	-0.21668900
H	2.11548300	-4.36296000	-0.07216700
H	2.54544300	-3.09456200	-1.24139400
H	2.96666500	-2.89668000	0.47377300
C	-0.63312100	3.09484500	-1.49418800
H	-1.64280600	2.67953400	-1.46447600
H	-0.68104800	4.18774400	-1.44305200
H	-0.16472900	2.79941500	-2.43724100
C	-0.45323100	3.15053500	1.39845800
H	-0.51671900	4.23990300	1.31021500
H	-1.45692900	2.72839800	1.50246200
H	0.12693600	2.89617600	2.29047700
C	1.91452000	3.41234500	-0.20596500
H	2.44140500	3.17138600	-1.13228800
H	1.68330700	4.48262900	-0.19847100
H	2.57275100	3.18448100	0.63539300
C	-5.49374600	1.32487200	0.87713300
H	-6.58049700	1.20625200	0.92965700
H	-5.09810300	1.38781100	1.89431400
H	-5.25778600	2.25433200	0.35080300
C	-5.28237100	-1.58821900	0.89535400
H	-6.36234100	-1.56740900	1.07339800
H	-5.02665000	-2.48063900	0.31733000
H	-4.75947800	-1.62792900	1.85494100
C	-5.52977400	-0.11896400	-1.66161900
H	-5.24952500	-1.02162500	-2.21008500
H	-6.61721100	-0.10477100	-1.53850100
H	-5.22699700	0.75942000	-2.23762800
P	2.08982200	0.14361800	1.69000500
P	2.08698500	-0.02088900	-1.68469300
F	3.36935900	1.08846900	1.61070100
F	2.84899700	-1.13823100	2.27029400
F	1.52383200	0.67360400	3.09126800
F	3.62748600	-0.31070500	-1.42321200
F	2.27656100	1.24823100	-2.63513800
F	1.86787100	-1.08568100	-2.85613800

Os.H (singlet)

Os	-0.79727600	-0.00000600	0.00393300
P	-2.13087400	1.88176400	-0.00806700
N	0.74488200	0.00727900	1.37957800
H	0.46175500	0.01236900	2.35294700
P	-2.13003100	-1.88210300	-0.00497200
C	2.05157700	-0.00687300	-1.22707600
C	2.07141400	0.00691100	1.26096100
C	2.73406200	0.00014100	0.03036100
C	0.68197200	-0.00764000	-1.41654000
H	2.64602400	0.01215500	2.18630700
H	0.43280400	-0.01354000	-2.47878500
H	2.68803100	-0.01190200	-2.11846200
P	4.50584800	0.00021800	-0.00782500
C	-1.70744900	3.05617600	1.35315600
H	-0.63855400	3.28584200	1.31679900
H	-2.27753400	3.98713300	1.25763000
H	-1.92985000	2.59174300	2.31753900
C	-1.91012200	2.92133000	-1.51632600
H	-2.47432300	3.85718100	-1.43556800
H	-0.84818400	3.14715200	-1.64678000
H	-2.25079200	2.36623100	-2.39462400
C	-3.96427100	1.76653000	0.12499400
H	-4.40589600	2.76903000	0.11824200
H	-4.36479800	1.19938200	-0.71920300
H	-4.23919600	1.26051000	1.05378400
C	-1.90655900	-2.92699900	-1.50913300
H	-0.84445800	-3.15369500	-1.63666000
H	-2.47127400	-3.86235100	-1.42625300
H	-2.24530300	-2.37485400	-2.39003900
C	-1.70866500	-3.05139100	1.36125300
H	-2.27810100	-3.98298100	1.26800500
H	-0.63957300	-3.28057400	1.32776100
H	-1.93306400	-2.58354300	2.32351200
C	-3.96366800	-1.76667700	0.12441200
H	-4.36274100	-1.20284200	-0.72270200
H	-4.40512600	-2.76926600	0.12071400
H	-4.24036800	-1.25715500	1.05074900
C	5.24312800	0.01003400	1.65985100
H	6.33322900	0.00980800	1.56411900
H	4.93979500	0.90489300	2.20990300
H	4.94033700	-0.87860100	2.22019400
C	5.16249500	1.46075300	-0.88749700
H	6.25428200	1.41419900	-0.95118800
H	4.74661100	1.50095500	-1.89819300

H	4.86632500	2.36866000	-0.35403300
C	5.16306100	-1.47013800	-0.87055700
H	4.74714500	-1.52218100	-1.88070300
H	6.25482700	-1.42388100	-0.93483800
H	4.86728500	-2.37194100	-0.32662300
H	-1.64008600	-0.00203900	-1.42434600
H	-1.66646400	0.00246200	1.48067900

Os.H (triplet)

Os	-1.16629500	0.00000400	-0.02261300
P	-1.64636600	2.33478300	-0.00093300
N	0.45354800	0.00002100	1.40692700
H	0.15971900	0.00001600	2.37722600
P	-1.64636600	-2.33480400	-0.00093100
C	1.73305800	0.00001700	-1.21788500
C	1.76414500	0.00002200	1.27984000
C	2.43303700	0.00001400	0.03688800
C	0.36232700	0.00001700	-1.34698000
H	2.35465200	0.00001900	2.19704200
H	0.00937200	-0.00001800	-2.38686400
H	2.34005300	0.00001000	-2.12725900
P	4.19916600	-0.00000300	-0.01133700
C	-0.68312800	3.37099200	1.18586700
H	0.38437700	3.28874100	0.96134900
H	-0.98315000	4.42290000	1.12705300
H	-0.85205300	3.00700200	2.20347500
C	-1.41821500	3.21421900	-1.60636100
H	-1.69522400	4.27095300	-1.52495100
H	-0.37295900	3.13754700	-1.91998300
H	-2.04074400	2.73665500	-2.36853100
C	-3.39582900	2.70659100	0.43613700
H	-3.58377000	3.78562200	0.41783200
H	-4.05860200	2.21054500	-0.27815400
H	-3.61233500	2.31460900	1.43340900
C	-1.41822700	-3.21422400	-1.60636700
H	-0.37297300	-3.13755000	-1.91999400
H	-1.69523800	-4.27095900	-1.52496900
H	-2.04075900	-2.73665000	-2.36852800
C	-0.68310900	-3.37100700	1.18585900
H	-0.98312600	-4.42291700	1.12706000
H	0.38439200	-3.28875200	0.96132100
H	-0.85201600	-3.00700800	2.20346600
C	-3.39582500	-2.70660200	0.43615600
H	-4.05860200	-2.21054700	-0.27812500

H	-3.58377600	-3.78563200	0.41784800
H	-3.61231700	-2.31462300	1.43343200
C	4.94571700	-0.00001600	1.65236800
H	6.03512800	-0.00002700	1.54893000
H	4.64751600	0.89182900	2.21006200
H	4.64749700	-0.89185800	2.21005600
C	4.86035300	1.46193800	-0.88895000
H	5.95115600	1.40672900	-0.96303800
H	4.43714400	1.51155700	-1.89632700
H	4.57749700	2.36963100	-0.34803700
C	4.86032300	-1.46195200	-0.88896100
H	4.43711200	-1.51155400	-1.89633800
H	5.95112700	-1.40676700	-0.96304900
H	4.57744500	-2.36964100	-0.34805500
H	-2.46297400	-0.00001900	-1.09163200
H	-1.95426400	-0.00000300	1.49668500

Ir.SnCl₃ (singlet)

P	-0.02722300	-0.14044900	2.47647600
N	-1.78317200	1.27578400	-0.20900700
H	-1.49899400	2.23199800	-0.45790000
P	0.16355600	0.00738500	-2.48943900
C	-3.00205900	-1.32109600	0.13204700
C	-3.07550100	1.12943800	-0.18209900
C	-3.71959400	-0.14420500	-0.01495000
C	-1.58678300	-1.45555800	0.24743600
H	-3.68514100	2.01628500	-0.34924800
H	-1.30584000	-2.45441800	0.58468200
H	-3.55838500	-2.25954100	0.16681500
P	-5.55191300	-0.24153400	-0.05040600
Ir	-0.20504800	-0.09381300	0.00008500
C	-0.47500600	-1.75566600	3.23749400
H	0.21047200	-2.54861500	2.92886600
H	-0.39935600	-1.64816600	4.32495300
H	-1.50032700	-2.03716400	2.98467400
C	-1.26688400	1.02656400	3.16842400
H	-2.27124000	0.76466000	2.82573900
H	-1.23491400	0.95788500	4.26160200
H	-1.02866700	2.05169300	2.87516900
C	1.54688700	0.32289300	3.29557500
H	1.73848300	1.39117400	3.18975500
H	1.42655600	0.09478200	4.36134300
H	2.38729900	-0.25803300	2.91519200
C	1.63974400	0.79806800	-3.23805400

H	1.62966800	0.55057300	-4.30601400
H	1.58872400	1.88390900	-3.13120700
H	2.56410700	0.41972800	-2.79941400
C	0.08936900	-1.67444800	-3.23407100
H	-0.74734700	-2.24781000	-2.82978000
H	-0.04419400	-1.54633100	-4.31455200
H	1.01587500	-2.22797900	-3.07112900
C	-1.24976000	0.86429500	-3.29889600
H	-1.10907100	0.78822000	-4.38276900
H	-2.19402200	0.38114600	-3.03463800
H	-1.27171300	1.92007900	-3.02339100
C	-6.16614500	-0.74877300	1.58649200
H	-7.25905100	-0.81802700	1.55427000
H	-5.75942500	-1.72675500	1.86105600
H	-5.87946600	-0.01192500	2.34304900
C	-6.27582700	1.37119000	-0.47667400
H	-6.03396900	2.12692100	0.27682600
H	-5.94033300	1.70724100	-1.46249600
H	-7.36513500	1.25650100	-0.50550400
C	-6.06952200	-1.46595300	-1.29370100
H	-5.67499600	-2.45831300	-1.05695600
H	-7.16369100	-1.52089700	-1.30067700
H	-5.72275100	-1.16596900	-2.28713000
Sn	1.37023500	2.20058400	0.10278000
Sn	1.69303000	-2.01232200	-0.01131900
Cl	1.20235100	3.59113700	2.00319200
Cl	3.60878400	2.28313600	-0.52396200
Cl	0.13122700	3.66191500	-1.38084200
Cl	3.39010800	-1.89348200	-1.61542700
Cl	2.88313500	-2.58724900	1.92459200
Cl	0.55467200	-4.04336000	-0.45939600

Ir.SnCl₃ (triplet)

P	-0.32238100	0.10911500	2.47152300
N	-1.82774000	1.41539800	-0.06402700
H	-1.53756500	2.39056500	-0.06412100
P	-0.29974200	-0.17110000	-2.46985800
C	-3.15387100	-1.20722700	0.05554900
C	-3.13198100	1.28620300	-0.05762800
C	-3.81939100	0.04249100	-0.00806000
C	-1.78020600	-1.42233500	0.06759400
H	-3.71209400	2.20782900	-0.08284600
H	-1.52829200	-2.48310200	0.09885500
H	-3.78070500	-2.10001400	0.09296900

P	-5.63525400	0.02515200	-0.01665800
Ir	-0.29983400	-0.03917000	0.00128100
C	-1.01438300	-1.38533200	3.29276300
H	-0.37940700	-2.25602300	3.11324500
H	-1.06386100	-1.20903200	4.37248600
H	-2.02023100	-1.58944500	2.91726000
C	-1.40134300	1.46527900	3.09173900
H	-2.43404700	1.31562700	2.76785300
H	-1.37354400	1.46059600	4.18653500
H	-1.04100400	2.43495800	2.73902100
C	1.25989100	0.41234000	3.35874200
H	1.65077800	1.40478800	3.12101200
H	1.06226200	0.37155300	4.43557700
H	2.00735000	-0.34668500	3.11924000
C	1.29711000	-0.40114900	-3.35324000
H	1.09786000	-0.36133100	-4.42987600
H	2.00982400	0.38883700	-3.10771900
H	1.73143200	-1.37727500	-3.12477600
C	-1.33722800	-1.53663100	-3.13658500
H	-2.37160500	-1.42902800	-2.80210500
H	-1.30909900	-1.50513400	-4.23086200
H	-0.94975700	-2.50313000	-2.80395000
C	-1.01041500	1.33618800	-3.25282500
H	-1.05092400	1.18656300	-4.33697300
H	-2.02254500	1.52121900	-2.88531600
H	-0.38381800	2.20903500	-3.05067600
C	-6.26158500	-0.76925500	1.49866800
H	-7.35574400	-0.80399600	1.46492200
H	-5.88127300	-1.79159700	1.58160400
H	-5.94988800	-0.19808100	2.37822500
C	-6.31701700	1.70987500	-0.10418700
H	-6.02060800	2.30299700	0.76597900
H	-6.00411000	2.21574300	-1.02236400
H	-7.40975300	1.63503900	-0.11041900
C	-6.24486800	-0.91361800	-1.45424600
H	-5.86568800	-1.93947900	-1.43233400
H	-7.33941300	-0.94421200	-1.43021800
H	-5.92207900	-0.43112700	-2.38164500
Sn	1.57118700	1.92310900	-0.12379200
Sn	1.51875600	-1.92857100	0.11070000
Cl	1.15114800	3.74819200	1.32311700
Cl	3.87747300	1.23525300	0.73255600
Cl	2.26427000	3.00972400	-2.08507100
Cl	3.82443600	-1.13165100	-0.55562700

Cl	2.11400400	-3.02137500	2.08931700
Cl	1.35009000	-3.69565800	-1.42307600

Ir.SiCl₃ (singlet)

P	-0.37624400	0.53766100	-2.41564500
N	1.42082500	1.39887000	0.16069200
H	1.07647300	2.36212400	0.24224200
P	-0.35177100	-0.42266700	2.44320400
C	2.73195400	-1.16901200	-0.02587100
C	2.71075600	1.29837000	0.19816600
C	3.40342300	0.03574800	0.05788800
C	1.32102300	-1.38877300	0.07723900
H	3.29909500	2.21204700	0.30956000
H	1.10765200	-2.43250700	0.32070100
H	3.32160600	-2.07159800	-0.18662300
P	5.22919800	0.08463400	-0.01446600
Ir	-0.14385900	-0.09182200	-0.01891500
C	0.97971500	-0.34446600	-3.30254900
H	0.84199100	-1.42345100	-3.21405400
H	0.94769200	-0.06003400	-4.36034700
H	1.94907000	-0.05915200	-2.88584500
C	0.00466800	2.30010100	-2.78801500
H	0.95890400	2.59420400	-2.34473100
H	0.07726600	2.40190700	-3.87657900
H	-0.77992600	2.96728600	-2.42885400
C	-1.88975000	0.15560000	-3.40020300
H	-2.10226600	1.01315900	-4.04530500
H	-1.70367800	-0.72879800	-4.01206300
H	-2.76052700	-0.02494200	-2.77120300
C	-1.93728600	-1.02004300	3.17161100
H	-2.09614300	-0.48737200	4.11472200
H	-2.79378700	-0.84005600	2.52464400
H	-1.85359700	-2.09077800	3.36465900
C	0.87398100	-1.61067300	3.14242500
H	1.89583600	-1.27644700	2.94384800
H	0.72288400	-1.65197300	4.22673200
H	0.72311300	-2.61183100	2.73454100
C	0.09968400	1.11862400	3.34518600
H	0.11011600	0.89051300	4.41686100
H	1.09759000	1.44854500	3.04530300
H	-0.61433600	1.92299200	3.16829200
C	5.90376800	-1.57966400	-0.28937800
H	6.99499800	-1.49797600	-0.34230300
H	5.64885300	-2.25048100	0.53617300

H	5.54374700	-1.99903200	-1.23359300
C	5.76608400	1.16704900	-1.37796200
H	5.39678700	0.78113500	-2.33296400
H	5.40059000	2.18830500	-1.23461800
H	6.86098600	1.19184600	-1.40503100
C	5.88915700	0.73745400	1.55276100
H	5.59843400	0.08694200	2.38321000
H	6.98257600	0.77311100	1.49485100
H	5.51830200	1.74968300	1.74051100
Si	-1.89008300	1.79663200	0.33735800
Si	-1.65719200	-1.94347400	-0.37242900
Cl	-1.33086300	-2.91389100	-2.19720700
Cl	-3.67647000	-1.51162600	-0.28426200
Cl	-1.33293300	-3.52190600	0.97365300
Cl	-3.22655800	2.22857900	-1.19923000
Cl	-3.12238000	1.80876400	2.01271800
Cl	-0.79538000	3.61950900	0.55113100

Ir.SiCl₃ (triplet)

P	-0.14120200	1.83716700	-1.65780400
N	1.44486900	0.80761000	1.09340600
H	1.16778700	1.42597900	1.85405500
P	-0.10002300	-2.08569600	1.41967600
C	2.68889500	-0.72601000	-1.02127800
C	2.74175000	0.74211500	0.97706200
C	3.40968300	-0.00524000	-0.04036300
C	1.31598100	-0.82314900	-1.12858700
H	3.34307000	1.30077600	1.69504800
H	0.93339800	-1.45649700	-1.93337400
H	3.26012100	-1.27728300	-1.77066900
P	5.22308000	-0.04828700	-0.10201300
Ir	-0.24100100	-0.08010900	-0.07410000
C	0.22803400	1.31493700	-3.38594500
H	-0.56779600	0.68765500	-3.78945000
H	0.31939200	2.21002800	-4.01025300
H	1.17222300	0.76491900	-3.41749600
C	1.27682300	2.95353000	-1.28569900
H	2.21898700	2.40194600	-1.31878900
H	1.30557100	3.74296300	-2.04412600
H	1.15710100	3.41604800	-0.30386000
C	-1.52926200	3.03170900	-1.81922600
H	-1.63903700	3.61643300	-0.90325500
H	-1.28512200	3.71319600	-2.64160300
H	-2.46927800	2.52827300	-2.04283200

C	-1.59913600	-2.95121800	2.03826300
H	-1.27074500	-3.68491700	2.78265900
H	-2.30423300	-2.26110200	2.50170200
H	-2.10011000	-3.47608300	1.22308500
C	0.84966800	-3.46843300	0.65426200
H	1.86823100	-3.15315300	0.41720100
H	0.89103700	-4.29962000	1.36597200
H	0.35732000	-3.80983800	-0.25861100
C	0.86825800	-1.75260900	2.95350100
H	0.92878300	-2.67888000	3.53433600
H	1.88085700	-1.42925800	2.70337500
H	0.38525800	-0.98903800	3.56596200
C	5.81076600	0.60459000	-1.69819700
H	6.90370300	0.54282400	-1.73439000
H	5.40009400	0.02107600	-2.52746600
H	5.50900100	1.65023700	-1.81047800
C	5.95041900	0.95133600	1.23243800
H	5.65847300	2.00185500	1.14265200
H	5.66077700	0.56866400	2.21554600
H	7.04083600	0.89024400	1.14866800
C	5.81344300	-1.76303800	0.07358200
H	5.40365700	-2.39369600	-0.72093600
H	6.90645000	-1.77912400	0.00476400
H	5.51148700	-2.16676000	1.04459500
Si	-1.66952900	1.34052200	1.53422400
Si	-2.12891600	-1.07961400	-1.25961600
Cl	-2.98410600	-0.02970000	-2.83728900
Cl	-3.75118900	-1.58644700	-0.08054600
Cl	-1.44729200	-2.85133500	-2.14545700
Cl	-3.48732200	1.89328500	0.76392200
Cl	-2.01881600	0.42023000	3.35220100
Cl	-0.64102700	3.09724300	2.00825900

Ir.CO (singlet)

P	0.98377300	-2.47471100	-0.05842900
N	-0.46633700	0.00006300	1.45214200
H	-0.20098700	0.00007000	2.42933400
P	0.98401300	2.47458500	-0.05836200
C	-1.74292100	0.00009100	-1.22794000
C	-1.78808100	0.00012800	1.27005600
C	-2.45247000	0.00011000	0.05073300
C	-0.40912700	0.00014000	-1.43542900
H	-2.37073600	0.00014600	2.19034800
H	-0.08527200	0.00008900	-2.47427500

H	-2.36594400	-0.00001100	-2.12497500
P	-4.23219500	0.00005600	0.01187600
Ir	1.08041300	0.00008900	0.03356600
C	0.96586300	-3.11078200	-1.77864200
H	1.89260500	-2.84423000	-2.29590000
H	0.87597200	-4.20202100	-1.76795600
H	0.12013800	-2.68512900	-2.32433500
C	-0.50093400	-3.18652400	0.74367200
H	-1.40148700	-2.77482900	0.28271000
H	-0.49135500	-4.27465900	0.62076400
H	-0.50534800	-2.94879800	1.81024000
C	2.41323000	-3.31051100	0.73976400
H	2.45513600	-3.06924800	1.80624700
H	2.31677500	-4.39625300	0.63265200
H	3.35074700	-2.99765800	0.26980600
C	2.41390500	3.31001700	0.73944400
H	2.31770600	4.39578500	0.63236700
H	2.45603800	3.06873700	1.80591400
H	3.35121100	2.99692300	0.26922700
C	0.96575600	3.11083200	-1.77850400
H	0.11976500	2.68546700	-2.32400600
H	0.87616200	4.20209300	-1.76764400
H	1.89227600	2.84409900	-2.29606600
C	-0.50024900	3.18677900	0.74422100
H	-0.49037200	4.27491200	0.62131700
H	-1.40107200	2.77537100	0.28353100
H	-0.50440800	2.94905200	1.81078900
C	-4.88783500	-1.46372400	-0.86130300
H	-5.97954600	-1.40737600	-0.92182100
H	-4.48436300	-1.51293900	-1.87704900
H	-4.60583300	-2.37387000	-0.32384700
C	-4.95329100	0.00002200	1.68477000
H	-4.65725300	-0.89389300	2.24075400
H	-4.65729500	0.89393700	2.24077800
H	-6.04379400	-0.00000200	1.58921100
C	-4.88791500	1.46380500	-0.86129100
H	-4.48441000	1.51306800	-1.87702200
H	-5.97961900	1.40737700	-0.92184500
H	-4.60600100	2.37396500	-0.32381000
C	2.40256900	-0.00002300	-1.34905200
C	2.41642700	-0.00016500	1.53343300
O	3.15614100	-0.00070400	2.40092100
O	3.16881600	-0.00024200	-2.19777800

Ir.CO_(triplet)

P	1.17957100	-2.44470200	0.05667700
N	-0.57647600	-0.00019700	1.34004600
H	-0.22405300	-0.00015800	2.29898000
P	1.17951800	2.44472300	0.05677500
C	-1.95764000	-0.00001500	-1.26565000
C	-1.88290500	-0.00023100	1.23826200
C	-2.59202900	-0.00013200	0.00526000
C	-0.58854400	0.00013600	-1.50649300
H	-2.44625500	-0.00022400	2.17031900
H	-0.34070300	0.00021100	-2.56870500
H	-2.61397200	0.00000300	-2.13936200
P	-4.40348600	-0.00001000	0.02442000
Ir	0.92375000	0.00001300	-0.11389800
C	0.24713600	-3.38848900	-1.21372800
H	0.59729000	-3.11178100	-2.21255400
H	0.39959800	-4.46355300	-1.07097800
H	-0.82009600	-3.16287700	-1.14270000
C	0.62515400	-3.11806000	1.67253600
H	-0.44243100	-2.93291500	1.81802900
H	0.80442200	-4.19784800	1.70393300
H	1.18273600	-2.64494700	2.48638300
C	2.91728000	-3.01160200	-0.11914900
H	3.55244200	-2.52538100	0.62627600
H	2.96834900	-4.09664900	0.02065300
H	3.29827100	-2.76969400	-1.11566900
C	2.91725700	3.01168000	-0.11852800
H	2.96825700	4.09671400	0.02139900
H	3.55225200	2.52539800	0.62699800
H	3.29850200	2.76989200	-1.11498000
C	0.24744500	3.38860300	-1.21381500
H	-0.81980100	3.16293900	-1.14315500
H	0.39981800	4.46365600	-1.07088700
H	0.59792500	3.11203700	-2.21256700
C	0.62459500	3.11779600	1.67257400
H	0.80378500	4.19758600	1.70430700
H	-0.44302200	2.93254400	1.81769400
H	1.18195300	2.64450100	2.48647000
C	-5.04614800	-1.47679600	-0.82857600
H	-6.14075500	-1.44532700	-0.83933000
H	-4.68568700	-1.50960300	-1.86079200
H	-4.71966300	-2.38136900	-0.30697100
C	-5.05641200	-0.00013500	1.72338900
H	-4.74095300	-0.89509100	2.26760500

H	-4.74086600	0.89469900	2.26775500
H	-6.15023200	-0.00007700	1.66939600
C	-5.04592600	1.47706000	-0.82826200
H	-4.68549500	1.50999800	-1.86048400
H	-6.14054100	1.44581400	-0.83897500
H	-4.71923600	2.38146300	-0.30649000
C	2.30949800	0.00015000	-1.39153500
C	2.29786900	-0.00013500	1.79296700
O	3.45873500	-0.00006600	1.87019900
O	3.13388100	0.00021900	-2.19212000

Ir.PF₃ (singlet)

P	0.42274700	-2.47558800	-0.10073800
N	-0.95590000	-0.02096000	1.41085200
H	-0.67603700	-0.08576300	2.38151300
P	0.46877700	2.47541600	0.00883800
C	-2.26743100	0.01943900	-1.24416500
C	-2.28011900	-0.01591300	1.24963400
C	-2.96197100	0.00427100	0.04158400
C	-0.93870500	0.02311100	-1.46936200
H	-2.84667000	-0.03687400	2.17994800
H	-0.63526300	0.05320600	-2.51357300
H	-2.89946000	0.04282000	-2.13469000
P	-4.74095200	0.01972200	0.02705600
Ir	0.56878500	-0.00351100	-0.02560400
C	-0.15781300	-3.14817600	-1.70617200
H	0.56126600	-2.92052400	-2.49696800
H	-0.25819700	-4.23556000	-1.62523600
H	-1.12248900	-2.70953600	-1.96801600
C	-0.73379800	-3.16319800	1.14608000
H	-1.74675900	-2.80101400	0.95823700
H	-0.72272600	-4.25616600	1.07914700
H	-0.42921100	-2.86812400	2.15345100
C	2.00290200	-3.36668500	0.21372700
H	2.36085900	-3.18699800	1.23098800
H	1.84090600	-4.44285100	0.09163100
H	2.77386600	-3.05058900	-0.49375700
C	2.08535100	3.32686600	-0.22173100
H	1.94140100	4.40698500	-0.11259800
H	2.81228600	2.99623300	0.52402300
H	2.48739000	3.13707000	-1.22084800
C	-0.60361800	3.21429000	-1.28121500
H	-1.62996500	2.86188500	-1.16669900
H	-0.57514400	4.30514500	-1.18906200

H	-0.24675100	2.93070800	-2.27470400
C	-0.16502200	3.13754700	1.59994000
H	-0.21076700	4.23015100	1.54330100
H	-1.16413700	2.74629100	1.80116800
H	0.50093000	2.86020600	2.42161700
C	-5.41826900	-1.41647000	-0.87443900
H	-6.51038900	-1.35250200	-0.91698400
H	-5.03036700	-1.44073400	-1.89711400
H	-5.13300500	-2.34201600	-0.36587800
C	-5.43914500	-0.01788600	1.70928000
H	-5.14038600	-0.92691100	2.23868100
H	-5.13052000	0.86026000	2.28323200
H	-6.53083300	-0.00969300	1.62900800
C	-5.39754300	1.51025300	-0.79897000
H	-5.01047900	1.57995200	-1.81996100
H	-6.49063500	1.46583400	-0.84267600
H	-5.09737100	2.40411100	-0.24429500
P	2.13771300	-0.06968500	1.73117700
P	2.11511200	0.05768600	-1.67054100
F	3.50784700	-0.81191000	1.52335000
F	2.66191100	1.26115800	2.39904600
F	1.60488200	-0.80651600	3.02477100
F	2.50178000	-1.26384700	-2.43320500
F	1.77837300	0.97787400	-2.89963000
F	3.55116700	0.58147200	-1.30981700

Ir.PF₃ (triplet)

P	0.49127900	-2.45213800	-0.06064600
N	-1.32654400	-0.04391400	1.72671400
H	-1.15346500	-0.10863500	2.73199700
P	0.57529700	2.46364200	0.09158500
C	-2.34828600	0.07806000	-1.08706500
C	-2.59288100	-0.05081000	1.45020300
C	-3.11048700	0.01275200	0.10748800
C	-0.96958800	0.09466900	-1.29340100
H	-3.32280300	-0.11113000	2.26205400
H	-0.73548000	0.18135000	-2.35632900
H	-2.93891800	0.13030000	-2.00549700
P	-4.91440700	0.02045400	-0.11706600
Ir	0.62525900	0.01209500	-0.01086000
C	-0.10303800	-3.12458500	-1.66591700
H	0.57342600	-2.82320300	-2.47025800
H	-0.13094500	-4.21836800	-1.62444300
H	-1.10488700	-2.74774100	-1.88665700

C	-0.60958600	-3.21902900	1.19650000
H	-1.63861800	-2.88300700	1.05105100
H	-0.57168500	-4.30964900	1.10465600
H	-0.28148000	-2.93579700	2.19975500
C	2.10117600	-3.31048600	0.19073500
H	2.49232300	-3.12180500	1.19416100
H	1.96289000	-4.39031600	0.07215400
H	2.83353000	-2.97044800	-0.54609000
C	2.22998600	3.27018400	0.12607500
H	2.10461100	4.35802700	0.13702000
H	2.78321100	2.97514900	1.02098400
H	2.81640800	2.99538800	-0.75418200
C	-0.24976700	3.26277100	-1.34422800
H	-1.30150700	2.96989000	-1.38913400
H	-0.18367300	4.35164100	-1.25129400
H	0.23983100	2.95657300	-2.27283900
C	-0.27853300	3.15709500	1.56516100
H	-0.25353100	4.25127400	1.52656800
H	-1.31737600	2.82110800	1.59257000
H	0.22537100	2.82527700	2.47668100
C	-5.43832100	-1.41165400	-1.11656000
H	-6.52163800	-1.37152300	-1.27169300
H	-4.94334500	-1.40135500	-2.09176500
H	-5.18653100	-2.34114600	-0.59730900
C	-5.80252300	-0.05325800	1.47029700
H	-5.56997400	-0.97441700	2.01224400
H	-5.56643700	0.81234400	2.09588900
H	-6.87710100	-0.04142700	1.25872900
C	-5.44042300	1.53927000	-0.97796100
H	-4.95148700	1.61823500	-1.95305000
H	-6.52471600	1.51522600	-1.12955100
H	-5.18356100	2.41646200	-0.37666000
P	2.08904900	-0.10647400	1.77628500
P	2.22683500	0.03390700	-1.78513200
F	3.58538900	-0.56674800	1.59632600
F	2.32466200	1.16974900	2.68341600
F	1.64960400	-1.12033400	2.91399100
F	2.69210300	-1.28852000	-2.54327900
F	1.67458300	0.83522200	-3.04341500
F	3.63157200	0.75808300	-1.64191600
Ir.H (singlet)			
P	2.03452400	-2.02260200	0.02358600
N	-0.64791400	0.00251000	1.37549500

H	-0.34894800	0.00424700	2.34726200
P	2.03578700	2.02212200	0.02261300
C	-1.97359700	-0.00202600	-1.21185500
C	-1.96432000	0.00235400	1.26572100
C	-2.64086800	0.00020300	0.02797600
C	-0.58726400	-0.00253300	-1.42520600
H	-2.53606500	0.00405400	2.19162800
H	-0.34409100	-0.00477900	-2.48801400
H	-2.60207500	-0.00347000	-2.10542300
P	-4.45266300	0.00035900	0.00274500
Ir	0.84641200	0.00002200	-0.04463600
C	1.59970200	-3.08891700	-1.40456500
H	1.86602400	-2.58652000	-2.33816500
H	2.14528700	-4.03696400	-1.33598400
H	0.52552500	-3.29091900	-1.40703900
C	1.64212900	-3.01926900	1.51264000
H	0.56411100	-3.19112800	1.57428000
H	2.15386200	-3.98644500	1.45268900
H	1.97262500	-2.49389900	2.41243100
C	3.85767700	-1.88736300	-0.01470200
H	4.21406900	-1.34446600	0.86406800
H	4.29561800	-2.89158100	-0.01596400
H	4.17680200	-1.36196700	-0.91846300
C	3.85885200	1.88601200	-0.01690500
H	4.29726500	2.89002100	-0.01910500
H	4.21563800	1.34348500	0.86193400
H	4.17706500	1.35990800	-0.92057700
C	1.60039100	3.08776600	-1.40588700
H	0.52625900	3.29002500	-1.40785500
H	2.14624500	4.03572100	-1.33813800
H	1.86602300	2.58476600	-2.33935600
C	1.64494900	3.01997000	1.51129500
H	2.15709400	3.98686300	1.45035400
H	0.56706100	3.19241800	1.57359000
H	1.97584800	2.49505500	2.41120700
C	-5.07093200	-1.47969500	-0.86097300
H	-6.16515100	-1.45569100	-0.89417000
H	-4.68830000	-1.51143700	-1.88521600
H	-4.74728100	-2.38117700	-0.33222400
C	-5.14379800	0.00345300	1.68619400
H	-4.83797300	-0.89026700	2.23777000
H	-4.83774600	0.89906200	2.23457200
H	-6.23613200	0.00345400	1.60939700
C	-5.07058200	1.47746300	-0.86625700

H	-4.68792600	1.50548000	-1.89059800
H	-6.16480500	1.45358200	-0.89938800
H	-4.74674000	2.38074800	-0.34071200
H	1.87976500	0.00061000	1.29975700
H	1.80399600	-0.00075600	-1.35505100

Ir.H (triplet)

P	1.62015800	-2.36904100	-0.00985900
N	-0.45514500	-0.00006100	1.42634000
H	-0.16519200	-0.00006500	2.40012100
P	1.61990000	2.36913700	-0.00985200
C	-1.71302300	-0.00004100	-1.18712300
C	-1.75786200	-0.00009200	1.29400100
C	-2.42800800	-0.00007500	0.04064500
C	-0.34472700	-0.00001100	-1.30515500
H	-2.35314700	-0.00011400	2.20691500
H	0.08368000	0.00001200	-2.31619100
H	-2.28608100	-0.00003200	-2.11593300
P	-4.23321600	-0.00010000	-0.02446200
Ir	1.19365000	0.00002300	-0.00693100
C	1.52754000	-3.12478100	-1.68143100
H	2.22946200	-2.62275300	-2.35348200
H	1.78522000	-4.18800000	-1.62961500
H	0.51705800	-3.02263600	-2.08744200
C	0.50442600	-3.38204000	1.04162600
H	-0.53093500	-3.26805000	0.70857300
H	0.78447900	-4.43892300	0.97777300
H	0.58017100	-3.06037200	2.08419000
C	3.31403400	-2.74144700	0.58783400
H	3.43527900	-2.39307600	1.61718200
H	3.49621900	-3.82081000	0.55003000
H	4.04890600	-2.23181900	-0.04142600
C	3.31375500	2.74171400	0.58779500
H	3.49582000	3.82109800	0.55001800
H	3.43507400	2.39332400	1.61712700
H	4.04866100	2.23218600	-0.04150700
C	1.52714600	3.12490400	-1.68140300
H	0.51666100	3.02266100	-2.08738300
H	1.78471700	4.18814900	-1.62957100
H	2.22909800	2.62296500	-2.35349000
C	0.50408900	3.38198700	1.04169400
H	0.78401900	4.43890300	0.97785200
H	-0.53127100	3.26788500	0.70867700
H	0.57991100	3.06030400	2.08424700

C	-4.83551400	-1.47659800	-0.90697500
H	-5.92849700	-1.44611900	-0.96795700
H	-4.42862600	-1.50856500	-1.92194600
H	-4.53169600	-2.38126200	-0.37205700
C	-4.95738900	-0.00014900	1.64471800
H	-4.66376500	-0.89500900	2.20112400
H	-4.66379600	0.89469600	2.20116300
H	-6.04794900	-0.00016600	1.54492400
C	-4.83556200	1.47641700	-0.90691100
H	-4.42867000	1.50844200	-1.92188000
H	-5.92854300	1.44590500	-0.96789800
H	-4.53177500	2.38106800	-0.37195300
H	1.91746000	0.00008100	1.47833400
H	2.52693600	0.00009400	-0.93247000

Re.BMe₂ (singlet)

P	-1.09013600	2.43405200	-0.01215800
N	0.97718900	0.26351900	1.52416200
H	0.75571000	0.36339800	2.50854000
P	-0.77899300	-2.35322200	-0.13892300
C	2.03160500	0.08854500	-1.15930200
C	2.26782100	0.23989700	1.33498600
C	2.86084300	0.12549800	0.05273400
C	0.67710000	0.05623000	-1.20546700
H	2.93591700	0.31089600	2.20378300
H	0.28349100	0.06215600	-2.23083100
H	2.57293800	0.11456600	-2.11201800
P	4.57017800	0.06471100	-0.12542200
C	0.08367900	3.35828400	1.09409900
H	1.10581400	3.04303800	0.87017400
H	-0.00698300	4.44266200	0.95862100
H	-0.12465800	3.10892600	2.13909100
C	-0.69181600	3.22355500	-1.64500300
H	-0.68893400	4.31796500	-1.57958400
H	0.29295600	2.87350500	-1.96945400
H	-1.42706500	2.90764100	-2.39074700
C	-2.68335600	3.29543200	0.40199200
H	-2.58260100	4.38489300	0.32869300
H	-3.46608700	2.96106700	-0.28573900
H	-2.99274100	3.03343900	1.41817200
C	-0.47992000	-3.07222000	-1.82641400
H	0.39140100	-2.57789000	-2.26606900
H	-0.30182100	-4.15316700	-1.78137800
H	-1.34354500	-2.87692200	-2.46888900

C	0.66350700	-3.08995100	0.77513200
H	0.73758600	-4.17184500	0.61104400
H	1.57924400	-2.60095300	0.43092200
H	0.55560100	-2.89390100	1.84540600
C	-2.15568000	-3.45272900	0.44875400
H	-3.07213500	-3.21113700	-0.09767000
H	-1.91743700	-4.51291600	0.30100600
H	-2.33890100	-3.27483000	1.51315800
C	5.47923200	0.12841400	1.46103500
H	6.55335900	0.07986300	1.25752100
H	5.26166000	1.05922800	1.99081200
H	5.20016900	-0.71606000	2.09603000
C	5.27865700	1.43005100	-1.14386000
H	6.34937900	1.28865700	-1.32761200
H	4.75401300	1.46933600	-2.10315700
H	5.11616100	2.38072300	-0.62759500
C	5.18510400	-1.44663400	-0.98345100
H	4.64237800	-1.56291800	-1.92639100
H	6.25918200	-1.39107000	-1.19188700
H	4.97503900	-2.32073900	-0.36013900
B	-1.70038400	-0.27613900	1.93879300
B	-2.57320900	-0.14902600	-1.43004700
C	-3.28009300	0.05568000	1.95551000
H	-3.86444800	-0.84937400	2.17995700
H	-3.44635000	0.74629200	2.79926700
H	-3.71658200	0.51959200	1.07059200
C	-1.15882200	-0.75599700	3.36605300
H	-1.87439900	-1.45045900	3.83272700
H	-0.17839200	-1.24504500	3.37230200
H	-1.10119500	0.09953600	4.06006800
C	-4.13111600	-0.51392200	-1.21145800
H	-4.51740700	-1.11186500	-2.05271600
H	-4.38390900	-1.04015300	-0.28615500
H	-4.72774300	0.41391900	-1.21679200
C	-2.30317100	0.08297400	-3.01035200
H	-1.32369000	0.47009700	-3.31095200
H	-2.45836100	-0.86368100	-3.55347100
H	-3.06472600	0.77103700	-3.41471600
Re	-1.03001900	0.01575900	-0.00705500

Re.BMe₂ (triplet)

P	-0.83863000	2.40786200	-0.03537800
N	0.90824100	-0.37718700	1.36864600
H	0.62871800	-0.58343100	2.32139500

P	-1.37657800	-2.36160200	-0.00691100
C	2.17740600	0.11195300	-1.23277800
C	2.21434900	-0.37809900	1.24060900
C	2.88326900	-0.12762400	0.02119500
C	0.81854300	0.15775300	-1.39288400
H	2.82006900	-0.58228400	2.13026000
H	0.55316700	0.35426700	-2.43765400
H	2.82261300	0.23813300	-2.11415500
P	4.61532900	-0.16397400	-0.03694700
C	0.52518100	3.15038600	0.98661500
H	1.48129100	2.75622800	0.62998500
H	0.53179400	4.24546000	0.92360500
H	0.39719400	2.84711900	2.02966800
C	-0.55574600	3.28351000	-1.65021400
H	-0.45904000	4.36775400	-1.51640300
H	0.35447700	2.88842800	-2.10995100
H	-1.39358200	3.07968300	-2.32426000
C	-2.29810600	3.36408100	0.59579100
H	-2.12971700	4.44373900	0.50349200
H	-3.19102700	3.09104300	0.02771900
H	-2.47375200	3.11738000	1.64673700
C	-0.67922900	-3.36601700	-1.40978700
H	0.40805900	-3.24382500	-1.42649200
H	-0.92765800	-4.43053400	-1.31584600
H	-1.07452300	-2.98107000	-2.35356100
C	-0.77065700	-3.37329600	1.43586500
H	-0.98061900	-4.44172800	1.30559700
H	0.30879300	-3.22948300	1.54378800
H	-1.25522300	-3.02349200	2.35312900
C	-3.15028000	-2.89777500	-0.06164100
H	-3.62046600	-2.51268100	-0.97067900
H	-3.22732900	-3.99146200	-0.05168200
H	-3.68731300	-2.48942100	0.79768200
C	5.40265000	-0.44553700	1.58944700
H	6.48993500	-0.43382400	1.46595800
H	5.11688600	0.34078100	2.29271000
H	5.10429900	-1.41428500	1.99819400
C	5.35262600	1.39248100	-0.68085600
H	6.43633300	1.30142600	-0.81089800
H	4.89346500	1.63236400	-1.64420700
H	5.13223000	2.20697900	0.01528200
C	5.29775700	-1.46418800	-1.14605400
H	4.84164600	-1.36362500	-2.13520700
H	6.38613600	-1.38517100	-1.24107500

H	5.03348900	-2.44782700	-0.74689300
B	-1.94826200	0.18580400	1.87992400
B	-2.23807800	0.12959700	-1.68492000
C	-3.54942000	0.07740400	2.00350400
H	-3.83623600	-0.58771300	2.83739100
H	-3.95240500	1.06687900	2.28058200
H	-4.08937600	-0.24427800	1.10893500
C	-1.31645700	0.45425200	3.34218000
H	-1.96981600	1.08238900	3.96856400
H	-1.25562900	-0.50928400	3.88026400
H	-0.31220200	0.89678300	3.37282400
C	-3.75478600	0.67422600	-1.58547100
H	-3.97976900	1.38983600	-2.39506000
H	-4.44578700	-0.16955500	-1.75555200
H	-4.05029600	1.13064800	-0.63583400
C	-1.91375800	-0.28365800	-3.21050000
H	-0.99291600	-0.85361800	-3.37551500
H	-2.74719100	-0.84265600	-3.66786700
H	-1.82750300	0.63784700	-3.81233700
Re	-0.84518800	-0.00672000	-0.04039700

Re.NH₂ (singlet)

P	-1.23435000	-2.38140300	0.02083800
N	0.47410500	-0.00035600	-1.39851100
H	0.14916600	-0.00046600	-2.35970500
P	-1.23372000	2.38157000	0.02067000
C	1.73089300	-0.00003800	1.24475700
C	1.78053700	-0.00056400	-1.28069900
C	2.45812200	-0.00048900	-0.03896800
C	0.37793900	0.00015700	1.36679900
H	2.37457200	-0.00083200	-2.19998000
H	0.04688000	0.00036400	2.41157000
H	2.35508100	0.00003500	2.14724500
P	4.17498100	-0.00026100	0.00632000
C	0.43637700	-3.18901200	-0.04270500
H	1.03798800	-2.79799600	0.78247700
H	0.37161900	-4.28189300	0.01929200
H	0.93059800	-2.90416800	-0.97610300
C	-1.96946500	-3.26323200	1.48979600
H	-1.83860600	-4.34898500	1.41704600
H	-1.48764700	-2.90629200	2.40576900
H	-3.04190800	-3.04964600	1.55867100
C	-2.09563400	-3.30890600	-1.35049700
H	-2.01778300	-4.39456300	-1.22060600

H	-3.15353300	-3.02755600	-1.37757200
H	-1.64731000	-3.04249900	-2.31416200
C	-1.96623400	3.26353000	1.49084300
H	-1.48282600	2.90654600	2.40595100
H	-1.83541200	4.34927100	1.41782400
H	-3.03857000	3.05006200	1.56164800
C	0.43715600	3.18867600	-0.04542500
H	0.37282700	4.28156800	0.01685800
H	1.03995800	2.79732700	0.77874700
H	0.92978100	2.90385200	-0.97968800
C	-2.09697700	3.30940900	-1.34920400
H	-3.15509200	3.02863300	-1.37420200
H	-2.01825700	4.39503800	-1.21954400
H	-1.65070200	3.04266600	-2.31374200
C	4.96791200	-0.00207700	-1.64378100
H	6.05491400	-0.00184700	-1.51746000
H	4.67783300	-0.89262400	-2.20700500
H	4.67774300	0.88712100	-2.20908500
C	4.91052300	-1.43912600	0.89812100
H	5.99497900	-1.33830100	1.01777000
H	4.44598900	-1.51515600	1.88573900
H	4.68368200	-2.35492700	0.34447500
C	4.91073400	1.44053200	0.89493000
H	4.44657100	1.51847700	1.88258000
H	5.99525900	1.34013700	1.01435100
H	4.68352800	2.35518500	0.33953500
H	-2.43038900	-0.82516000	-2.31928900
H	-2.43044000	0.82547000	-2.31919900
H	-2.98899900	-0.82586400	1.90620600
H	-2.98869000	0.82662300	1.90628600
N	-2.26461500	0.00013200	-1.75008200
N	-2.60552400	0.00032700	1.45470400
Re	-1.28247400	0.00010600	0.01364400

Re.NH₂ (triplet)

P	1.18547000	2.42684200	0.05758400
N	-0.38298200	-0.00278400	-1.45528200
H	-0.06304800	-0.00599500	-2.42076800
P	1.15821800	-2.42632700	0.05824500
C	-1.67200400	0.01065200	1.26027100
C	-1.69761100	0.00070100	-1.30056900
C	-2.35127200	0.00764600	-0.04739100
C	-0.31201500	0.00757200	1.42527100
H	-2.30692600	-0.00194500	-2.20727300

H	-0.02153400	0.01321800	2.48981800
H	-2.33478100	0.01742400	2.13556000
P	-4.08067500	0.01207400	-0.01434900
C	-0.38044500	3.26643900	-0.46778700
H	-1.20557000	2.84400700	0.11315700
H	-0.33744000	4.35153600	-0.31770400
H	-0.56687700	3.05430600	-1.52503400
C	1.43788700	3.11726400	1.75534100
H	1.48839400	4.21239300	1.76121200
H	0.61222800	2.78421900	2.39188800
H	2.36483600	2.69597800	2.15426100
C	2.45637800	3.37748300	-0.91034700
H	2.35934900	4.46073600	-0.77154600
H	3.45555800	3.06550800	-0.58931400
H	2.35223800	3.14321300	-1.97505300
C	1.41639500	-3.14006800	1.74866700
H	0.61927000	-2.77545500	2.40397900
H	1.41540900	-4.23637900	1.74474100
H	2.37036700	-2.77539200	2.14036000
C	-0.42800800	-3.24071400	-0.44545200
H	-0.39761500	-4.32693000	-0.30039400
H	-1.23718100	-2.80832300	0.15030000
H	-0.62791000	-3.02078800	-1.49844400
C	2.39717100	-3.40266000	-0.92819100
H	3.40884500	-3.11459100	-0.62392200
H	2.27868300	-4.48389100	-0.79019400
H	2.28253900	-3.16431300	-1.99091200
C	-4.86885300	0.01066200	-1.66593300
H	-5.95616800	0.01466200	-1.54212900
H	-4.57351700	0.89808600	-2.23130700
H	-4.57965800	-0.88136800	-2.22720500
C	-4.80136800	1.46064200	0.86624800
H	-5.88710900	1.37008500	0.98023100
H	-4.33956600	1.53772600	1.85468300
H	-4.56458800	2.37080200	0.30736700
C	-4.81017000	-1.42823800	0.87283600
H	-4.34934600	-1.50293100	1.86193400
H	-5.89545800	-1.33110300	0.98581900
H	-4.57823500	-2.34247600	0.31858200
H	3.08513900	0.79888400	-1.93553100
H	3.05461500	-0.83519000	-1.95832500
H	3.69620800	-0.16029300	1.02532100
H	2.62257600	-0.13139500	2.30444600
N	2.51820100	-0.01134900	-1.69391400

N	2.73712100	0.02331900	1.30540500
Re	1.19984200	-0.00361900	-0.05082700

Re.OH (singlet)

P	-1.44041700	2.35876700	-0.02873000
N	0.46445700	0.11062700	1.35852300
H	0.10298800	0.19073400	2.30424900
P	-1.08623100	-2.40881200	0.00368500
C	1.73834500	0.05322900	-1.25892000
C	1.77072000	0.16478300	1.25885800
C	2.46310500	0.12062400	0.02459400
C	0.38769400	-0.00996500	-1.36355000
H	2.34619300	0.25330400	2.18440800
H	0.01571000	-0.01412500	-2.39656000
H	2.34972300	0.08857800	-2.16719600
P	4.17984700	0.14693100	-0.00786200
C	-1.35166400	3.12618500	1.65319700
H	-0.33404900	3.01666200	2.04248600
H	-1.62233400	4.18825100	1.64565400
H	-2.02539100	2.56621500	2.30764400
C	-0.22196400	3.37466800	-0.98678900
H	-0.38111600	4.45016500	-0.84449500
H	0.79062900	3.10531300	-0.67277400
H	-0.31331100	3.13426700	-2.05062300
C	-3.05809700	2.99446200	-0.66662400
H	-3.08508300	4.08875800	-0.72634300
H	-3.23685600	2.55683100	-1.65233000
H	-3.85582200	2.64699500	-0.00262800
C	0.60793100	-3.16787200	0.02810300
H	1.12173200	-2.85094200	0.94058000
H	0.57363900	-4.26297100	-0.01213500
H	1.17226200	-2.77529700	-0.82230300
C	-1.87107800	-3.31188600	1.43982000
H	-1.73447400	-4.39673700	1.36449000
H	-1.42066600	-2.97309300	2.38003800
H	-2.94516700	-3.09729800	1.47631800
C	-1.85794900	-3.35160100	-1.41176600
H	-1.40112900	-3.02970600	-2.35380600
H	-1.72230100	-4.43392500	-1.30523600
H	-2.93381200	-3.14611800	-1.46261600
C	4.95297900	0.27001300	1.64661600
H	6.04096900	0.29040300	1.53139000
H	4.63379800	1.18610800	2.15009300
H	4.67919100	-0.58955400	2.26348600

C	4.89350300	1.54226700	-0.98208700
H	5.98034100	1.45410000	-1.08856300
H	4.43587200	1.55103700	-1.97574100
H	4.64708800	2.48561400	-0.48604200
C	4.95288500	-1.33096300	-0.79912400
H	4.49878000	-1.47887200	-1.78360100
H	6.03621800	-1.21611700	-0.91669300
H	4.73918100	-2.21412100	-0.19004200
O	-2.12779600	0.06130900	1.76913000
H	-2.32531700	-0.81680400	2.12664100
O	-2.61985100	-0.01601100	-1.43288600
H	-2.87863400	-0.89303000	-1.75655600
Re	-1.23273800	-0.05997800	-0.04334900

Re.OH (triplet)

P	-1.37497600	2.41197500	-0.06910000
N	0.41064500	0.08780100	1.38413600
H	0.05613000	0.16338100	2.33536000
P	-1.15135300	-2.45801900	0.02573000
C	1.74563400	-0.07642600	-1.27617900
C	1.73228600	0.11799100	1.26703500
C	2.40421300	0.03929800	0.02660300
C	0.38235800	-0.12275400	-1.45666300
H	2.31527500	0.20703900	2.18497000
H	0.10226000	-0.19530300	-2.52190200
H	2.41242400	-0.11712200	-2.14601000
P	4.13584400	0.10975500	0.01159800
C	-0.98435600	3.24214400	1.53409700
H	0.08667300	3.15431200	1.74351100
H	-1.26979600	4.30048400	1.54154600
H	-1.53786200	2.69839200	2.30542200
C	-0.46981900	3.44086100	-1.31464400
H	-0.66328500	4.51306600	-1.19199900
H	0.60420500	3.25020900	-1.22503800
H	-0.77896000	3.13439600	-2.31917600
C	-3.14209500	2.85096900	-0.33826300
H	-3.31211200	3.93340400	-0.36240100
H	-3.47530400	2.38250000	-1.26764300
H	-3.70159000	2.39007900	0.48020500
C	-1.58996600	-3.27347100	-1.57721200
H	-0.81404100	-3.04438300	-2.31475800
H	-1.69217500	-4.36053600	-1.48229000
H	-2.53359600	-2.84320300	-1.92519300
C	0.43536500	-3.29166100	0.48268900

H	0.35978500	-4.38395100	0.43239600
H	1.21382100	-2.94043400	-0.20141700
H	0.71701700	-2.99291100	1.49699800
C	-2.36673400	-3.25417600	1.18225200
H	-3.37886300	-2.95178000	0.89268400
H	-2.30600000	-4.34871300	1.16675700
H	-2.18373500	-2.89664100	2.20083800
C	4.89465200	0.24762200	1.67032900
H	5.98327300	0.27985400	1.56382400
H	4.56043000	1.16121200	2.16844100
H	4.62394000	-0.61311500	2.28699800
C	4.80781200	1.52534900	-0.95338400
H	5.89813000	1.47437000	-1.04535900
H	4.35955700	1.51739300	-1.95095700
H	4.52354000	2.45913600	-0.45941400
C	4.92111400	-1.36054900	-0.76747000
H	4.47741000	-1.51689000	-1.75482600
H	6.00405900	-1.23483000	-0.87313800
H	4.71103600	-2.24248400	-0.15527700
O	-2.37552800	0.28968600	1.64534700
H	-3.02231400	-0.42590500	1.72998500
O	-2.69859600	-0.16141200	-1.29587000
H	-2.39348600	-0.35130300	-2.19766700
Re	-1.10657200	-0.03556500	-0.02691700

Re.H₂O (singlet)

P	1.28079200	-2.33936900	-0.02542900
N	-0.30535300	0.01023600	1.49944600
H	-0.01285900	0.03692700	2.47550100
P	0.96080300	2.40729900	-0.03192800
C	-1.60129500	-0.11232800	-1.28084400
C	-1.61467700	-0.04008800	1.31339800
C	-2.25668600	-0.09138900	0.04485200
C	-0.24743400	-0.05986600	-1.49191000
H	-2.23445100	-0.04768700	2.21181500
H	0.04842000	-0.13158800	-2.55353700
H	-2.27374700	-0.20956200	-2.14162300
P	-3.98219800	-0.14056800	0.01399500
C	-0.31630700	-3.28280600	0.15211100
H	-1.00944100	-2.91157200	-0.60882500
H	-0.18284300	-4.36562000	0.04052200
H	-0.75137000	-3.07015000	1.13397000
C	1.95094100	-3.09401900	-1.58364100
H	1.99666800	-4.18817800	-1.52462500

H	1.30149900	-2.80102500	-2.41440900
H	2.94630400	-2.69132700	-1.78759100
C	2.31500600	-3.23568600	1.25259400
H	2.26589300	-4.32476900	1.13233900
H	3.36385400	-2.92843300	1.16753000
H	1.95780900	-2.98720000	2.25980500
C	1.58288800	3.30235300	-1.55044800
H	1.02880800	2.94707700	-2.42749400
H	1.44909800	4.38795900	-1.47197200
H	2.64866300	3.09753400	-1.70290700
C	-0.74279500	3.16423600	0.07631900
H	-0.72510300	4.25750300	-0.00917300
H	-1.35551000	2.73577800	-0.72234300
H	-1.19290900	2.88308500	1.03317900
C	1.82880500	3.39018600	1.29523800
H	2.90970300	3.22938900	1.22942200
H	1.62278500	4.46463300	1.21439300
H	1.50040300	3.03357400	2.27687000
C	-4.77446200	-0.12425200	1.66456900
H	-5.86073600	-0.16449300	1.53803300
H	-4.45495000	-0.98921200	2.25135300
H	-4.51514800	0.78903800	2.20586700
C	-4.67595900	-1.62670300	-0.83080700
H	-5.76422300	-1.56422600	-0.94063200
H	-4.21890200	-1.71695000	-1.82025100
H	-4.41455100	-2.51793300	-0.25274400
C	-4.76132200	1.25546500	-0.90570400
H	-4.30764700	1.31776300	-1.89899200
H	-5.84407000	1.12439800	-1.01028400
H	-4.55166200	2.18991700	-0.37700400
O	2.57941400	0.18705100	2.13585100
H	2.91445300	0.42491400	1.20806100
H	2.82957400	-0.74667800	2.21844700
O	2.69581900	0.00856800	-1.91465500
H	3.00109700	0.38161400	-1.02334300
H	2.31967200	0.76656800	-2.39025700
Re	1.11319800	0.04095000	0.01241700

Re.H₂O (triplet)

P	-1.07553900	-2.39596300	0.05543600
N	0.31883000	-0.00055000	-1.46710000
H	0.01678000	-0.00356900	-2.43784100
P	-1.06929800	2.39760200	0.05636000
C	1.60490400	-0.00068700	1.25672200

C	1.62972100	-0.00157700	-1.30605600
C	2.28894000	-0.00051600	-0.05243400
C	0.24990200	-0.00052800	1.41702500
H	2.23227000	-0.00376500	-2.21596800
H	-0.08922800	-0.00315800	2.46319000
H	2.25022300	-0.00250400	2.14172700
P	4.01386000	-0.00308400	-0.02089500
C	0.62030400	-3.09395000	-0.26999700
H	1.31810300	-2.61007200	0.41827900
H	0.64834700	-4.18156200	-0.13520700
H	0.92421300	-2.84465200	-1.29092200
C	-1.41418200	-3.17543200	1.71077400
H	-1.24564100	-4.25898200	1.69002800
H	-0.74619600	-2.71880300	2.44788400
H	-2.44568100	-2.98279300	2.02084300
C	-2.08213000	-3.51197100	-1.05408300
H	-1.80523200	-4.56689400	-0.92790500
H	-3.14750900	-3.39449500	-0.83085800
H	-1.92314600	-3.22767600	-2.10074300
C	-1.40791700	3.18296100	1.70949700
H	-0.74909000	2.72024800	2.45106200
H	-1.22724500	4.26456300	1.68802200
H	-2.44351300	3.00383400	2.01453200
C	0.62842500	3.09186200	-0.26791300
H	0.65826800	4.17974900	-0.13578000
H	1.32434300	2.60837900	0.42255400
H	0.93340600	2.83934400	-1.28770200
C	-2.07212400	3.51490700	-1.05561200
H	-3.13822300	3.39945100	-0.83460100
H	-1.79389700	4.56947500	-0.92935600
H	-1.91126300	3.23024600	-2.10192200
C	4.79468400	-0.00306800	-1.67555100
H	5.88242100	-0.00363000	-1.55563100
H	4.50057900	-0.89307200	-2.23779000
H	4.50133800	0.88742800	-2.23738700
C	4.74347900	-1.44742100	0.86104900
H	5.82973300	-1.35374400	0.96794900
H	4.28920500	-1.52194700	1.85347900
H	4.50412400	-2.36049600	0.30811600
C	4.74680300	1.43823900	0.86303700
H	4.29221000	1.51283100	1.85530900
H	5.83274600	1.34155500	0.97038300
H	4.51016400	2.35256500	0.31100200
O	-2.67401800	0.00142800	-1.92955800

H	-3.25968000	-0.76039700	-1.70820600
H	-3.24530200	0.77794600	-1.72521400
O	-2.88464500	-0.00957100	1.52008100
H	-3.46381000	-0.76385800	1.24462100
H	-3.43798400	0.78071800	1.30342300
Re	-1.20211400	0.00162000	-0.03354800

Re.NH₃ (singlet)

P	-1.11268600	2.36152700	-0.02521500
N	0.32221500	0.00022000	1.49311200
H	0.09606800	0.00025700	2.49538100
P	-1.11161000	-2.36183100	-0.02510500
C	1.62577000	0.00037900	-1.28091100
C	1.63370900	0.00055200	1.30875700
C	2.28519100	0.00075000	0.04355900
C	0.26439000	0.00001800	-1.45494100
H	2.25868100	0.00075900	2.20638500
H	0.00019600	-0.00016800	-2.54510000
H	2.30024000	0.00041000	-2.14801600
P	4.00550900	0.00049200	0.01647500
C	0.56855100	3.16086800	0.13026900
H	1.20866600	2.73757200	-0.64938800
H	0.53287000	4.25377800	0.04063200
H	1.00017900	2.88818300	1.09818100
C	-1.70732200	3.25841400	-1.56073500
H	-1.54891100	4.34182400	-1.49474300
H	-1.15922900	2.87331200	-2.42783600
H	-2.77815500	3.08337100	-1.72287600
C	-2.03020900	3.38945700	1.25709700
H	-1.86576200	4.46623100	1.12478700
H	-3.10900100	3.19890600	1.19599200
H	-1.68896800	3.11110200	2.26181600
C	-1.70521800	-3.25881800	-1.56095400
H	-1.15699400	-2.87320700	-2.42774500
H	-1.54619900	-4.34215100	-1.49511700
H	-2.77609000	-3.08438700	-1.72349400
C	0.56997600	-3.16034900	0.13084500
H	0.53482300	-4.25328200	0.04129600
H	1.21003200	-2.73683000	-0.64874300
H	1.00127600	-2.88735900	1.09881500
C	-2.02904400	-3.39032200	1.25680700
H	-3.10788800	-3.20015500	1.19545400
H	-1.86415600	-4.46701500	1.12438300
H	-1.68816500	-3.11199200	2.26165700

C	4.80565900	0.00213000	1.66509900
H	5.89223600	0.00272300	1.53376100
H	4.51696500	0.89199700	2.23005000
H	4.51813700	-0.88730600	2.23132900
C	4.75397400	1.43842900	-0.87152700
H	5.83821200	1.33284300	-0.99116000
H	4.28777800	1.51873200	-1.85767700
H	4.53111200	2.35365500	-0.31515500
C	4.75431200	-1.43913300	-0.86863000
H	4.28839800	-1.52122600	-1.85477600
H	5.83859200	-1.33381000	-0.98815000
H	4.53126100	-2.35333700	-0.31065200
N	-2.59905000	-0.00037300	1.89588300
H	-2.06852100	-0.00020700	2.77791900
H	-3.20262100	0.81680700	1.92138700
N	-2.58554800	-0.00051800	-1.77700200
H	-1.99566300	-0.00051700	-2.62178700
H	-3.18955900	-0.81574100	-1.84200000
H	-3.20236700	-0.81773700	1.92153400
H	-3.18979300	0.81451800	-1.84215600
Re	-1.18223500	-0.00017200	0.01601500

Re.NH₃ (triplet)

P	-1.12313900	2.45256800	-0.03562800
N	0.31301600	0.00005100	1.47536400
H	0.06940300	0.00006800	2.46991400
P	-1.12351100	-2.45249700	-0.03555900
C	1.62364000	-0.00017800	-1.25211200
C	1.63589400	-0.00004200	1.30842300
C	2.28124100	-0.00013300	0.04855700
C	0.24987400	-0.00010900	-1.42566500
H	2.24777900	-0.00005500	2.21266600
H	-0.01849400	-0.00012000	-2.50740000
H	2.28577900	-0.00028300	-2.12846400
P	4.01756600	-0.00016200	0.01444000
C	0.59890700	3.09995900	0.21578800
H	1.24404900	2.62789300	-0.52973100
H	0.64255000	4.19197200	0.12596100
H	0.95378400	2.79430700	1.20410200
C	-1.54994100	3.29416000	-1.64054200
H	-1.31913900	4.36604100	-1.60244000
H	-0.96917500	2.82937300	-2.44405500
H	-2.61395100	3.17338400	-1.86436300
C	-2.05444800	3.53388300	1.16745200

H	-1.79121800	4.59290500	1.04293300
H	-3.13190600	3.41359600	1.01885200
H	-1.81691600	3.22821100	2.19288600
C	-1.55006300	-3.29384800	-1.64066100
H	-0.96907900	-2.82902600	-2.44399500
H	-1.31939400	-4.36576100	-1.60263700
H	-2.61401300	-3.17291700	-1.86468000
C	0.59843600	-3.10006000	0.21612900
H	0.64201100	-4.19206800	0.12620700
H	1.24376400	-2.62797800	-0.52921900
H	0.95314800	-2.79453500	1.20454200
C	-2.05512600	-3.53394800	1.16717500
H	-3.13255100	-3.41354700	1.01841500
H	-1.79194200	-4.59296000	1.04245700
H	-1.81775900	-3.22853500	2.19272400
C	4.80141000	-0.00014000	1.66687600
H	5.88928500	-0.00016000	1.54634900
H	4.50523900	0.89003300	2.22842600
H	4.50521000	-0.89028000	2.22846200
C	4.73249600	1.44716000	-0.86633800
H	5.82035800	1.36346700	-0.96451200
H	4.28234400	1.51368300	-1.86132400
H	4.48027300	2.35846800	-0.31602400
C	4.73244800	-1.44755200	-0.86626400
H	4.28231700	-1.51410400	-1.86125700
H	5.82031500	-1.36390300	-0.96441800
H	4.48017900	-2.35882400	-0.31591300
N	-2.78996400	0.00011700	1.70784800
H	-2.49719900	0.00014300	2.69800100
H	-3.41067900	0.81040000	1.58299900
N	-2.72296200	0.00001100	-1.57960300
H	-2.33686400	-0.00040400	-2.53690800
H	-3.35408900	-0.80842300	-1.50183100
H	-3.41034200	-0.81041200	1.58291000
H	-3.35354500	0.80890700	-1.50233000
Re	-1.16150000	0.00008800	0.03541000

Re.PMe₃ (singlet)

P	0.27672500	-2.39827300	-0.12853400
N	-1.01666700	-0.04198800	1.43898500
H	-0.76101500	-0.09236300	2.41872000
P	0.33268100	2.40822200	0.00281700
C	-2.32114800	0.14587300	-1.26239600
C	-2.32456400	-0.04750000	1.28582100

C	-2.99897900	0.03706600	0.04509700
C	-0.97336100	0.12848000	-1.46004800
H	-2.93156100	-0.10614000	2.19476300
H	-0.73659900	0.21201500	-2.52903400
H	-2.99497300	0.22444300	-2.12752300
P	-4.72407900	0.00504000	0.02073400
C	-0.49342200	-3.19199500	1.38231900
H	-1.42923500	-2.67990400	1.61759800
H	-0.69518300	-4.25686000	1.21615500
H	0.17449300	-3.09147600	2.24384600
C	-0.91779100	-3.04442200	-1.40753900
H	-1.05498700	-4.12834700	-1.31047300
H	-1.87514900	-2.53144700	-1.29974700
H	-0.53615100	-2.81978100	-2.40852500
C	1.61215200	-3.67676400	-0.42992100
H	1.21848800	-4.68912700	-0.27702300
H	1.96245600	-3.60274900	-1.46385200
H	2.46529500	-3.52474700	0.23451300
C	-0.12369000	3.23388200	-1.60788400
H	-1.00416700	2.72529300	-2.00839000
H	-0.34207900	4.29914000	-1.46510600
H	0.68446100	3.13560800	-2.33785500
C	-1.09499700	3.04664300	1.02200600
H	-1.17959300	4.13648500	0.93588500
H	-2.02005600	2.58002200	0.67508300
H	-0.95210400	2.78124300	2.07389700
C	1.61110700	3.64374500	0.59085100
H	2.54902800	3.51850600	0.04374400
H	1.25761000	4.67305100	0.45281800
H	1.81129000	3.48833000	1.65601500
C	-5.50286900	-0.13033300	1.67203100
H	-6.59061900	-0.13925700	1.55244800
H	-5.19406400	-1.05444000	2.16708800
H	-5.22334000	0.72024200	2.29881000
C	-5.43693600	-1.38138100	-0.96393000
H	-6.52489700	-1.29705700	-1.06158800
H	-4.98461900	-1.37451200	-1.95986100
H	-5.18285200	-2.32932600	-0.48054500
C	-5.48754100	1.49486400	-0.75186700
H	-5.02687000	1.65917000	-1.73025500
H	-6.56999600	1.38183800	-0.87709800
H	-5.27823000	2.36741900	-0.12601200
P	2.21239500	-0.08369800	1.77263700
P	2.29207200	0.04473400	-1.67948500

C	1.58834400	0.34907900	3.50017200
H	2.39440600	0.33751900	4.24332900
H	1.12908800	1.34379500	3.49597500
H	0.82971300	-0.37573000	3.82098000
C	3.75532600	0.98707700	1.81693400
H	3.49038300	2.04323500	1.73565400
H	4.32882900	0.83614600	2.74026500
H	4.39669400	0.73596500	0.96577900
C	3.08719400	-1.67269500	2.27032300
H	3.71339800	-2.01998300	1.44249700
H	3.72340700	-1.53090600	3.15307700
H	2.35487300	-2.45541900	2.49177100
C	3.77726900	-1.10471900	-1.62274900
H	4.44861300	-0.93569500	-2.47390000
H	4.33882000	-0.93368400	-0.69849700
H	3.45931200	-2.14857100	-1.63186100
C	3.30493600	1.59377400	-2.01668200
H	3.86709200	1.86750100	-1.11829200
H	4.01496300	1.43932000	-2.83849200
H	2.65433600	2.43276000	-2.27725700
C	1.80230500	-0.29524300	-3.46053100
H	2.66766000	-0.27262300	-4.13342000
H	1.32270400	-1.27730200	-3.53216100
H	1.07694300	0.45251300	-3.79646000
Re	0.62458300	0.00315800	-0.01886600

Re.PMe₃ (triplet)

P	0.28886700	-2.44060100	0.05285800
N	-0.94623200	0.17957500	1.40473200
H	-0.70097600	0.33675600	2.37741500
P	0.53451000	2.42055200	-0.27493400
C	-2.28406300	0.03518000	-1.20023700
C	-2.28257100	0.16408700	1.26358000
C	-2.96190400	0.07211900	0.05069600
C	-0.90736600	-0.00944500	-1.39470700
H	-2.86059600	0.25474500	2.18599200
H	-0.67510200	0.01039900	-2.46875200
H	-2.92905500	0.07484400	-2.08588300
P	-4.93220700	0.30240900	-0.05215500
C	-1.16926300	-3.00016100	1.05752700
H	-2.06436700	-2.47262800	0.72021200
H	-1.31835000	-4.08195300	0.96243000
H	-1.00729300	-2.74996000	2.11038300
C	-0.15309300	-3.21387300	-1.58130100

H	-0.46146700	-4.25838000	-1.45575900
H	-0.96875500	-2.64037000	-2.02832200
H	0.70332100	-3.18296600	-2.26188500
C	1.52094200	-3.71999600	0.63987200
H	1.16654800	-4.72785200	0.39367800
H	2.49981700	-3.57015000	0.17783200
H	1.64107300	-3.65361400	1.72352800
C	0.19934800	3.04564700	-1.99537200
H	-0.70042600	2.55114700	-2.37055700
H	0.04819100	4.13125900	-2.00120600
H	1.02818500	2.80295500	-2.66669200
C	-0.88984400	3.22222300	0.60513000
H	-0.94465300	4.29133700	0.36972200
H	-1.81816000	2.73085200	0.30354000
H	-0.77768000	3.09765600	1.68624500
C	1.88703900	3.61272500	0.21488800
H	2.81437100	3.38654900	-0.31805800
H	1.59499700	4.64471600	-0.01257000
H	2.08343400	3.53902700	1.28890100
C	-5.36939500	-0.34535900	1.64092200
H	-6.40270500	-0.70563700	1.64202800
H	-4.70620700	-1.16378400	1.93358700
H	-5.29065800	0.45015600	2.38993300
C	-5.31288200	-1.15979800	-1.14316400
H	-6.28858400	-1.58101500	-0.87735700
H	-5.35509700	-0.84576400	-2.19108100
H	-4.54524400	-1.93078500	-1.04351000
C	-6.71230300	1.18350200	-0.33794000
H	-6.74145500	1.56073000	-1.36526000
H	-7.55900000	0.50125000	-0.17157100
H	-6.78688300	2.03270300	0.34936300
P	2.20522100	0.14061100	1.88548900
P	2.29938200	-0.20877300	-1.71211300
C	1.61580100	1.13680100	3.36698300
H	2.39596100	1.21173700	4.13319400
H	1.32301700	2.14648300	3.06339600
H	0.74400500	0.65726300	3.82703900
C	3.91059100	0.90131900	1.73325000
H	3.84609900	1.90850600	1.31449800
H	4.41975200	0.95459500	2.70357700
H	4.51752700	0.29062500	1.05645600
C	2.74163400	-1.37021600	2.85233500
H	3.30899500	-2.04698600	2.20746700
H	3.36895900	-1.09418100	3.70850500

H	1.86174200	-1.90621700	3.22203700
C	3.50026100	-1.64582600	-1.68535700
H	4.24004700	-1.56686500	-2.49075500
H	4.02418100	-1.67070700	-0.72417800
H	2.96320700	-2.59111100	-1.80406300
C	3.57770400	1.13268200	-1.99677500
H	4.16950900	1.28581300	-1.09050100
H	4.25318500	0.86659000	-2.81848400
H	3.08969100	2.07835300	-2.24858800
C	1.74562200	-0.37447000	-3.49490100
H	2.60306100	-0.50109200	-4.16564600
H	1.07711400	-1.23265900	-3.60723100
H	1.19171000	0.51862000	-3.80033100
Re	0.64899300	-0.00818400	0.00432600

Os.BMe₂ (singlet)

P	0.86720900	2.36148800	0.16128700
N	-0.92755700	-0.37462400	-1.50538800
H	-0.73105900	-0.51187700	-2.49116500
P	1.01095700	-2.48293900	-0.01135900
C	-1.97429800	0.04279800	1.15651000
C	-2.22192900	-0.29009700	-1.30059800
C	-2.80569800	-0.08541100	-0.03656600
C	-0.62696000	0.08183900	1.23722200
H	-2.88555800	-0.38740900	-2.16590000
H	-0.23058900	0.18505100	2.25010500
H	-2.50575400	0.10222800	2.11086400
P	-4.53712400	-0.00926800	0.14598000
C	0.79470600	3.03624400	1.87974400
H	1.72404600	2.81266900	2.41110600
H	0.65446800	4.12201700	1.85544700
H	-0.03678000	2.57938700	2.42169200
C	-0.64296100	3.10515200	-0.59759300
H	-1.52610600	2.62049300	-0.17400600
H	-0.68352300	4.18243100	-0.40389800
H	-0.63989500	2.93572700	-1.67685500
C	2.22794700	3.38026600	-0.56444800
H	2.29405800	3.21857300	-1.64415800
H	2.04783100	4.44489400	-0.38132100
H	3.18347000	3.10034000	-0.11259400
C	2.58064900	-3.32731800	0.47745900
H	2.46589300	-4.41625900	0.44928400
H	3.38915700	-3.04285100	-0.20288100
H	2.86188700	-3.02652400	1.49093500

C	-0.22128000	-3.24500200	1.12914800
H	-1.22038200	-2.88294500	0.87537300
H	-0.19047300	-4.33712700	1.05410300
H	-0.00421300	-2.95002500	2.15962200
C	0.62467600	-3.29678300	-1.62393400
H	0.60646300	-4.38631500	-1.51466300
H	-0.34919600	-2.95018500	-1.97716200
H	1.38244200	-3.03084700	-2.36752600
C	-5.12219200	1.57316000	0.86625700
H	-6.20211200	1.54991600	1.04515000
H	-4.61009800	1.75474900	1.81604000
H	-4.88359600	2.39275400	0.18220400
C	-5.42266100	-0.20645100	-1.43800500
H	-5.14788300	0.58799700	-2.13670700
H	-5.19786100	-1.17663800	-1.88865000
H	-6.49873000	-0.14946200	-1.24808000
C	-5.20453800	-1.29991000	1.26631500
H	-4.70501100	-1.24086000	2.23794300
H	-6.28171900	-1.17199300	1.41501000
H	-5.01060000	-2.28724100	0.83729400
B	1.60436800	0.38102400	-1.91912600
B	2.52299300	0.06733300	1.42465900
C	3.10712900	-0.17840100	-1.87421700
H	3.17649200	-0.89519900	-2.70613800
H	3.80211900	0.64272300	-2.09324500
H	3.47755900	-0.68682400	-0.98247600
C	1.07840200	0.99073300	-3.27336400
H	1.81531300	1.69214100	-3.68972200
H	0.99283700	0.19408000	-4.02936000
H	0.11219300	1.49949600	-3.22421500
C	4.04518800	0.50131400	1.21717800
H	4.29111300	1.05163500	0.30478200
H	4.39368700	1.09284400	2.07702800
H	4.67601300	-0.40245200	1.22377200
C	2.21212500	-0.34644300	2.94419200
H	1.32919600	-0.96822600	3.12455700
H	3.07964600	-0.85524400	3.38927700
H	2.07943000	0.56962800	3.54145400
Os	1.01153200	-0.02431700	-0.01819300

Os.BMe₂ (triplet)

Os	-0.86161100	-0.00292400	-0.05050000
P	-0.89970900	2.40432700	-0.06826800
N	0.89407700	-0.29212100	1.40250700

H	0.62448700	-0.47512800	2.36366100
P	-1.23478700	-2.39004400	0.01329800
C	2.13189000	0.08756500	-1.20006900
C	2.19811600	-0.29121100	1.26723600
C	2.85130200	-0.08452100	0.02916800
C	0.75954700	0.10250700	-1.34839800
H	2.81030100	-0.46361600	2.15632800
H	0.46979800	0.23498400	-2.39525300
H	2.74108200	0.18632200	-2.10487300
P	4.61639500	-0.09587500	-0.05354900
C	0.54743600	3.15599500	0.80110800
H	1.46962200	2.78224700	0.34802500
H	0.52080700	4.24885500	0.73000400
H	0.53459700	2.86344500	1.85426600
C	-0.81304600	3.20741500	-1.72980300
H	-0.73764600	4.29605700	-1.63489900
H	0.05762900	2.83099900	-2.27379400
H	-1.71118500	2.96510400	-2.30537000
C	-2.31699200	3.30136100	0.70478700
H	-2.18234700	4.38339800	0.59929800
H	-3.25413400	3.01241400	0.22328300
H	-2.38164300	3.05572500	1.76850400
C	-0.13373400	-3.34174300	-1.12753200
H	0.91045000	-3.12409600	-0.88717600
H	-0.31429800	-4.41880800	-1.03924700
H	-0.32037000	-3.02835900	-2.15809100
C	-0.92522900	-3.23647200	1.62922400
H	-1.04175700	-4.32126000	1.53182400
H	0.09078100	-3.01728700	1.96995600
H	-1.63179700	-2.87269600	2.38123800
C	-2.90257600	-3.03781200	-0.43832400
H	-3.15252300	-2.73821200	-1.45993300
H	-2.91562700	-4.13129400	-0.37566500
H	-3.66036900	-2.63406900	0.23743200
C	5.39429800	-0.30931500	1.58210300
H	6.48156200	-0.28689100	1.45986600
H	5.10066000	0.49874900	2.25748900
H	5.11238200	-1.26901900	2.02342000
C	5.27394600	1.46137600	-0.75192700
H	6.36223700	1.40759200	-0.85730700
H	4.82964500	1.64221900	-1.73492700
H	5.01289100	2.29458400	-0.09302100
C	5.25364200	-1.43803600	-1.12121100
H	4.81095000	-1.35888000	-2.11829600

H	6.34321200	-1.37764500	-1.20884100
H	4.97603000	-2.40581300	-0.69353600
B	-1.92403500	0.17245700	1.85984400
B	-2.28735700	0.07140400	-1.60568900
C	-3.48744900	-0.14060900	1.94052200
H	-3.69917300	-0.78146500	2.81201900
H	-4.01497200	0.80409800	2.14981800
H	-3.96382600	-0.58065800	1.06263600
C	-1.31497700	0.58425600	3.27736300
H	-2.04429300	1.13849700	3.88507900
H	-1.11941700	-0.33473800	3.85767100
H	-0.38155100	1.15931100	3.26983200
C	-3.79008400	0.59944300	-1.45909600
H	-4.05639300	1.25506300	-2.30294500
H	-4.46679800	-0.26518200	-1.55378300
H	-4.05860600	1.10639000	-0.52911500
C	-1.96310800	-0.39092000	-3.10608200
H	-1.12876600	-1.08836100	-3.23712200
H	-2.84504900	-0.80894000	-3.61228700
H	-1.70213000	0.51229800	-3.68310500

Os.NH₂ (singlet)

Os	-1.26500900	-0.00116300	0.01097100
P	-1.22137500	-2.41602600	0.02036700
N	0.45460500	0.00345800	-1.38965700
H	0.15022900	0.00457900	-2.35604600
P	-1.22922800	2.41393500	0.02140400
C	1.71068800	0.00116000	1.23305400
C	1.76865800	0.00457000	-1.25914900
C	2.44680800	0.00336700	-0.03520700
C	0.36715500	-0.00028800	1.36666300
H	2.34773500	0.00660400	-2.18474700
H	0.01838300	-0.00121600	2.40090500
H	2.31316100	0.00096600	2.14606400
P	4.18842600	0.00335100	0.01257900
C	0.45264400	-3.18120700	-0.05946600
H	1.05047900	-2.81142400	0.77703700
H	0.38762700	-4.27338400	-0.02013600
H	0.94239000	-2.87751700	-0.98781100
C	-1.95765600	-3.22812800	1.50996100
H	-1.81689100	-4.31296700	1.46533400
H	-1.47954200	-2.84819900	2.41733600
H	-3.03346100	-3.02921200	1.56563800
C	-2.11591900	-3.27068200	-1.35490300

H	-2.08161300	-4.35720200	-1.22395800
H	-3.16222700	-2.95014300	-1.38055300
H	-1.65227900	-3.02900500	-2.31744200
C	-1.97994500	3.22428300	1.50477000
H	-1.50720600	2.84652800	2.41676600
H	-1.84250800	4.30945900	1.46078900
H	-3.05512700	3.02140400	1.55253100
C	0.44247100	3.18465100	-0.04635900
H	0.37364000	4.27673600	-0.00816400
H	1.03579500	2.81717300	0.79450500
H	0.94013700	2.88206300	-0.97129800
C	-2.11662000	3.26546300	-1.36080200
H	-3.16177900	2.94248900	-1.39297800
H	-2.08603200	4.35200600	-1.23031400
H	-1.64595600	3.02422400	-2.31987100
C	4.94604300	0.00905700	-1.64828500
H	6.03476200	0.00839800	-1.53911600
H	4.65091700	-0.88024200	-2.21129800
H	4.65129200	0.90266100	-2.20481300
C	4.88429200	-1.45077800	0.88747100
H	5.97332400	-1.37568000	0.97211300
H	4.45469700	-1.51410900	1.89175000
H	4.62268300	-2.36177900	0.34150000
C	4.88379600	1.45166500	0.89729000
H	4.45407200	1.50828500	1.90200200
H	5.97269000	1.37598500	0.98157600
H	4.62230900	2.36628700	0.35740700
H	-2.32076700	-0.82937100	-2.29417400
H	-2.32260800	0.82431200	-2.29453600
H	-2.92394300	-0.83511300	1.87501100
H	-2.92760600	0.82670700	1.87420800
N	-2.23261100	-0.00254400	-1.71066600
N	-2.55027400	-0.00371700	1.42682700

Os.NH₂ (triplet)

Os	1.18926900	-0.00079500	-0.04761100
P	1.16566200	2.43576500	0.04446800
N	-0.36633900	0.00053900	-1.44287600
H	-0.07681600	0.00051200	-2.41534600
P	1.15837400	-2.43754200	0.04471300
C	-1.65319400	0.00285000	1.25303900
C	-1.68730500	0.00147500	-1.27730600
C	-2.34337500	0.00244700	-0.04264100
C	-0.30314800	0.00177000	1.41494200

H	-2.28290700	0.00148800	-2.19034600
H	0.01128100	0.00257600	2.46750500
H	-2.29508000	0.00441900	2.13900200
P	-4.09892700	0.00299100	-0.00864200
C	-0.35312400	3.24752200	-0.61274100
H	-1.22362600	2.84608400	-0.08701800
H	-0.31059100	4.33317000	-0.47654400
H	-0.45979700	3.02316400	-1.67781500
C	1.29512600	3.10670700	1.75438900
H	1.27826500	4.20146500	1.75526200
H	0.45925600	2.72952300	2.35058400
H	2.22729800	2.75826300	2.20740000
C	2.52328000	3.31855000	-0.84605200
H	2.46301800	4.39974000	-0.68329900
H	3.49393300	2.96152700	-0.48844600
H	2.45599100	3.12684100	-1.92201900
C	1.28472900	-3.10815900	1.75497300
H	0.44947400	-2.72832100	2.35034200
H	1.26482800	-4.20286500	1.75630700
H	2.21749700	-2.76202000	2.20850400
C	-0.36195800	-3.24577200	-0.61334300
H	-0.32202100	-4.33149900	-0.47697900
H	-1.23185700	-2.84228400	-0.08820100
H	-0.46749100	-3.02132900	-1.67851000
C	2.51434200	-3.32414500	-0.84453800
H	3.48563600	-2.96836300	-0.48749100
H	2.45203000	-4.40499300	-0.68029100
H	2.44743000	-3.13387100	-1.92078900
C	-4.85374200	0.00131100	-1.67040600
H	-5.94255300	0.00190600	-1.56150800
H	-4.55801200	0.89207400	-2.23083700
H	-4.55873700	-0.89107800	-2.22863200
C	-4.78239400	1.45982000	0.86679000
H	-5.87169300	1.38988100	0.95029300
H	-4.35151500	1.52054700	1.87026200
H	-4.51723200	2.36931100	0.31985800
C	-4.78300100	-1.45163000	0.86997600
H	-4.35208400	-1.51039000	1.87354500
H	-5.87226100	-1.38101300	0.95339500
H	-4.51829400	-2.36242300	0.32499500
H	2.97681000	-0.82826500	-1.98042200
H	2.98452900	0.82094100	-1.97567900
H	3.60607300	-0.00633100	1.14163900
H	2.44211600	-0.00109300	2.35896000

N	2.57407700	-0.00300800	-1.54462800
N	2.61492100	-0.00346500	1.35753200

Os.OH (singlet)

Os	-0.68514700	0.00059600	-0.00936700
P	-1.88107500	2.03588800	-0.00500900
N	0.73503900	-0.03487800	1.37508200
H	0.44100300	-0.07090600	2.35253200
P	-1.86088400	-2.04571300	-0.01983600
C	2.06687400	0.02880800	-1.23576600
C	2.07040700	-0.03472300	1.26046300
C	2.72980400	0.00040000	0.02459100
C	0.68445600	0.02221900	-1.42462600
H	2.63796300	-0.06475800	2.18706000
H	0.41318100	0.03831600	-2.49109900
H	2.70343800	0.05473100	-2.12439200
P	4.50976500	0.00781800	-0.00368100
C	-1.44292200	3.10783300	1.42758700
H	-0.37378500	3.34068100	1.41383500
H	-2.01117500	4.04400900	1.39751200
H	-1.68564600	2.56698200	2.34438800
C	-1.52849000	3.08848100	-1.47147600
H	-2.11680000	4.01182300	-1.43093700
H	-0.46501200	3.34148400	-1.50746100
H	-1.79664800	2.52658200	-2.36784700
C	-3.69911900	1.88279200	0.05589300
H	-4.14922500	2.88118300	0.07577100
H	-4.02498200	1.33843900	-0.83091900
H	-3.95892100	1.32850000	0.95835600
C	-1.50654600	-3.07887600	-1.49867100
H	-0.44148200	-3.32405800	-1.54102000
H	-2.08856100	-4.00653300	-1.46682800
H	-1.78150600	-2.50797300	-2.38732200
C	-1.41065700	-3.11980300	1.40592200
H	-1.97920400	-4.05592500	1.38132100
H	-0.34154200	-3.35200700	1.38343700
H	-1.64673200	-2.57391100	2.32160400
C	-3.67902000	-1.90022400	0.05080400
H	-4.01189100	-1.35258400	-0.83137200
H	-4.12549500	-2.90026800	0.06871100
H	-3.93591400	-1.35169000	0.95780500
C	5.23439900	-0.04204400	1.66809100
H	6.32516700	-0.03573500	1.57992100
H	4.92507400	0.83122300	2.24876800

H	4.93078700	-0.95201900	2.19274600
C	5.15599900	1.50523600	-0.82436600
H	6.24867400	1.47098500	-0.87995100
H	4.74846600	1.57845800	-1.83658000
H	4.84755600	2.39029500	-0.26025600
C	5.16731200	-1.43027500	-0.91621900
H	4.76147900	-1.44287100	-1.93163600
H	6.25974100	-1.38451100	-0.96797900
H	4.86495400	-2.35126300	-0.40923400
O	-2.08945500	-0.01239300	1.72394500
H	-1.56699300	0.06785200	2.53842800
O	-2.11994500	0.00643200	-1.63820800
H	-1.57696600	0.01318500	-2.44238300

Os.OH (triplet)

Os	-1.07392100	0.02168500	-0.03317400
P	-1.21177500	2.45421700	0.02921500
N	0.43579500	-0.15179500	1.35501500
H	0.06549100	-0.24625600	2.29938800
P	-1.39291400	-2.40593800	-0.06398700
C	1.75711900	0.08929000	-1.24153700
C	1.75229400	-0.15827100	1.25474200
C	2.43225500	-0.04352400	0.02450100
C	0.38763800	0.13179600	-1.41120100
H	2.31884100	-0.26235100	2.17890600
H	0.06503300	0.23981700	-2.45248300
H	2.38969600	0.15901200	-2.13017000
P	4.19971700	-0.07788000	-0.00003200
C	0.18669500	3.34568500	0.83168400
H	1.12014400	3.07393700	0.32991700
H	0.05121800	4.43090400	0.77696200
H	0.25834200	3.04714200	1.88191100
C	-1.34522100	3.19111800	-1.64685700
H	-1.56993400	4.26159800	-1.60044200
H	-0.40543600	3.03976200	-2.18610400
H	-2.13889200	2.66109600	-2.17975800
C	-2.70410300	3.07946300	0.90934500
H	-2.76478900	4.17145200	0.85721100
H	-3.59430000	2.65067900	0.43933100
H	-2.67615100	2.77941000	1.96172000
C	-0.32162000	-3.40061900	-1.18534400
H	0.72882900	-3.22246000	-0.93720800
H	-0.53619600	-4.47111400	-1.10019500
H	-0.48433300	-3.08245900	-2.21954800

C	-1.18222500	-3.16461400	1.59643600
H	-1.49459600	-4.21381000	1.60222100
H	-0.13288000	-3.10179500	1.90054700
H	-1.78904500	-2.58536900	2.29769300
C	-3.10473000	-2.89001500	-0.54357700
H	-3.30528000	-2.61294300	-1.58393000
H	-3.24819500	-3.97070400	-0.44269600
H	-3.81122100	-2.37307300	0.11263700
C	4.92157400	-0.24884500	1.66586400
H	6.01223700	-0.25952800	1.57742300
H	4.63057200	0.59162500	2.30170900
H	4.59985800	-1.18372500	2.13264500
C	4.90209900	1.44513400	-0.72886100
H	5.99212700	1.37230300	-0.79864700
H	4.49051200	1.59948600	-1.73041800
H	4.63425000	2.30369100	-0.10620600
C	4.84475100	-1.46552900	-1.00149000
H	4.43373000	-1.41348400	-2.01374200
H	5.93729000	-1.42572800	-1.05762700
H	4.53820800	-2.41345600	-0.54979700
O	-2.28116500	-0.23025900	1.63850500
H	-2.91056400	0.49505500	1.76362300
O	-2.56007200	0.32544000	-1.33087200
H	-3.19182000	-0.40809600	-1.36999900

Os.H₂O (singlet)

Os	-1.13202000	0.00735800	-0.00492200
P	-1.10140500	-2.38200600	0.01391800
N	0.31910000	0.01226500	-1.45956000
H	0.03423400	-0.00050200	-2.43582600
P	-1.08649100	2.37988400	0.01740800
C	1.61921300	-0.00968300	1.27466300
C	1.63187300	0.00412100	-1.28119300
C	2.29228100	-0.00273000	-0.03692400
C	0.27044000	-0.00244300	1.45577900
H	2.23354400	-0.00026700	-2.19108600
H	-0.03353200	-0.00894000	2.52086100
H	2.27116000	-0.02204800	2.15329800
P	4.03684800	-0.00770600	-0.01550000
C	0.51073800	-3.18634600	-0.39240500
H	1.27266500	-2.79827900	0.28853400
H	0.44869500	-4.27582600	-0.30067600
H	0.79948600	-2.92498600	-1.41409200
C	-1.52348700	-3.17413900	1.63505700

H	-1.46739400	-4.26638100	1.57746500
H	-0.81871100	-2.82690800	2.39808700
H	-2.53938900	-2.89677300	1.93672200
C	-2.26734300	-3.26521600	-1.13240600
H	-2.14404700	-4.35189000	-1.07090300
H	-3.30604200	-3.03015600	-0.87044900
H	-2.08401500	-2.95392300	-2.16641500
C	-1.71746900	3.19823200	1.56283400
H	-1.15668000	2.82636400	2.42676400
H	-1.60394000	4.28656600	1.51625600
H	-2.78496800	2.98944400	1.71217100
C	0.57023200	3.17650200	-0.16383800
H	0.50418000	4.26675000	-0.08510700
H	1.22848600	2.78348000	0.61521500
H	0.99246300	2.90662400	-1.13541300
C	-2.07401600	3.27947200	-1.27780900
H	-3.14307000	3.05760100	-1.16967300
H	-1.94998600	4.36503100	-1.19968600
H	-1.74849400	2.96727800	-2.27625800
C	4.79033500	0.00007300	-1.67969100
H	5.87922000	-0.00322000	-1.57221800
H	4.49211900	-0.88734300	-2.24394600
H	4.49630100	0.89510700	-2.23396800
C	4.74529900	-1.46494800	0.84743500
H	5.83481700	-1.38841900	0.92402200
H	4.32231700	-1.53453800	1.85378000
H	4.48153400	-2.37359200	0.29840100
C	4.75385300	1.43442700	0.86553200
H	4.33370800	1.49167900	1.87385100
H	5.84320400	1.35187300	0.93831900
H	4.49267700	2.35172300	0.32989400
O	-2.67506300	-0.03530800	-1.84687600
H	-3.33980600	-0.72270700	-1.68261200
H	-3.17074200	0.79708100	-1.89129000
O	-2.70766000	-0.07329800	1.66070000
H	-2.93221600	0.82878500	1.94040100
H	-2.22214400	-0.45140800	2.41641200

Os.H₂O (triplet)

Os	-0.84013700	0.06135700	0.43200900
P	-1.85296000	-2.09232500	0.07299000
N	0.49372000	-0.15112900	-1.08409200
H	0.14850500	-0.30491900	-2.03180100
P	-1.68601700	2.16269100	-0.36675200

C	2.00680300	0.18789700	1.46858000
C	1.81724700	-0.16164500	-1.02216500
C	2.57904000	0.00072700	0.15091800
C	0.65581300	0.22894900	1.73931400
H	2.32895100	-0.30993800	-1.97282300
H	0.44142200	0.37455900	2.81565000
H	2.70920500	0.30233300	2.29981100
P	4.32943800	-0.03392300	0.04479500
C	-0.63101100	-3.47934700	-0.06289700
H	-0.08789800	-3.57552000	0.88194000
H	-1.12081100	-4.43176000	-0.29698800
H	0.09499800	-3.24169900	-0.84624500
C	-3.03111900	-2.73587000	1.34468400
H	-3.40085600	-3.73084800	1.07312600
H	-2.52843200	-2.79414800	2.31445400
H	-3.87825100	-2.05166000	1.44368300
C	-2.82065600	-2.30292400	-1.49942600
H	-3.12812500	-3.34576200	-1.64537500
H	-3.71360100	-1.67132300	-1.46319300
H	-2.20863100	-1.97974800	-2.34751800
C	-2.83048200	3.14890400	0.71760300
H	-2.34693700	3.36600100	1.67726900
H	-3.09602900	4.10436200	0.25153500
H	-3.75826300	2.59366700	0.89863600
C	-0.36190800	3.40629900	-0.73219100
H	-0.77314600	4.32945600	-1.15673700
H	0.17935500	3.63872200	0.18969200
H	0.34906300	2.96698600	-1.43830600
C	-2.62880800	2.15021100	-1.96752300
H	-3.55588300	1.58292300	-1.84247300
H	-2.86998500	3.16540200	-2.30535500
H	-2.02602900	1.65189800	-2.73312700
C	4.94039200	-0.28628300	-1.65687800
H	6.03446500	-0.29343200	-1.64144900
H	4.58908300	-1.24192900	-2.05467300
H	4.60392000	0.52204500	-2.31133900
C	5.07099900	-1.36704300	1.05978500
H	6.16437800	-1.31554700	1.03778800
H	4.72966600	-1.27194100	2.09453300
H	4.74238600	-2.33749100	0.67671100
C	5.10444100	1.51500100	0.64309300
H	4.76416900	1.72490800	1.66115200
H	6.19625200	1.43393000	0.64089200
H	4.79794300	2.34438400	-0.00086300

O	-0.33882500	-0.87621700	-3.92904000
H	-0.27138200	-1.78519300	-4.25878800
H	-0.79497600	-0.39155100	-4.63384300
O	-2.14471700	0.21124900	2.30944600
H	-2.62668100	1.05318400	2.32824700
H	-1.50651700	0.25827000	3.04563000

Os.NH₃ (singlet)

Os	-1.17280900	0.00000800	0.02461500
P	-1.07797700	2.37513900	-0.02801500
N	0.33293100	0.00005200	1.48111400
H	0.09371900	0.00005800	2.47066800
P	-1.07779500	-2.37521600	-0.02803700
C	1.61800800	0.00006200	-1.26319400
C	1.64587600	0.00004000	1.29108400
C	2.29925000	0.00003900	0.04493100
C	0.26801800	0.00005900	-1.43405700
H	2.25850000	0.00003800	2.19431900
H	-0.02731900	0.00008800	-2.50174500
H	2.26871400	0.00011000	-2.14348200
P	4.04262800	0.00006600	0.01284000
C	0.54935200	3.14274400	0.39578800
H	1.31206900	2.71941200	-0.26237500
H	0.51870400	4.23145800	0.28108500
H	0.81226200	2.89452800	1.42757100
C	-1.42000200	3.16769300	-1.67155700
H	-1.27823600	4.25296300	-1.63104000
H	-0.73713200	2.74656800	-2.41591900
H	-2.44911800	2.97574400	-1.99641600
C	-2.22468600	3.35485700	1.06592200
H	-2.07546600	4.43296100	0.94192800
H	-3.27134900	3.12970200	0.82840000
H	-2.04599500	3.10497800	2.11783600
C	-1.41968600	-3.16769600	-1.67163400
H	-0.73685500	-2.74644800	-2.41595900
H	-1.27782000	-4.25295800	-1.63120100
H	-2.44882500	-2.97582300	-1.99647300
C	0.54953400	-3.14274900	0.39589300
H	0.51894100	-4.23146200	0.28115900
H	1.31231400	-2.71937000	-0.26216400
H	0.81231700	-2.89455400	1.42771700
C	-2.22450500	-3.35504600	1.06580600
H	-3.27117800	-3.12991400	0.82829500
H	-2.07525500	-4.43313500	0.94176200

H	-2.04581900	-3.10521800	2.11773700
C	4.81074100	-0.00001700	1.67080700
H	5.89868100	-0.00003900	1.55403500
H	4.51928200	0.89120400	2.23253600
H	4.51923500	-0.89126600	2.23246500
C	4.75051700	1.44941800	-0.86457400
H	5.83892200	1.36767800	-0.95123300
H	4.31761400	1.51494100	-1.86693400
H	4.49578300	2.36229400	-0.31828400
C	4.75051000	-1.44918900	-0.86473800
H	4.31755300	-1.51463500	-1.86707800
H	5.83890800	-1.36741600	-0.95144700
H	4.49582800	-2.36211800	-0.31851200
N	-2.74256700	-0.00013600	1.73310800
H	-2.29200500	0.00020800	2.65060900
H	-3.35254900	0.81630000	1.72352800
N	-2.67242300	-0.00008400	-1.61820000
H	-2.15465600	-0.00019800	-2.50231000
H	-3.28528300	-0.81428200	-1.65013000
H	-3.35181500	-0.81712100	1.72375300
H	-3.28521200	0.81415700	-1.65031500

Os.NH₃ (triplet)

Os	-0.30329900	-0.37252900	-0.03645600
P	0.14488300	-2.84564000	0.03103700
N	1.10341400	0.04695300	-1.43659600
H	0.91458900	-0.15369500	-2.41749100
P	-4.79734200	1.54981400	0.02028500
C	2.21861000	0.69277500	1.24610500
C	2.29616100	0.62143200	-1.27666400
C	2.85829400	0.93976800	-0.02981500
C	0.95864600	0.15299800	1.40177000
H	2.85844200	0.83154200	-2.18586700
H	0.67458400	0.05189700	2.46541600
H	2.79064700	0.95883900	2.14012900
P	4.43361600	1.71355200	0.01807700
C	-0.41984700	-3.78979600	1.53078300
H	-1.51495200	-3.82985700	1.56606700
H	-0.04311500	-4.81923800	1.53113200
H	-0.06219700	-3.28503500	2.43411100
C	-0.38619900	-4.01032700	-1.32419700
H	-0.01198300	-5.02838700	-1.16273700
H	-1.48007300	-4.05154200	-1.37834500
H	-0.00911100	-3.64982000	-2.28725200

C	1.96952500	-3.14795100	0.07218500
H	2.20741200	-4.21301700	0.17241400
H	2.41523100	-2.76203300	-0.84976000
H	2.39900400	-2.59098200	0.90987100
C	-4.86479900	2.67564700	1.50062600
H	-3.93005200	3.24076400	1.58029200
H	-5.69809400	3.38495300	1.43561700
H	-4.98202700	2.08501100	2.41551100
C	-4.86794500	2.79891400	-1.35748400
H	-5.70027900	3.50076500	-1.22974700
H	-3.93274000	3.36799100	-1.38994100
H	-4.98785200	2.28940300	-2.31962100
C	-6.53971400	0.90086800	-0.00520600
H	-6.70262200	0.23872100	0.85162300
H	-7.27830100	1.71002200	0.03208800
H	-6.70635400	0.31659400	-0.91625400
C	5.16933800	1.96244300	-1.63420700
H	6.14834500	2.43695300	-1.51719900
H	5.30204600	1.00493100	-2.14470300
H	4.53574300	2.61133700	-2.24436900
C	5.65614800	0.74782200	0.98209900
H	6.60288700	1.29044000	1.06970000
H	5.26190300	0.55332300	1.98340400
H	5.82963600	-0.21184600	0.48671100
C	4.38260600	3.36372500	0.81177600
H	3.93572800	3.27407000	1.80597200
H	5.38749400	3.78815200	0.90550600
H	3.75668500	4.03142500	0.21267600
N	-1.94861300	-0.38581500	-1.67828900
H	-1.66404700	0.12299600	-2.51625400
H	-2.25226400	-1.31107900	-1.98007800
N	-1.88166600	-0.43421500	1.50676500
H	-1.53020500	-0.00894000	2.36824400
H	-2.70379900	0.10610700	1.21501200
H	-2.77777300	0.09365200	-1.31275900
H	-2.21608100	-1.36642700	1.75073800

Os.PMe₃ (singlet)

Os	0.60812400	0.00299700	-0.02599400
P	0.27075000	-2.41007100	-0.10614700
N	-0.98408000	-0.04195900	1.42764000
H	-0.72295100	-0.08926400	2.40445100
P	0.32463600	2.41486500	-0.00716900
C	-2.28838200	0.12674000	-1.25317400

C	-2.29765400	-0.05244900	1.27097500
C	-2.97428500	0.02360300	0.04449800
C	-0.94722700	0.11386000	-1.45626400
H	-2.89017900	-0.11028700	2.18669900
H	-0.69057500	0.19061300	-2.51592100
H	-2.94507900	0.19745400	-2.12748700
P	-4.72016500	0.00740300	0.02328700
C	-0.45790400	-3.14884200	1.43621600
H	-1.41955100	-2.67740400	1.64642000
H	-0.60665700	-4.22609100	1.30749300
H	0.19768600	-2.98739000	2.29645500
C	-0.95150500	-3.03334500	-1.35210800
H	-1.05231600	-4.12094700	-1.26749000
H	-1.91870400	-2.55545500	-1.19203800
H	-0.61927900	-2.78273300	-2.36345600
C	1.62300100	-3.64607000	-0.43382300
H	1.24859800	-4.65874100	-0.24904400
H	1.93237200	-3.59048400	-1.48128100
H	2.49527800	-3.47484100	0.19901900
C	-0.14931500	3.20497900	-1.61745500
H	-1.04697800	2.71179100	-1.99568000
H	-0.34710200	4.27260400	-1.47415600
H	0.63980000	3.09421000	-2.36490100
C	-1.07914200	3.01451100	1.04348300
H	-1.16248900	4.10387500	0.96653800
H	-2.01032800	2.55348400	0.70817700
H	-0.91609100	2.74298000	2.08986600
C	1.63149700	3.60713100	0.56938300
H	2.56304700	3.47816800	0.01433000
H	1.28484900	4.63725100	0.43252600
H	1.83424300	3.45594000	1.63387100
C	-5.46749600	-0.12346400	1.68484600
H	-6.55671700	-0.12742900	1.58080300
H	-5.15966200	-1.05023400	2.17594100
H	-5.17905900	0.72743600	2.30746400
C	-5.41512900	-1.38101000	-0.95428900
H	-6.50525300	-1.30728400	-1.02468100
H	-4.99216400	-1.36451000	-1.96294300
H	-5.14400500	-2.32908500	-0.48070200
C	-5.44168800	1.51254000	-0.73870500
H	-5.01154300	1.65945200	-1.73365100
H	-6.52931600	1.42662000	-0.83003700
H	-5.19529500	2.38319200	-0.12394000
P	2.23654800	-0.06693500	1.78863900

P	2.27636500	0.03249000	-1.70755600
C	1.58056800	0.42810500	3.46382500
H	2.38733600	0.46796100	4.20311300
H	1.10086900	1.41078200	3.41563900
H	0.84257200	-0.30011700	3.81897100
C	3.76945000	0.98992600	1.74927400
H	3.51432200	2.04675600	1.66195700
H	4.35941200	0.84578300	2.66108000
H	4.39242200	0.71887700	0.89208100
C	3.06614900	-1.66126300	2.28409800
H	3.70226900	-2.02208000	1.47059100
H	3.69245000	-1.51266200	3.17063400
H	2.32698400	-2.43435600	2.50951800
C	3.74416300	-1.10795300	-1.58783200
H	4.43499300	-0.92149000	-2.41707900
H	4.28197000	-0.94373100	-0.64988800
H	3.43755800	-2.15321800	-1.62414600
C	3.24244600	1.59064900	-2.04391500
H	3.82405600	1.87211900	-1.16149700
H	3.93577300	1.43258400	-2.87693900
H	2.58357600	2.42224500	-2.30144100
C	1.74147800	-0.35778600	-3.44473100
H	2.60695400	-0.39315000	-4.11434700
H	1.22795400	-1.32335800	-3.47828300
H	1.04893000	0.40465500	-3.81215100

Os.PMe₃ (triplet)

Os	-0.59340700	-0.00527100	-0.06203500
P	-0.39979400	2.39761200	0.19360800
N	1.01169900	-0.04157200	1.36355100
H	0.75480100	-0.10938000	2.34164300
P	-0.34666100	-2.43691700	-0.11687000
C	2.31333800	0.06488800	-1.30186200
C	2.30485900	-0.48150000	1.16679000
C	2.98042300	-0.16858900	-0.09176600
C	0.91601800	0.08262700	-1.48465200
H	2.90889300	-0.63712100	2.06081400
H	0.67216600	0.22320600	-2.54207000
H	2.93138400	0.26841800	-2.17868300
P	4.72934100	0.07402000	-0.02079800
C	0.11045900	2.96381900	1.88336200
H	1.02146700	2.43418700	2.16929800
H	0.29296600	4.04359400	1.88834700
H	-0.66604400	2.74087100	2.62065600

C	0.91965900	3.20067400	-0.82571000
H	0.98101900	4.27119700	-0.60146300
H	1.87809100	2.72264300	-0.61010900
H	0.70902000	3.06678500	-1.88996200
C	-1.80628400	3.56957800	-0.13084200
H	-1.49014900	4.59657500	0.08222200
H	-2.12321700	3.52101400	-1.17546300
H	-2.66694400	3.33443800	0.49843600
C	0.98494700	-3.09006600	-1.22266700
H	1.94615300	-2.67177200	-0.91977400
H	1.02277800	-4.18349800	-1.16330800
H	0.79168600	-2.78984300	-2.25637700
C	0.17720000	-3.18699400	1.49533000
H	0.36585100	-4.25836000	1.36851300
H	1.09559900	-2.69498700	1.82565900
H	-0.59619900	-3.06079100	2.25824800
C	-1.71197300	-3.61177000	-0.59222600
H	-1.82145200	-3.63692900	-1.67807300
H	-1.45602500	-4.62192000	-0.25482300
H	-2.67058900	-3.32969100	-0.15385400
C	5.52159700	-1.34942300	0.83088200
H	6.60226100	-1.19578800	0.91229000
H	5.10472600	-1.46755100	1.83469900
H	5.32774300	-2.26534200	0.26511800
C	5.26757300	1.54033200	0.94958100
H	6.34043800	1.49832900	1.16610500
H	5.04471000	2.45388500	0.39155000
H	4.71341200	1.55936900	1.89234100
C	5.54005100	0.16430100	-1.65753100
H	5.25914800	1.08151800	-2.18065700
H	6.62612400	0.15275200	-1.52117600
H	5.25061100	-0.69694500	-2.26534700
P	-2.22384700	-0.15662300	1.78553000
P	-2.17027700	0.17717500	-1.83674000
C	-1.49828400	-0.32030000	3.49501200
H	-2.29207100	-0.41827400	4.24294100
H	-0.85058200	-1.19905000	3.56203900
H	-0.90388800	0.56506000	3.74316500
C	-3.43349900	-1.57077800	1.84568200
H	-2.90688400	-2.52416400	1.93629900
H	-4.10664000	-1.46780300	2.70360300
H	-4.03500100	-1.59698900	0.93192600
C	-3.42111200	1.22501200	2.14462000
H	-4.06472600	1.41201900	1.28192500

H	-4.05312100	0.96642500	3.00109800
H	-2.88552200	2.14732700	2.38392700
C	-3.90782800	0.74854200	-1.50119300
H	-4.48922500	0.79138600	-2.42866200
H	-4.40470200	0.05588100	-0.81486000
H	-3.90638600	1.74241200	-1.04650700
C	-2.57223500	-1.29142200	-2.90455800
H	-3.16316400	-2.02072000	-2.34630000
H	-3.15109000	-0.97672400	-3.77950400
H	-1.65238400	-1.77249500	-3.25054600
C	-1.72119000	1.35175200	-3.21402200
H	-2.55316900	1.43917900	-3.92051900
H	-1.47996200	2.34672900	-2.83398400
H	-0.84864200	0.97939800	-3.75738200

Ir.BMe₂ (singlet)

P	0.93585400	-2.37675900	-0.30689900
N	-0.86808900	0.50079100	1.52759400
H	-0.72184800	0.70130300	2.51179900
P	0.99978300	2.53291300	0.01266700
C	-1.87893200	-0.01749400	-1.17787600
C	-2.15894700	0.33371200	1.27331400
C	-2.70791200	0.09622300	0.01063300
C	-0.53705500	-0.05318400	-1.30473100
H	-2.83920000	0.42753700	2.12233900
H	-0.12371700	-0.17313700	-2.30245800
H	-2.40862000	-0.08272700	-2.13179700
P	-4.46722600	-0.01005100	-0.18865700
Ir	0.96245400	0.04319100	0.08368100
C	1.14273300	-2.84236000	-2.07650000
H	2.14183000	-2.57853700	-2.43191300
H	1.02029900	-3.92680100	-2.16602400
H	0.39499400	-2.35112700	-2.70177400
C	-0.64444100	-3.19724300	0.15149800
H	-1.47200500	-2.68615900	-0.34436900
H	-0.61532200	-4.24359500	-0.16971200
H	-0.80150100	-3.16462500	1.23073600
C	2.23846600	-3.40253600	0.49953400
H	2.15520100	-3.38034600	1.58823300
H	2.12721200	-4.44067000	0.16916600
H	3.23200800	-3.05106900	0.21029400
C	2.53977300	3.32681200	-0.61386600
H	2.44126300	4.41621400	-0.56044800
H	3.40066300	3.02903700	-0.00715200

H	2.72603300	3.04372400	-1.65247100
C	-0.33721700	3.25566600	-1.01549500
H	-1.30782900	2.91424400	-0.64893400
H	-0.28789500	4.34830000	-0.96475900
H	-0.22708900	2.94047400	-2.05616200
C	0.77743700	3.31838100	1.66300100
H	0.78918400	4.40755400	1.55042300
H	-0.17762400	3.01643500	2.09669600
H	1.58880700	3.03459700	2.33938500
C	-4.99092300	-1.62030400	-0.87639600
H	-6.07366600	-1.62969900	-1.03847000
H	-4.49359000	-1.80127200	-1.83415600
H	-4.72533100	-2.42286800	-0.18205400
C	-5.34785400	0.20677900	1.39163800
H	-5.07212300	-0.57368900	2.10604800
H	-5.14075500	1.18958100	1.82388600
H	-6.42291000	0.13412400	1.19897000
C	-5.10191600	1.26493600	-1.33374600
H	-4.61331000	1.18066500	-2.30900500
H	-6.18091000	1.14269100	-1.47331400
H	-4.90273300	2.25974700	-0.92477400
B	1.29772700	-0.65808700	1.98555700
B	2.55023100	0.02591900	-1.30476600
C	2.68265000	0.10891900	2.12216800
H	2.57494200	0.76356500	2.99801700
H	3.44576500	-0.64584000	2.35282900
H	3.08983200	0.72569300	1.31373800
C	0.67759700	-1.50537200	3.13206300
H	1.39303800	-2.25717300	3.49294300
H	0.51123000	-0.84737300	3.99910700
H	-0.27103200	-1.99742600	2.91276900
C	4.02162400	-0.40428900	-0.91839000
H	4.17471800	-0.96847500	0.00478300
H	4.48561100	-0.96255200	-1.74435300
H	4.63019000	0.51144400	-0.83617200
C	2.34199200	0.51781800	-2.79722000
H	1.48074600	1.16089600	-3.00187300
H	3.24460500	1.02154300	-3.16882400
H	2.23007600	-0.36495700	-3.44615100

Ir.BMe₂ (triplet)

P	0.98827300	-2.40837600	-0.12268700
N	-0.91839100	0.14553400	1.50055700
H	-0.66872200	0.24054100	2.48220300

P	1.02610100	2.43330000	0.01203000
C	-2.10511200	-0.08498400	-1.14983600
C	-2.20947400	0.14885000	1.33883300
C	-2.83657800	0.02139700	0.05802600
C	-0.72741600	-0.07473100	-1.31136100
H	-2.85201200	0.24866000	2.21652500
H	-0.41856800	-0.13586500	-2.35690200
H	-2.69129600	-0.16766100	-2.06854800
P	-4.63973700	0.00833700	-0.06112800
Ir	0.89965800	0.00585900	-0.04475500
C	0.99294200	-3.11050100	-1.82494200
H	1.90194700	-2.81444500	-2.35598700
H	0.95930700	-4.20392800	-1.77761100
H	0.12597100	-2.75233600	-2.38685500
C	-0.47060800	-3.21324900	0.66125900
H	-1.38688700	-2.86498000	0.17757800
H	-0.39902400	-4.30073400	0.55506200
H	-0.51531900	-2.96430000	1.72438300
C	2.41688200	-3.25341300	0.67334000
H	2.44489000	-3.03948000	1.74496700
H	2.32089900	-4.33589300	0.53676500
H	3.35551300	-2.92599100	0.22049000
C	2.57110700	3.21603400	-0.61107500
H	2.48380500	4.30534700	-0.53891800
H	3.43353200	2.89607600	-0.02154800
H	2.73824000	2.94702100	-1.65741700
C	-0.28342000	3.25990400	-0.98545900
H	-1.27089400	2.95150400	-0.63259100
H	-0.19220300	4.34753900	-0.89775800
H	-0.18456200	2.98060900	-2.03801600
C	0.81817100	3.18364800	1.68268300
H	0.83360400	4.27601300	1.60723700
H	-0.13510800	2.87406400	2.11970300
H	1.63061000	2.87099200	2.34456400
C	-5.21766600	-1.54920000	-0.81248000
H	-6.30788600	-1.52660300	-0.91247500
H	-4.77632500	-1.68117200	-1.80458200
H	-4.93368800	-2.39549900	-0.17999600
C	-5.42360200	0.16692400	1.57401600
H	-5.14590500	-0.66631200	2.22592700
H	-5.15225800	1.11349600	2.05020400
H	-6.50989300	0.14968900	1.43674200
C	-5.22375300	1.38763800	-1.10078500
H	-4.78308300	1.32598700	-2.10001700

H	-6.31392600	1.34199000	-1.19320900
H	-4.94274300	2.34203000	-0.64574600
B	1.99443600	-0.13845800	1.85713700
B	2.35061700	0.01713700	-1.53345200
C	3.46252700	0.44120300	1.89545300
H	3.56851500	1.06979900	2.79389700
H	4.14825600	-0.40527900	2.05613600
H	3.83269800	0.99524300	1.03381200
C	1.42294500	-0.74170300	3.19608300
H	2.21780000	-1.26399200	3.74645700
H	1.13489100	0.08672800	3.86558900
H	0.56549800	-1.41813500	3.12528400
C	3.85408700	-0.43695000	-1.33011900
H	4.12423000	-0.92737000	-0.39365400
H	4.16268000	-1.08282600	-2.16601600
H	4.49579600	0.45327200	-1.42417900
C	1.98832600	0.47808100	-3.01382200
H	1.16244600	1.18835400	-3.12630100
H	2.86552100	0.88885300	-3.53047200
H	1.70777900	-0.41687800	-3.59305300

Ir.NH₂ (singlet)

P	1.21101300	-2.48111500	-0.03299800
N	-0.37896400	0.00275000	1.41633800
H	-0.08304200	0.00466700	2.39143300
P	1.22455300	2.47742600	-0.03325000
C	-1.68017100	0.00326400	-1.21574800
C	-1.69384300	0.00391200	1.28089000
C	-2.35614700	0.00356200	0.03062900
C	-0.29406000	0.00236600	-1.39026900
H	-2.27951600	0.00559400	2.19747200
H	0.00971900	0.00428100	-2.44223700
H	-2.29777800	0.00446100	-2.11574200
P	-4.16510900	0.00546700	-0.00702500
Ir	1.08807200	-0.00135600	0.01959200
C	0.71924100	-3.20902500	-1.64451700
H	1.35978100	-2.80899400	-2.43573000
H	0.82591600	-4.29837900	-1.62139100
H	-0.31960000	-2.95654700	-1.87542400
C	0.18342700	-3.34539000	1.22367600
H	-0.87496600	-3.11365400	1.07494200
H	0.32149100	-4.42886300	1.14675700
H	0.47695800	-3.02864700	2.22891400
C	2.91631900	-3.08799800	0.25666000

H	3.26475500	-2.75486200	1.23716600
H	2.94235600	-4.18168200	0.21392600
H	3.58056000	-2.68663300	-0.51333800
C	2.93344800	3.07584800	0.25306800
H	2.96460800	4.16940800	0.21058300
H	3.28216200	2.74099400	1.23289700
H	3.59431500	2.67173400	-0.51839900
C	0.73306200	3.20855400	-1.64338800
H	-0.30761000	2.96167900	-1.87210000
H	0.84547700	4.29732600	-1.61998800
H	1.36974000	2.80551800	-2.43619500
C	0.20407500	3.34616700	1.22608200
H	0.34695300	4.42900700	1.14908800
H	-0.85575400	3.11939000	1.07993800
H	0.49869300	3.02780200	2.23049200
C	-4.78472000	-1.46911600	-0.88100100
H	-5.87832200	-1.43639700	-0.92649300
H	-4.39160900	-1.50166500	-1.90121800
H	-4.47573100	-2.37462300	-0.35049900
C	-4.87432000	0.00524800	1.66918700
H	-4.57577800	-0.88965800	2.22274900
H	-4.57482100	0.89942500	2.22341200
H	-5.96572500	0.00589500	1.57992800
C	-4.78183100	1.48222300	-0.87939600
H	-4.38877200	1.51500600	-1.89962600
H	-5.87550500	1.45181200	-0.92476800
H	-4.47088200	2.38653800	-0.34800600
H	3.53243800	-0.00455700	-1.08917300
H	3.52989000	-0.00262500	1.28542400
H	2.40307900	-0.00858700	-2.33664400
H	2.38237700	-0.00862100	2.48146900
N	2.53121300	-0.00499600	1.47505700
N	2.54759000	-0.00568000	-1.33201400

Ir.NH₂ (triplet)

P	1.17543900	-2.47975000	-0.04142900
N	-0.35631700	0.00018400	1.43633300
H	-0.08014500	0.00025300	2.41456800
P	1.17651200	2.47919700	-0.04141200
C	-1.64278000	0.00036000	-1.23142300
C	-1.67671700	0.00030700	1.27295100
C	-2.33661200	0.00034600	0.03963000
C	-0.28737300	0.00028600	-1.41093300
H	-2.26452200	0.00033500	2.18925000

H	0.03340000	0.00027700	-2.45717800
H	-2.26657100	0.00041300	-2.12742300
P	-4.12742800	0.00043000	-0.00062100
Ir	1.13216300	0.00003200	0.02800300
C	0.85792900	-3.16719900	-1.71321100
H	1.62008800	-2.80940100	-2.41164500
H	0.89179000	-4.26116400	-1.68736500
H	-0.12321300	-2.84489900	-2.07160600
C	-0.04072700	-3.31112600	1.05676200
H	-1.05551100	-3.01309200	0.78016200
H	0.05003500	-4.39840400	0.96515200
H	0.13710400	-3.03119400	2.09899600
C	2.80414600	-3.17507400	0.44466300
H	3.05249400	-2.87466500	1.46644400
H	2.78225300	-4.26842900	0.39028500
H	3.58326300	-2.80765200	-0.22961500
C	2.80548500	3.17378700	0.44479600
H	2.78399400	4.26715700	0.39054700
H	3.05368300	2.87314200	1.46654000
H	3.58446800	2.80616300	-0.22952400
C	0.85936300	3.16692000	-1.71313700
H	-0.12195900	2.84520600	-2.07156100
H	0.89382600	4.26086200	-1.68715600
H	1.62133100	2.80877800	-2.41160000
C	-0.03936100	3.31095000	1.05679000
H	0.05175700	4.39819700	0.96515800
H	-1.05424300	3.01324000	0.78020600
H	0.13841500	3.03097600	2.09902100
C	-4.76561700	-1.46817000	-0.87570900
H	-5.85795100	-1.42177100	-0.93415200
H	-4.36179500	-1.51070400	-1.89143600
H	-4.47367200	-2.37601200	-0.33971200
C	-4.84983800	0.00031600	1.67111900
H	-4.55410000	-0.89377800	2.22714500
H	-4.55408500	0.89432100	2.22728100
H	-5.94037200	0.00033500	1.57458000
C	-4.76548500	1.46923400	-0.87546300
H	-4.36165700	1.51189700	-1.89118200
H	-5.85782300	1.42295100	-0.93391200
H	-4.47345000	2.37695900	-0.33931600
H	3.55494000	-0.00057700	-1.16625200
H	3.55857900	-0.00070100	1.40604600
H	2.36670300	-0.00038400	-2.35502500
H	2.35139500	-0.00089800	2.54059800

N	2.54679700	-0.00046200	1.53897900
N	2.55419100	-0.00029100	-1.35411400
Ir:OH (singlet)			
P	1.81092400	-2.13222300	0.01779500
N	-0.69303800	-0.00149700	1.35796700
H	-0.38166800	-0.00292400	2.32922100
P	1.81194500	2.13170300	0.01838300
C	-2.02733100	0.00107000	-1.21691900
C	-2.01529700	-0.00144300	1.25578900
C	-2.69642800	0.00000600	0.02232100
C	-0.63833400	0.00082200	-1.41093200
H	-2.57339400	-0.00262000	2.18844400
H	-0.35644600	0.00156100	-2.46936400
H	-2.64348300	0.00213500	-2.11739200
P	-4.51079800	0.00040400	0.00252200
Ir	0.73136800	0.00000500	-0.03807200
C	1.32382700	-3.13587300	-1.43588700
H	1.61414300	-2.60823700	-2.34661400
H	1.84758100	-4.09823300	-1.39976400
H	0.24569100	-3.31506200	-1.44065900
C	1.31621900	-3.09730300	1.49418600
H	0.23442800	-3.25521000	1.51064700
H	1.81573900	-4.07267700	1.46769700
H	1.63032000	-2.56353800	2.39310200
C	3.62638300	-2.03540800	0.01046300
H	3.95533300	-1.49222400	0.89601900
H	4.01763200	-3.05935600	0.02158800
H	3.94874100	-1.51809700	-0.89328600
C	3.62741400	2.03483100	0.01129500
H	4.01863800	3.05878700	0.02280700
H	3.95622400	1.49135500	0.89671400
H	3.94993400	1.51784300	-0.89257600
C	1.32521200	3.13609600	-1.43494500
H	0.24712400	3.31556600	-1.43971100
H	1.84919600	4.09831300	-1.39830300
H	1.61548700	2.60885700	-2.34590600
C	1.31714100	3.09682400	1.49477800
H	1.81640800	4.07232400	1.46804700
H	0.23531300	3.25448200	1.51127800
H	1.63137000	2.56349300	2.39390100
C	-5.12730000	-1.47807700	-0.86426300
H	-6.22176000	-1.45539500	-0.89322900
H	-4.74927000	-1.50557500	-1.89039800
H	-4.80111000	-2.38110700	-0.33967900

C	-5.19162800	-0.00139700	1.68972700
H	-4.88378900	-0.89723100	2.23688700
H	-4.88339300	0.89302500	2.23896800
H	-6.28445000	-0.00107400	1.61862300
C	-5.12662000	1.48115800	-0.86086300
H	-4.74852000	1.51085300	-1.88691300
H	-6.22108900	1.45903700	-0.88993600
H	-4.80004800	2.38282600	-0.33417800
O	2.17458900	0.00042500	-1.56021600
O	2.20792500	-0.00054200	1.57023400
H	1.69095200	0.00076200	-2.40225400
H	1.74332500	0.00228400	2.42281700

Ir.OH (triplet)

P	1.45217100	-2.40266300	-0.06062300
N	-0.45134800	-0.18396800	1.35284300
H	-0.07376300	-0.30097100	2.29288400
P	1.20020200	2.47345000	0.03280300
C	-1.76999500	0.07553500	-1.22443900
C	-1.75762800	-0.19185100	1.25113500
C	-2.44874700	-0.06345200	0.01742700
C	-0.39668600	0.12163500	-1.39560100
H	-2.32116300	-0.31235400	2.17446600
H	-0.05846900	0.23504600	-2.42731100
H	-2.38082700	0.14790300	-2.12506900
P	-4.25673400	-0.10115600	-0.00784000
Ir	1.06401200	0.02402300	-0.03139700
C	0.49640300	-3.38416500	-1.28280900
H	0.71103800	-3.03104400	-2.29591600
H	0.76372900	-4.44387800	-1.21364600
H	-0.57556800	-3.27533800	-1.09535300
C	1.13902000	-3.15813200	1.57848600
H	0.07179400	-3.12481400	1.81567600
H	1.46884000	-4.20207100	1.58210100
H	1.69689300	-2.59548800	2.33164300
C	3.21883700	-2.75768500	-0.41282300
H	3.84667500	-2.16688700	0.26015000
H	3.42135500	-3.82119400	-0.24728000
H	3.47492300	-2.53175200	-1.45351400
C	2.79986500	3.01639700	0.74996900
H	2.91296900	4.09860300	0.62526000
H	2.85164100	2.79448700	1.82069500
H	3.61933300	2.51207400	0.23005000
C	1.16161600	3.19059100	-1.65119400

H	0.17441300	3.04731200	-2.09955700
H	1.38613500	4.26144900	-1.61361900
H	1.90858900	2.68093300	-2.26517600
C	-0.09756400	3.33856000	1.00097500
H	0.06011500	4.42155100	0.96274200
H	-1.08444300	3.11115400	0.58784000
H	-0.06634000	3.01555100	2.04569400
C	-4.84714300	-1.49838400	-1.01800400
H	-5.94159500	-1.48704200	-1.05420800
H	-4.46121400	-1.42227200	-2.03874900
H	-4.51352500	-2.44352800	-0.57949000
C	-4.94228000	-0.28107900	1.66817700
H	-4.62232700	-1.22178000	2.12575500
H	-4.65026200	0.55868500	2.30551600
H	-6.03474000	-0.29094800	1.59254200
C	-4.90997200	1.44006000	-0.72827300
H	-4.52297900	1.58249200	-1.74149800
H	-6.00289600	1.38823500	-0.77374700
H	-4.61811700	2.29455600	-0.11058200
O	2.45811500	0.32906600	-1.37670200
O	2.20472200	-0.18412500	1.65281700
H	2.99791700	-0.45456500	-1.57125100
H	2.68071800	0.62175100	1.90843800

Ir.H₂O (singlet)

P	1.10218900	-2.42444000	-0.02233400
N	-0.31763600	-0.02316100	1.41778300
H	0.00292400	0.02119100	2.37977500
P	1.07699700	2.42364500	-0.01394600
C	-1.61845900	-0.00094300	-1.26235000
C	-1.63886500	-0.01051200	1.24980300
C	-2.31227800	-0.00520600	0.03007500
C	-0.28121800	-0.00290400	-1.45092900
H	-2.21116800	-0.00257600	2.17620100
H	0.08350300	-0.00984600	-2.48328400
H	-2.24310700	0.00115600	-2.15750700
P	-4.08512400	-0.00767100	0.01207700
Ir	1.11342100	-0.00066500	-0.00383200
C	1.83852900	-3.16575000	-1.54435300
H	2.91188900	-2.94935600	-1.61239900
H	1.73309400	-4.25560600	-1.52876000
H	1.32896400	-2.78547700	-2.43555200
C	-0.55505600	-3.20342600	0.08946800
H	-1.17911400	-2.83999800	-0.73009200

H	-0.46669300	-4.29282500	0.03128200
H	-1.02439900	-2.92980600	1.03746500
C	2.05784500	-3.22042700	1.34236500
H	1.67070300	-2.89988400	2.31550800
H	1.97180500	-4.31069400	1.28666800
H	3.12218800	-2.96883200	1.27103900
C	2.35925200	3.22234400	1.04416400
H	2.25977000	4.31220400	1.00641800
H	2.24901300	2.90130300	2.08458800
H	3.36354900	2.96474700	0.68970600
C	1.36966500	3.15976900	-1.67826900
H	0.63980700	2.76840300	-2.39337900
H	1.26871800	4.24925900	-1.63691100
H	2.38380800	2.93861100	-2.03007200
C	-0.49868300	3.18423200	0.53968100
H	-0.44387700	4.27355300	0.44748300
H	-1.31931300	2.80506900	-0.07369200
H	-0.68919900	2.92381800	1.58390700
C	-4.75972900	-1.46904800	-0.85358400
H	-5.85219300	-1.41274100	-0.89736800
H	-4.37124800	-1.51563300	-1.87530000
H	-4.46810900	-2.38024500	-0.32327300
C	-4.79401300	-0.00819500	1.69102900
H	-4.49221900	-0.90162900	2.24449500
H	-4.49246600	0.88542000	2.24439200
H	-5.88516500	-0.00830700	1.60504800
C	-4.76142200	1.45293200	-0.85329300
H	-4.36667100	1.50521100	-1.87229700
H	-5.85330000	1.39158300	-0.90400200
H	-4.47783100	2.36387500	-0.31807500
O	2.75782500	0.07869900	-1.50486600
H	2.98850800	-0.78148200	-1.89696900
O	2.67728500	0.06553200	1.75633300
H	3.44073800	0.64954600	1.61269100
H	2.53652400	0.65706200	-2.25649500
H	3.04540800	-0.77776700	2.06779400

Ir.H₂O (triplet)

P	1.24204898	2.36823373	0.33391639
N	-0.61516302	0.07051594	-1.52161712
H	-0.29866458	0.15004949	-2.48668669
P	1.29285317	-2.35070834	0.31570151
C	-1.94141448	-0.04435448	1.11277535
C	-1.92703268	0.05552581	-1.39767294

C	-2.59960999	-0.00917123	-0.15514426
C	-0.57531659	-0.03151042	1.34599091
H	-2.51421894	0.10229997	-2.31457088
H	-0.29819862	-0.04771876	2.40577334
H	-2.57976412	-0.07761802	1.99739799
P	-4.39893558	-0.02975130	-0.13715314
Ir	0.84722942	0.00438598	0.01012017
C	1.59922380	2.81253410	2.08416148
H	2.49049988	2.28246377	2.43237448
H	1.76689057	3.89074457	2.18022212
H	0.75680239	2.52648279	2.72054070
C	-0.16906305	3.45759968	-0.12584270
H	-1.05492276	3.16730751	0.44597196
H	0.06731995	4.50581050	0.08533339
H	-0.38698698	3.34928300	-1.19220519
C	2.66259761	3.05016766	-0.61596237
H	2.48341243	2.93426022	-1.68809407
H	2.79300922	4.11271582	-0.38536144
H	3.58264666	2.51665086	-0.36064974
C	2.62115785	-3.05324936	-0.75418849
H	2.82856021	-4.08816378	-0.46209887
H	2.30381316	-3.05963113	-1.80296194
H	3.54264899	-2.47097991	-0.65965517
C	1.84252063	-2.74837999	2.02714256
H	1.07498789	-2.44345711	2.74431746
H	2.02126343	-3.82388264	2.13369908
H	2.76558496	-2.20954014	2.25944663
C	-0.13986219	-3.47233862	0.03304113
H	0.13670531	-4.51291357	0.23282701
H	-0.96071081	-3.18518464	0.69598984
H	-0.47989787	-3.38559119	-1.00315752
C	-5.05564942	1.39949283	0.78632771
H	-6.14876277	1.34807215	0.82131766
H	-4.67064222	1.40108399	1.81008129
H	-4.75561766	2.32865816	0.29292429
C	-5.09884292	0.02985378	-1.81700448
H	-4.80765812	0.95020168	-2.33111472
H	-4.78258512	-0.83622491	-2.40519838
H	-6.19051252	0.01135754	-1.73535673
C	-5.02101057	-1.54327830	0.66839717
H	-4.63367480	-1.61761058	1.68862243
H	-6.11494014	-1.52016647	0.70785548
H	-4.70063473	-2.42268575	0.10202401
O	5.00574593	-0.04912736	-0.76459046

H	5.73710451	0.11343174	-1.38264972
O	2.45334328	0.10166369	-1.62882910
H	2.43557741	-0.66974401	-2.21707099
H	5.38177612	0.06593732	0.12199155
H	3.38086501	0.12871875	-1.27155352

Ir.NH₃ (singlet)

P	1.07147600	-2.41847800	-0.03680000
N	-0.32773600	-0.00055900	1.44899800
H	-0.05677200	-0.00238700	2.42652000
P	1.06885100	2.41880400	-0.03716500
C	-1.61008400	-0.00084400	-1.24454800
C	-1.64821500	-0.00095400	1.26832800
C	-2.31276400	-0.00057600	0.04369200
C	-0.27063300	-0.00103100	-1.42341400
H	-2.23461300	-0.00152700	2.18629400
H	0.06930500	-0.00124400	-2.46567200
H	-2.23398400	-0.00107900	-2.14056500
P	-4.08385700	-0.00082300	0.01037900
Ir	1.15525600	0.00023000	0.02648500
C	1.22320600	-3.12386300	-1.73281800
H	2.20274500	-2.90355300	-2.17019600
H	1.10673300	-4.21199200	-1.70452900
H	0.44685500	-2.69953900	-2.37539300
C	-0.48251200	-3.16198900	0.59895900
H	-1.33146000	-2.74435600	0.05313200
H	-0.46004000	-4.24858200	0.46874700
H	-0.60094200	-2.93125800	1.66063300
C	2.38438100	-3.31621600	0.90641400
H	2.31304900	-3.09110400	1.97577900
H	2.26972900	-4.39819500	0.78280300
H	3.38444000	-3.04405600	0.55040000
C	2.38750300	3.31727900	0.89722000
H	2.27113000	4.39922000	0.77490400
H	2.32417600	3.09134600	1.96687400
H	3.38521500	3.04600000	0.53402800
C	1.20928500	3.12370600	-1.73431700
H	0.42907400	2.69864300	-2.37165900
H	1.09265700	4.21180400	-1.70561100
H	2.18598200	2.90345600	-2.17803300
C	-0.48143500	3.16152300	0.60852700
H	-0.46043400	4.24811600	0.47805100
H	-1.33371200	2.74336400	0.06830500
H	-0.59298500	2.93087400	1.67097500

C	-4.75351000	-1.46116900	-0.86177100
H	-5.84471600	-1.39920400	-0.92443000
H	-4.34717300	-1.51367500	-1.87616100
H	-4.47608500	-2.37229500	-0.32362000
C	-4.81191900	-0.00075600	1.68145900
H	-4.51598600	-0.89413600	2.23812400
H	-4.51602100	0.89268300	2.23804500
H	-5.90202300	-0.00078600	1.58342300
C	-4.75391100	1.45915300	-0.86207900
H	-4.34742800	1.51164100	-1.87641300
H	-5.84508700	1.39680000	-0.92489500
H	-4.47688500	2.37046400	-0.32403600
N	2.75504500	0.00331700	1.68731300
H	3.35393900	-0.82287700	1.67922300
H	3.38080600	0.80858100	1.65010000
N	2.69738700	0.00068300	-1.52614900
H	2.24722400	-0.00764100	-2.44523500
H	3.30866500	0.81854400	-1.51960800
H	2.33476200	0.02733000	2.61853000
H	3.31887600	-0.80931300	-1.50946400

Ir.NH₃ (triplet)

P	-1.35160100	-2.81411200	-0.03008500
N	0.43035300	0.01245500	-1.39489800
H	0.14254100	0.01409000	-2.37147900
P	-1.38841400	2.79910600	-0.02567300
C	1.73921000	0.00154300	1.22171600
C	1.75026300	0.01602500	-1.26728900
C	2.42300600	0.01136900	-0.03114000
C	0.36289300	-0.00506000	1.38632100
H	2.32288700	0.02237200	-2.19218400
H	0.05440800	-0.01153100	2.43983800
H	2.35087800	-0.00101300	2.12550500
P	4.21678400	0.01936300	-0.00040000
Ir	-1.01440800	-0.00307800	0.00203100
C	-1.51815800	-3.50830500	1.68006500
H	-2.52400300	-3.32555700	2.07434900
H	-1.34915800	-4.59083100	1.68450100
H	-0.78590000	-3.04170600	2.34709800
C	0.27879500	-3.49246700	-0.57330100
H	1.07889600	-3.01982600	0.00359900
H	0.32309200	-4.57744600	-0.43010700
H	0.43905500	-3.27045300	-1.63292100
C	-2.55211300	-3.85794300	-0.99281400

H	-2.46955700	-3.64277600	-2.06356300
H	-2.35613400	-4.92609600	-0.84302700
H	-3.57941100	-3.65042400	-0.67489800
C	-1.69763200	3.49715000	1.66377200
H	-1.54352100	4.58189800	1.67679500
H	-2.72949800	3.30417600	1.97853500
H	-1.01429900	3.04428700	2.38981400
C	0.26705900	3.50291400	-0.44533700
H	0.51349100	3.27506200	-1.48699900
H	0.28127200	4.58954900	-0.30903800
H	1.02713400	3.04864500	0.19674500
C	-2.52981800	3.81659200	-1.08239700
H	-2.36038100	4.88869300	-0.92905900
H	-2.36695300	3.59209200	-2.14177000
H	-3.57456200	3.59694200	-0.83776200
C	4.86108000	-1.45222500	0.86359600
H	5.95401400	-1.40852700	0.91100500
H	4.46584600	-1.49629500	1.88256500
H	4.56025300	-2.35729500	0.32780600
C	4.92618900	0.02912400	-1.67751700
H	4.62758000	-0.86380500	-2.23392200
H	4.62021000	0.92404600	-2.22666100
H	6.01755500	0.03330800	-1.59159300
C	4.84787600	1.48983500	0.87515600
H	4.45255400	1.52205700	1.89453300
H	5.94118500	1.45583800	0.92190900
H	4.53846900	2.39631200	0.34669300
N	-2.63710100	-0.00331500	-1.66852000
H	-3.32205500	0.74379600	-1.54650500
H	-2.25600400	0.12888800	-2.60771700
N	-2.51060300	-0.02665800	1.61359100
H	-2.32247100	-0.78253600	2.27452200
H	-2.49449000	0.83965000	2.15414300
H	-3.16081900	-0.87891900	-1.70218300
H	-3.47464800	-0.15366900	1.30121400

Ir.PMe₃ (singlet)

P	-0.35388300	2.45803900	-0.17068200
N	0.94878500	0.07698500	1.41151100
H	0.66718800	0.09796000	2.38200100
P	-0.29507700	-2.41935900	0.09195400
C	2.27227700	0.05136500	-1.24077500
C	2.26953700	0.03889700	1.26332200
C	2.95922800	0.02149500	0.05310000

C	0.93968600	0.03270300	-1.46132500
H	2.84005500	0.03643200	2.19269000
H	0.65739300	0.07311100	-2.51267200
H	2.91549200	0.08175500	-2.12401900
P	4.72827700	-0.00804100	0.04605000
Ir	-0.58548400	0.00739200	-0.04457500
C	0.17160300	3.16737800	-1.79222800
H	-0.65119600	3.17407100	-2.50849500
H	0.49589500	4.20136100	-1.63623700
H	1.00011500	2.58759700	-2.20200100
C	0.97971700	3.09123800	0.93414700
H	1.93797800	2.65954100	0.63848700
H	1.02992400	4.18099600	0.84220900
H	0.78712100	2.83115000	1.97694300
C	-1.74681000	3.59156900	0.27843400
H	-2.02361100	3.47835100	1.32962100
H	-1.42708400	4.62714000	0.12164600
H	-2.62935500	3.41188200	-0.34059100
C	-1.74295300	-3.56044300	-0.07002700
H	-1.39143100	-4.59421300	0.01234200
H	-2.47544500	-3.38511500	0.71976000
H	-2.23691600	-3.44883400	-1.03772400
C	0.87887300	-3.14600500	-1.12983300
H	1.85771100	-2.67753800	-1.01998300
H	0.96293100	-4.22295500	-0.95027500
H	0.53705000	-2.98200600	-2.15374000
C	0.45115100	-2.99678600	1.68016400
H	0.48409900	-4.09106800	1.68589900
H	1.46802000	-2.61144900	1.77106400
H	-0.12632000	-2.66162400	2.54459300
C	5.43788300	1.44806800	-0.80220200
H	6.52855600	1.36697500	-0.85056800
H	5.04624300	1.51791700	-1.82127900
H	5.16863000	2.35871700	-0.25915600
C	5.43187100	-0.03508900	1.72765500
H	5.14482900	0.85968900	2.28667600
H	5.10963200	-0.92619300	2.27313500
H	6.52308800	-0.05573400	1.64594200
C	5.38963500	-1.47016400	-0.83008700
H	4.99835200	-1.50485600	-1.85118100
H	6.48256700	-1.42560000	-0.87525400
H	5.08863300	-2.38209500	-0.30620800
P	-2.28252300	0.13071900	1.83901200
P	-2.20269400	-0.19970200	-1.81055600

C	-3.86627000	1.07253100	1.61815100
H	-4.59830300	0.44736700	1.10211800
H	-4.28070900	1.32878600	2.59865200
H	-3.72775700	1.98980600	1.04683600
C	-2.98433100	-1.40466400	2.60567100
H	-2.19939300	-2.08739200	2.93923500
H	-3.59314000	-1.13310600	3.47455400
H	-3.62835000	-1.92786800	1.89379900
C	-1.58348300	0.94512200	3.35395200
H	-1.16252900	1.92740900	3.12350200
H	-2.37152300	1.07240700	4.10285900
H	-0.80138800	0.32753000	3.80806800
C	-3.87890900	-0.85810900	-1.38994300
H	-4.48224900	-0.07465300	-0.92685200
H	-4.38597800	-1.17407200	-2.30744600
H	-3.82343400	-1.71114700	-0.71118600
C	-2.67555200	1.29778600	-2.78345300
H	-3.02103300	2.10563100	-2.13408900
H	-1.82851600	1.64970800	-3.37656700
H	-3.48739100	1.03740900	-3.47040500
C	-1.70558700	-1.32400500	-3.19266200
H	-1.61977600	-2.35837900	-2.85345000
H	-2.46656300	-1.28458600	-3.97851900
H	-0.74825500	-1.02047100	-3.62206100

Ir.PMe₃ (triplet)

P	0.36001800	-2.41238000	0.20198000
N	-1.55154400	0.18592200	1.86112000
H	-1.49271000	0.29221600	2.87679100
P	0.35009900	2.42590700	0.05617800
C	-2.35463800	-0.10317400	-1.05163400
C	-2.78285600	0.15900700	1.47137600
C	-3.18668400	0.00906500	0.08941500
C	-0.95892600	-0.09804200	-1.21802800
H	-3.59728400	0.24489000	2.20465800
H	-0.73654200	-0.19859200	-2.28378600
H	-2.90287300	-0.19780800	-1.98923500
P	-4.98044000	-0.02030700	-0.15177800
Ir	0.66946900	0.00468000	-0.01516200
C	-0.28134300	-3.24173300	-1.32260300
H	0.42498000	-3.14536900	-2.15071100
H	-0.44435200	-4.30688400	-1.12864800
H	-1.22707700	-2.78528900	-1.62370200
C	-0.91490300	-2.92549400	1.43801300

H	-1.88570900	-2.51190900	1.16026600
H	-0.98304600	-4.01824900	1.46869600
H	-0.65541500	-2.55570700	2.43282700
C	1.74132800	-3.55581300	0.65826400
H	2.08316000	-3.36726100	1.67919500
H	1.38214000	-4.58910400	0.60806300
H	2.58553600	-3.45030000	-0.02633200
C	1.70818400	3.57275500	-0.45975300
H	1.41831600	4.60496700	-0.23655200
H	2.64738500	3.35585400	0.04966000
H	1.86601400	3.49243000	-1.53874200
C	-1.00316400	3.06935300	-1.02643500
H	-1.96278400	2.64449900	-0.72626300
H	-1.05298800	4.16039400	-0.94739200
H	-0.81561100	2.79962100	-2.06967400
C	-0.16063600	3.13564400	1.68813300
H	-0.26699700	4.22257000	1.60655500
H	-1.11812800	2.70218200	1.98241100
H	0.56785800	2.91480100	2.47098000
C	-5.43562400	-0.22546300	-1.90192200
H	-6.52832900	-0.24146500	-1.96996000
H	-5.06213400	0.60672500	-2.50473000
H	-5.04861700	-1.16749400	-2.29967300
C	-5.74867400	-1.39573700	0.77148900
H	-5.35335700	-2.34991800	0.41069200
H	-5.54080600	-1.30710800	1.84161600
H	-6.83352200	-1.37888300	0.62344900
C	-5.75213600	1.52932400	0.42987600
H	-5.35758400	2.37566900	-0.14018900
H	-6.83679300	1.47720500	0.28872000
H	-5.54516900	1.68918800	1.49190100
P	2.46498200	0.05850600	1.69690300
P	2.30034100	-0.07263400	-1.95816600
C	3.99392800	-0.96885700	1.48040900
H	4.56220900	-0.61676200	0.61470200
H	4.63019300	-0.87162500	2.36642100
H	3.76493700	-2.02383200	1.33453800
C	3.30142200	1.65255000	2.14171500
H	2.59005800	2.43098000	2.42200700
H	3.97334100	1.48294000	2.98945500
H	3.90121600	2.01172600	1.30073600
C	1.86107300	-0.49118700	3.35802200
H	1.46220600	-1.50819900	3.30583100
H	2.66908800	-0.46906800	4.09676500

H	1.05933600	0.17306200	3.69416100
C	3.76896500	1.06173800	-1.96682600
H	4.37534300	0.91753600	-1.06809700
H	4.39702500	0.85751200	-2.84091800
H	3.45678400	2.10645100	-2.00479000
C	3.16145900	-1.67314400	-2.33560200
H	3.80631400	-1.96271600	-1.50082400
H	2.44296500	-2.47674600	-2.51466500
H	3.78525000	-1.56702900	-3.23000000
C	1.55592500	0.31684400	-3.61066200
H	1.07207500	1.29841400	-3.59263300
H	2.32869300	0.32331000	-4.38662600
H	0.80591800	-0.43185700	-3.88356300