

Penta- *versus* hexa-coordinated iridium catalysts control the reactivity of the direct reductive amination between both aliphatic amines and ketones: a DFT-guided mechanism

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1. Computational methods and results.

Table S1. The computed potential energies (E , a.u.) and relative potential energies (ΔE , kcal/mol) at the ω B97X-D/BS-II level. The relative Gibbs energies (ΔG ; at 298.15 K and 1 atm) are in kcal/mol.

Complex	E	ΔE	G	ΔG
A1	-908.1088	0.0	-2437.2736	0.0
A2	-1434.9651	-18.2	-1434.6103	7.1
A3	-1434.9913	-34.7	-1434.6276	-3.8
A4	-908.1275	-11.7	-907.7958	4.6
3'	-832.1452	-26.4	-831.8255	-23.5
3''	-831.6687	-4.1	-831.3633	-1.7
TS _{A2-A3}	-1434.9596	-14.8	-1434.6030	11.6
TS _{A4-3'}	-1434.9646	-17.9	-1434.6067	9.3
B1	-2694.7487	-26.4	-2694.0908	-23.5
B2	-2694.0174	-36.8	-2693.3717	-36.5
B3	-2695.1963	-38.8	-2694.5311	-25.3
TS _{B1-B2}	-3526.8849	-20.8	-3525.8855	-4.2
TS _{B3-B1'}	-3221.5838	-39.5	-3220.9043	-14.3
C1	-3221.1436	-31.8	-3220.4748	-19.3
C2	-3220.4204	-47.3	-3219.7549	-31.7
C3	-3221.5981	-48.5	-3220.9145	-20.7
TS _{C1-C2}	-4053.2712	-20.7	-4052.2530	10.4
TS _{C3-B1}	-3221.5851	-40.3	-3220.9056	-15.1
D1	-2695.9244	-26.3	-2695.2518	-13.3
D2	-3222.3201	-32.2	-3221.6349	-4.2
D3	-3222.2967	-17.5	-3221.6088	7.9
D4	-2695.4453	-2.3	-2694.7867	10.2
TS _{D2-D3}	-3222.2946	-16.4	-3221.6108	6.6
TS _{D4-B1}	-3527.5825	2.7	-3526.5777	31.9
E1	-2829.2880	-26.4	-2828.7378	-23.5
E2	-2828.5392	-25.9	-2827.9929	-20.3
E3	-2829.7171	-27.2	-2829.1545	-10.5
TS _{E1-E2}	-3661.4142	-14.5	-3660.5178	5.0
TS _{E3-E1}	-3356.1098	-31.2	-3355.5341	-3.5
F1	-3355.6946	-39.1	-3355.1248	-21.1
F2	-3354.9378	-33.6	-3354.3738	-14.1
F3	-3356.1398	-50.0	-3355.5557	-17.0
TS _{F1-F2}	-4187.8254	-30.1	-4186.9105	3.9
TS _{F3-E1}	-3356.1240	-40.1	-3355.5446	-10.1
E2c	-2830.4613	-24.8	-2829.8945	-10.6
E3c	-3356.8596	-32.3	-3356.2750	-4.2
E4c	-3356.8379	-18.7	-3356.2535	9.4
E5c	-2829.9828	-1.2	-2829.4284	13.6
TS _{E2c-E3c}	-3356.8363	-17.7	-3356.2550	8.4
TS _{E5c-E1}	-3662.1299	-2.4	-3661.2277	30.1
G1	-2623.4030	-26.4	-2622.6682	-23.5
G2	-2622.6690	-35.2	-2621.9343	-27.2
G3	-2623.8494	-38.0	-2623.0998	-19.8
TS _{G1-G2}	-3455.5331	-16.9	-3454.4496	4.2
TS _{G3-G1}	-3150.2395	-40.4	-3149.4746	-9.8
H1	-3149.7954	-30.2	-3149.0415	-12.6
H2	-3149.0538	-34.2	-3148.3026	-13.1
H3	-3150.2500	-47.0	-3149.4827	-14.9
TS _{H1-H2}	-3981.9223	-18.8	-3980.8175	18.6
TS _{H3-G1}	-3150.2388	-39.9	-3149.4746	-9.8
G2c	-2624.5838	-29.5	-2623.8321	-15.1
G3c	-3150.9796	-35.5	-3150.2114	-7.9
G4c	-3150.9567	-21.1	-3150.1843	9.1
G5c	-2624.1034	-4.7	-2623.3614	12.0
TS _{G2c-G3c}	-3150.9552	-20.1	-3150.1882	6.6
TS _{G5c-G1}	-3456.2416	-0.3	-3455.1555	31.7
I1	-2483.4123	-26.4	-2482.9369	-23.5
I2	-2482.6713	-30.8	-2482.2008	-25.8
I3	-2483.8542	-35.2	-2483.3651	-17.7

TS_{I1-I2}	-3315.5640	-30.5	-3314.7363	-7.1
TS_{I3-I1}	-3010.2437	-37.2	-3009.7384	-6.8
J1	-3009.8152	-36.8	-3009.3181	-17.5
J2	-3009.0855	-48.2	-3008.5952	-28.1
J3	-3010.2648	-50.4	-3009.7549	-17.1
TS_{J1-J2}	-3841.9700	-42.8	-3841.1222	-4.1
TS_{J3-I1}	-3010.2527	-42.8	-3009.7472	-12.3
I2c	-2484.5960	-31.3	-2484.1026	-16.2
I3c	-3010.9919	-37.3	-3010.4818	-9.0
I4c	-3010.9781	-28.7	-3010.4648	1.7
I5c	-2484.1242	-11.9	-2483.6412	5.0
TS_{I2c-I3c}	-3010.9734	-25.7	-3010.4638	2.3
TS_{I5c-I1}	-3316.2798	-18.4	-3315.4483	16.5
A3'	-908.5816	-20.0	-908.2316	-0.5
TS_{A3'-3'}	-908.5180	19.8	-908.1749	35.0
TS_{A3*-3'}	-1435.3810	-2.6	-1435.0044	28.1

Table S2. The imaginary frequencies (in cm^{-1}) of transition states at the $\omega\text{B97X-D/BS-I}$ level.

Complex	Imaginary frequencies (in cm^{-1})
TS _{A2-A3}	100.6 <i>i</i>
TS _{A4-3'}	280.6 <i>i</i>
TS _{B1-B2}	980.2 <i>i</i>
TS _{B3-B1}	1105.2 <i>i</i>
TS _{C2-C3}	1036.2 <i>i</i>
TS _{C4-C1}	1052.6 <i>i</i>
TS _{D3-D4}	1138.4 <i>i</i>
TS _{D5-D1}	1076.8 <i>i</i>
TS _{E1-E2}	782.5 <i>i</i>
TS _{E3-E1}	1063.6 <i>i</i>
TS _{F1-F2}	-831.5 <i>i</i>
TS _{F3-E1}	1296.8 <i>i</i>
TS _{E3c-E4c}	1149.2 <i>i</i>
TS _{E5c-E1}	735.6 <i>i</i>
TS _{G1-G2}	1081.1 <i>i</i>
TS _{G3-G1}	1131.5 <i>i</i>
TS _{H1-H2}	1084.4 <i>i</i>
TS _{H3-G1}	1003.4 <i>i</i>
TS _{G3c-G4c}	1157.6 <i>i</i>
TS _{G5c-G1}	837.4 <i>i</i>
TS _{I1-I2}	585.6 <i>i</i>
TS _{I3-I1}	883.9 <i>i</i>
TS _{J1-J2}	869.2 <i>i</i>
TS _{J3-I1}	1231.2 <i>i</i>
TS _{I3c-I4c}	1266.7 <i>i</i>
TS _{I5c-I1}	633.7 <i>i</i>
TS _{A3'-3'}	285.4 <i>i</i>
TS _{A3*-3'}	1554.0 <i>i</i>

2. Additional figures.

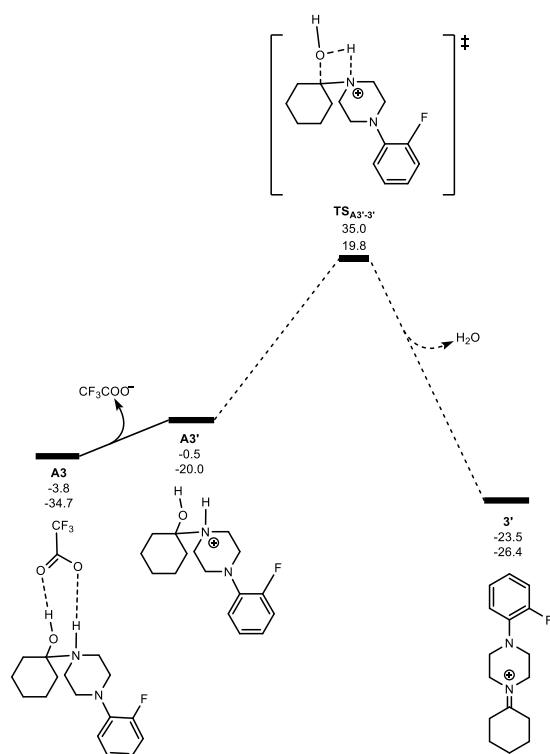


Fig. S1. Alternative formation of iminium **3'** without involving TFA in the transition state.

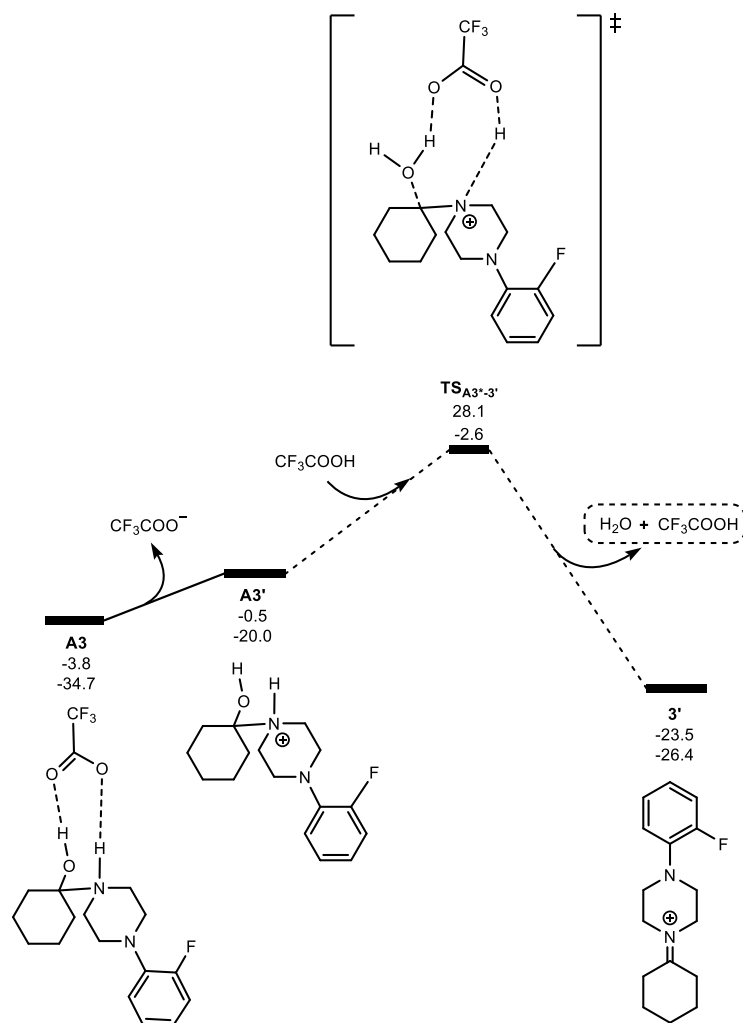


Fig. S2. Alternative formation of iminium **3'** involving a cationic, protonated aminoalcohol.

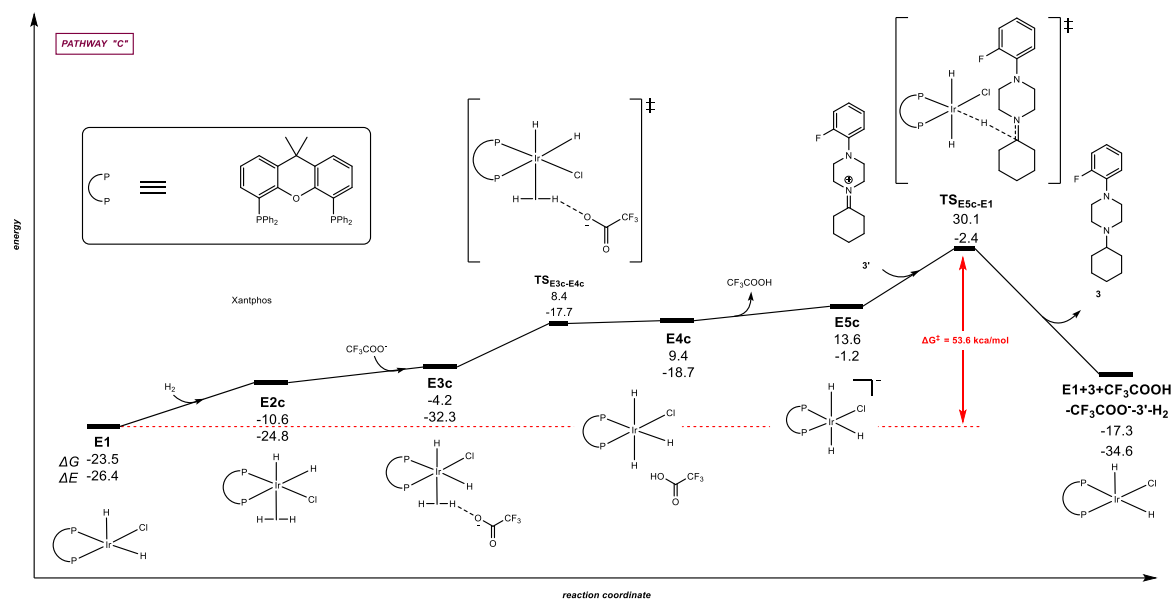


Fig. S3. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **E2c** with initial H₂ activation. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand Xantphos.

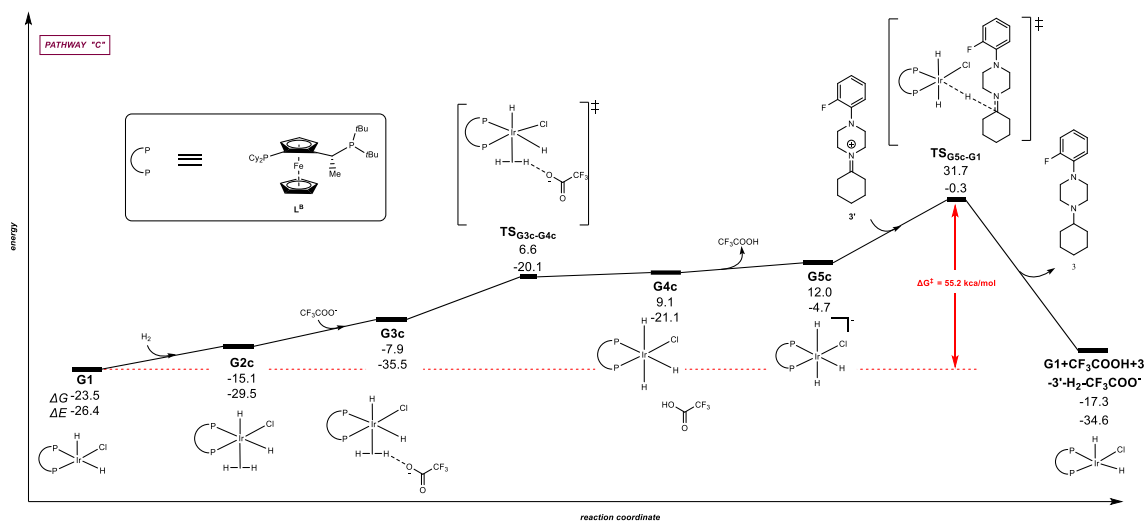


Fig. S4. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **G2c** with initial H₂ activation. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^B**.

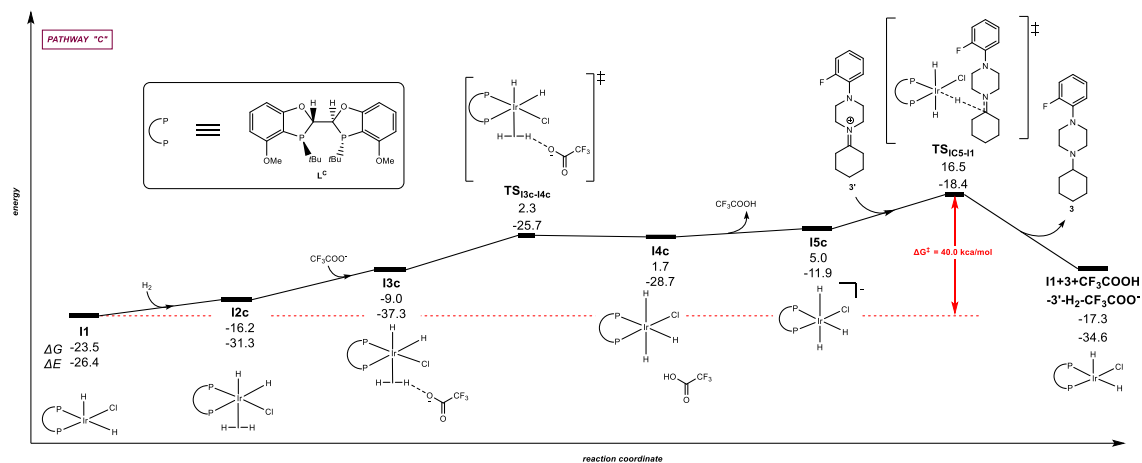


Fig. S5. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **I2c** with initial H₂ activation. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand L^c.

3. The formation of the associated complexes between the methanol solvent molecule and TFA derivatives

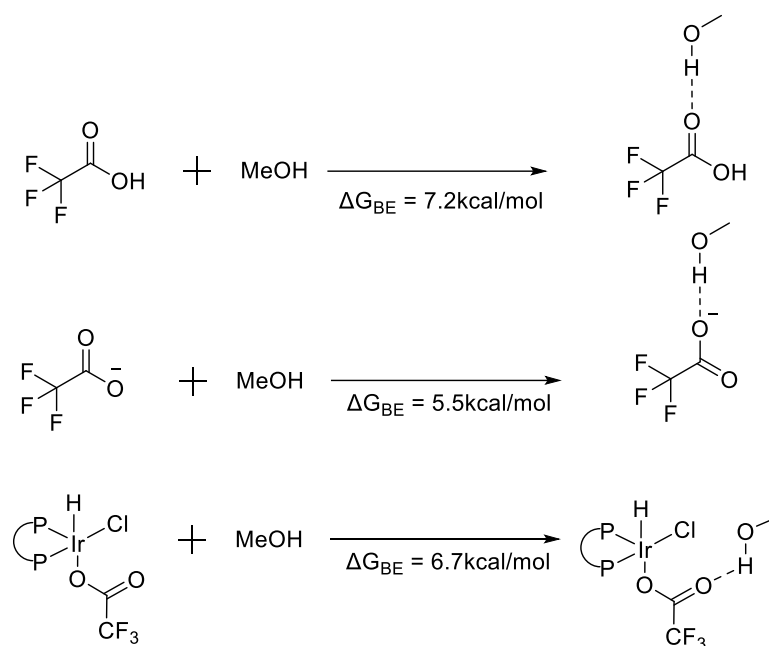


Fig. S6. The formation of the associated complexes between the methanol solvent molecule and TFA derivatives (CF_3COOH , CF_3COO^- , TFA-derived metal complex). The binding free energies (ΔG_{BE}) were computed at (SMD: methanol) $\omega\text{B97X-D}/6-311++\text{G}(2\text{d}, \text{p})/\text{SDD}(\text{Ir}, \text{Fe})//\omega\text{B97X-D}/6-311\text{G}(\text{d}, \text{p})/\text{SDD}(\text{Ir}, \text{Fe})$ level.

The formation of the hydrogen-bond complexes between the methanol solvent molecule and TFA derivatives (CF_3COOH , CF_3COO^- , TFA-derived metal complex) are endothermic reactions, suggesting TFA derivatives can not form associated complexes. The addition of solvent molecules could cause to estimate the energy wrongly.

4. The pathway computed at ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

The geometric structures in methanol solution were optimized using def2-SVP basis sets, and the def2-TZVPP basis sets were further used for single point energy refinements. The refined energies were then corrected to Gibbs energies at 298.15 K and 1 atm by using the ω B97X-D/def2-SVP harmonic frequencies. The solvent effect was evaluated using SMD (density-based solution model) solvation model.

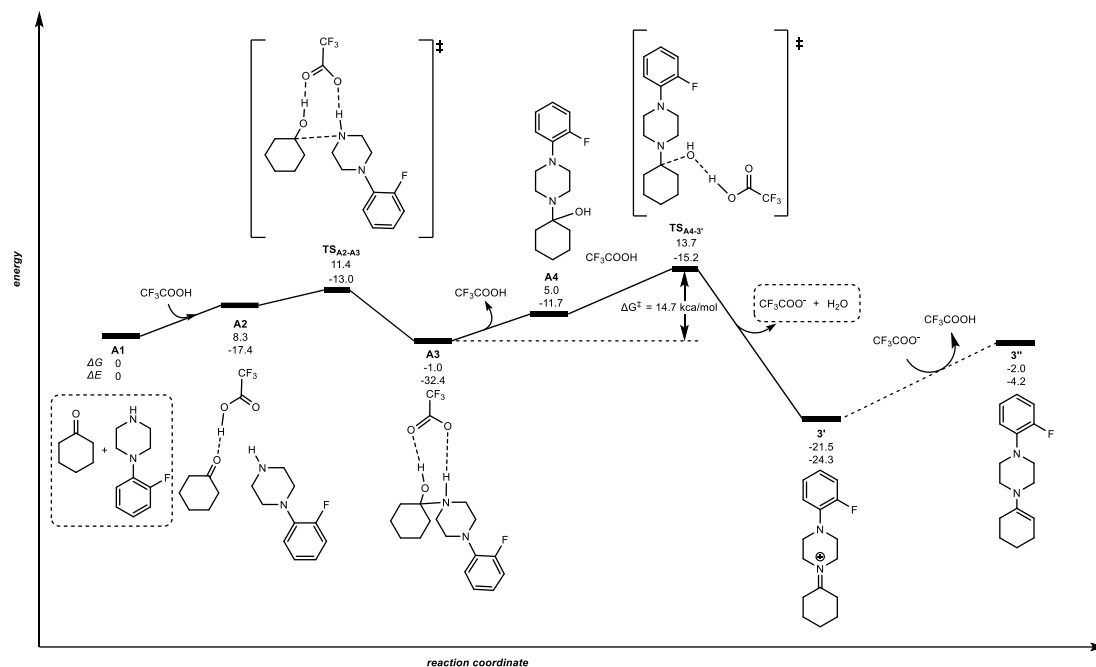


Fig. S7. Reaction coordinate for the TFA-mediated condensation of ketone **1** and amine **2**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP // ω B97X-D/def2-SVP.

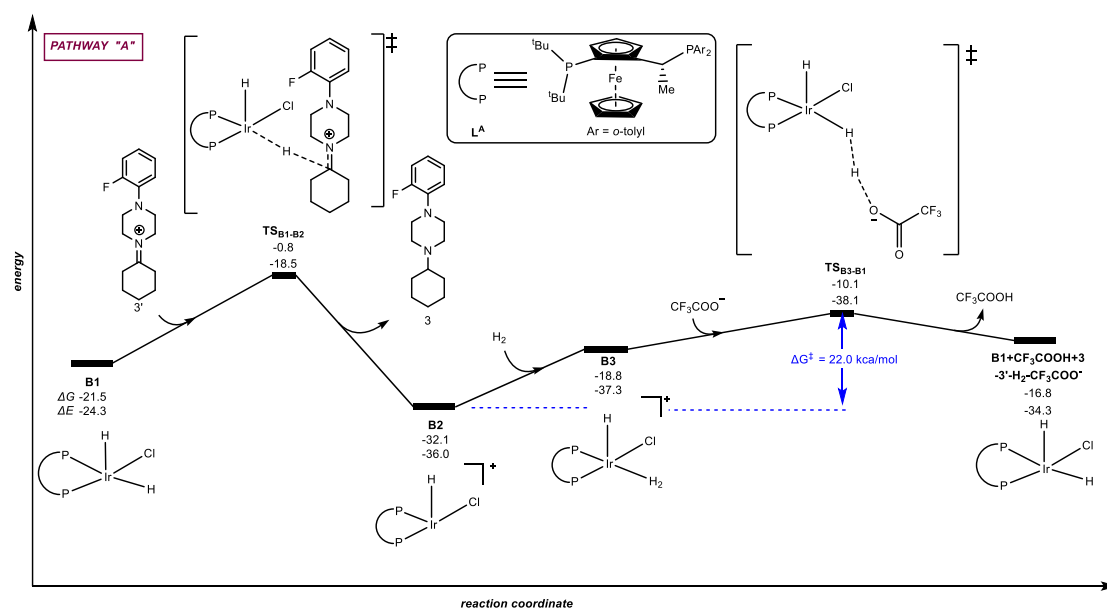


Fig. S8. Pathway "A": reaction coordinate for the hydride/hydrogen transfer pathway occurring in a penta-coordinated iridium complex **B1**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^A**. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP // ω B97X-D/def2-SVP.

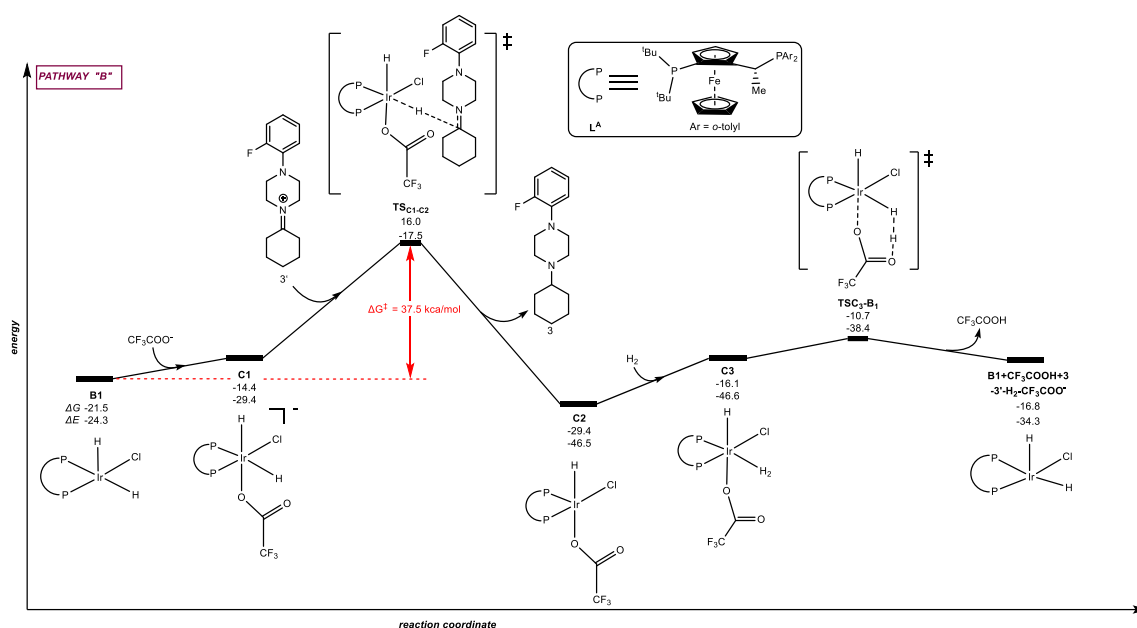


Fig. S9. Pathway "B": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **C1**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^A**. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP // ω B97X-D/def2-SVP.

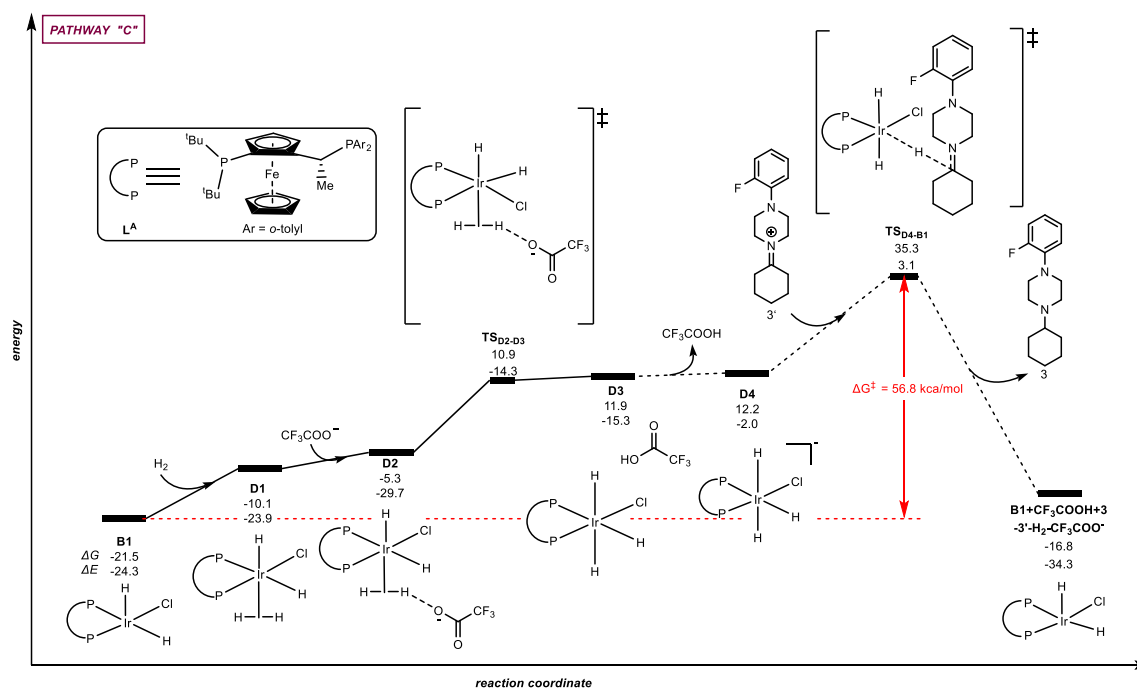


Fig. S10. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **D1** with initial H₂ activation. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^A**. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP // ω B97X-D/def2-SVP.

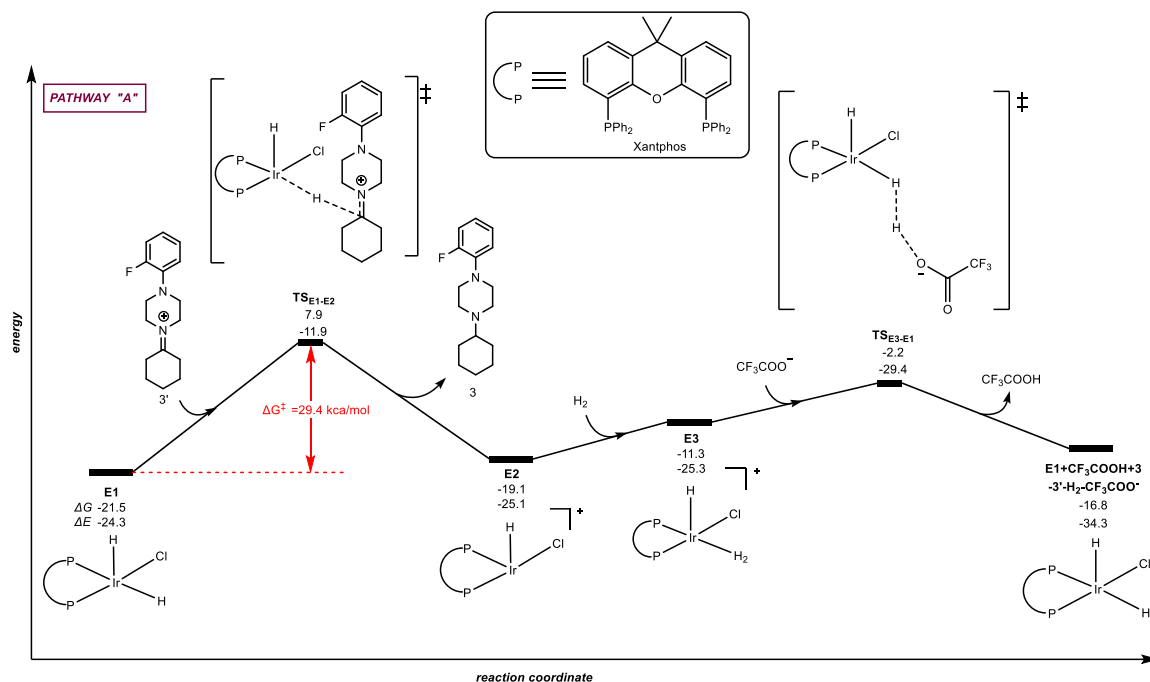


Fig. S11. Pathway "A": reaction coordinate for the hydride/hydrogen transfer pathway occurring in a penta-coordinated iridium complex **E1**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand Xantphos. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

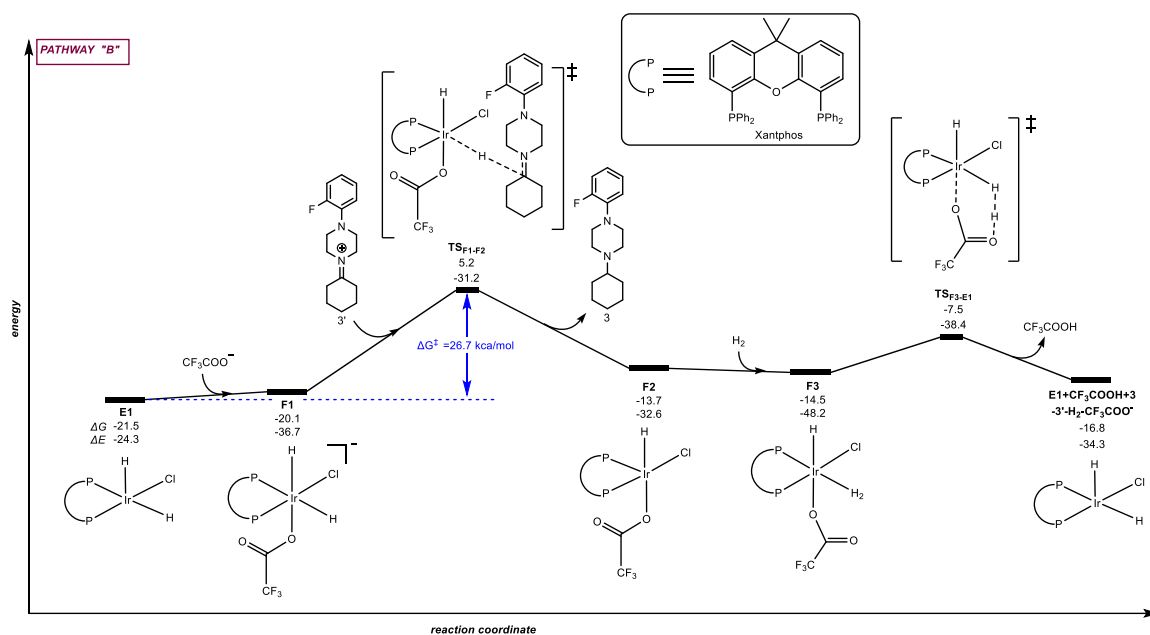


Fig. S12. Pathway "B": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **F1**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand Xantphos. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

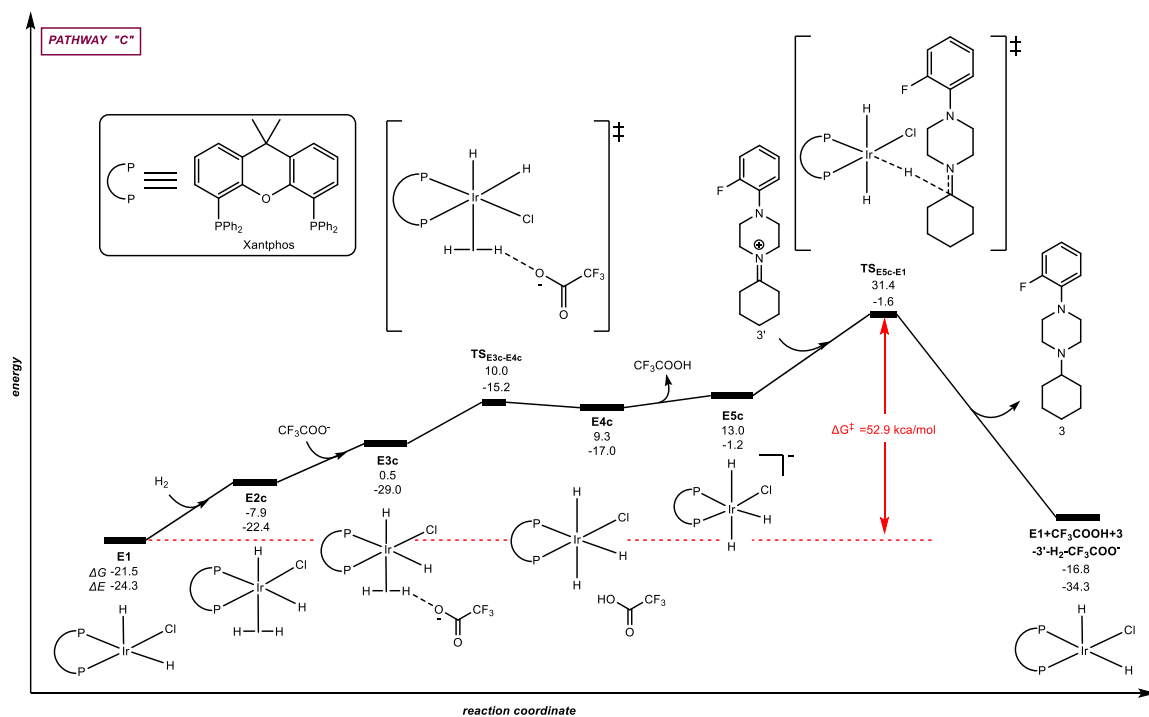


Fig. S13. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **E2c** with initial H_2 activation. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand Xantphos. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

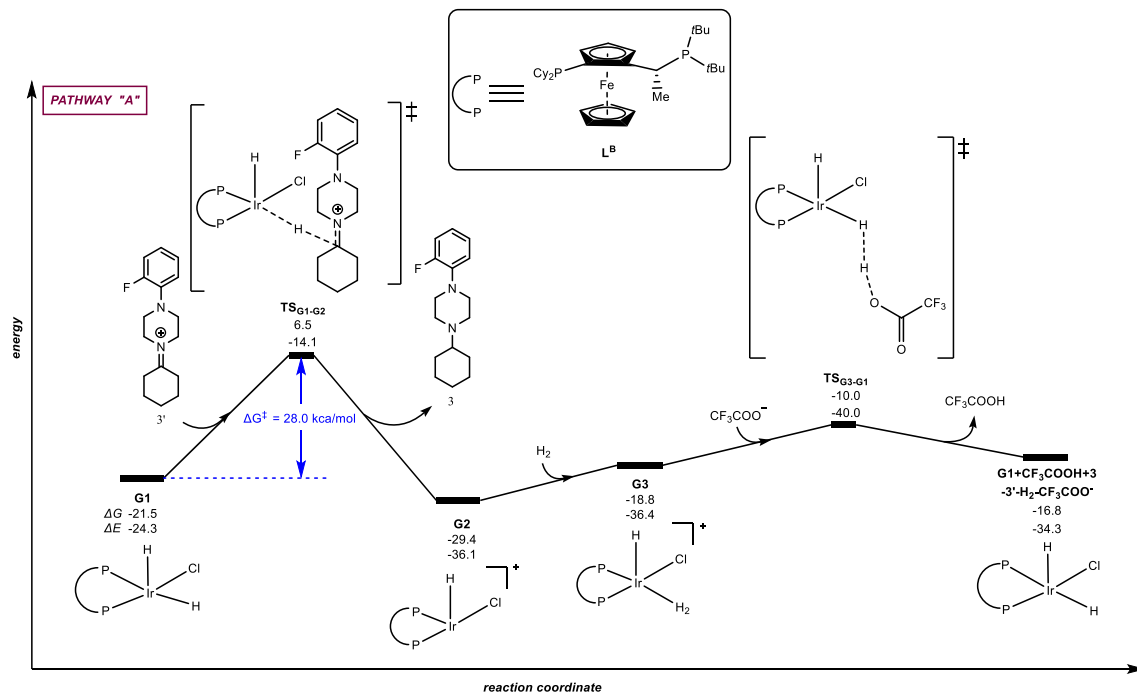


Fig. S14. Pathway "A": reaction coordinate for the hydride/hydrogen transfer pathway occurring in a penta-coordinated iridium complex **G1**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand L^{B} . Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

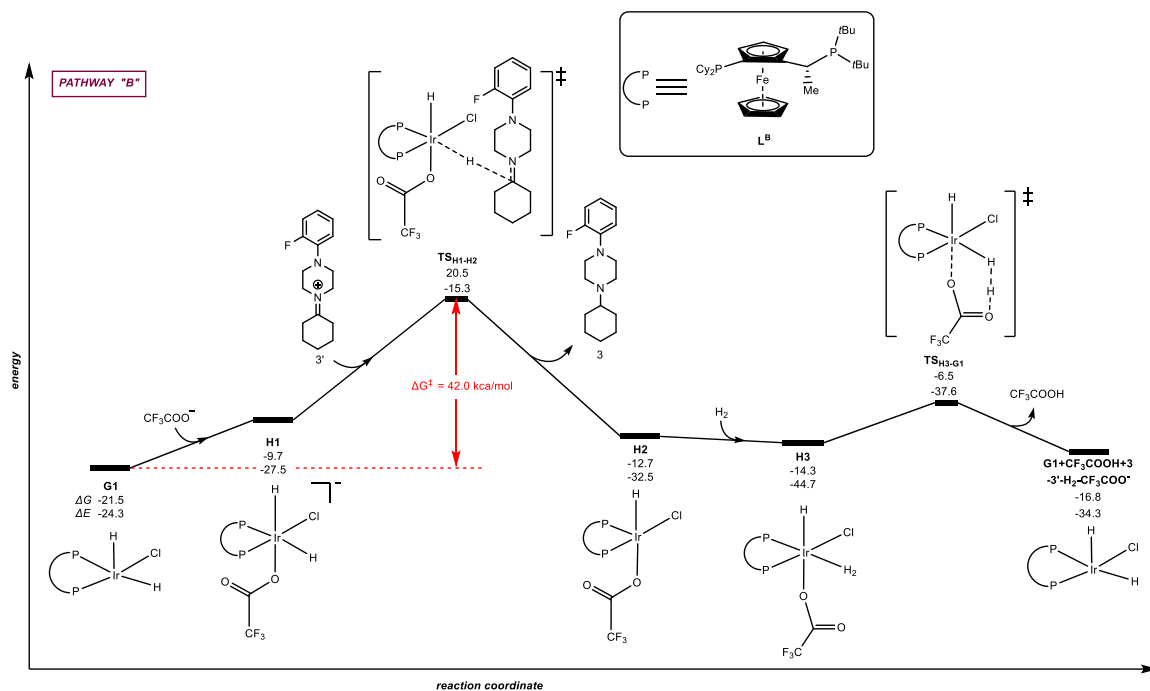


Fig. S15. Pathway "B": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **H1**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^B**. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

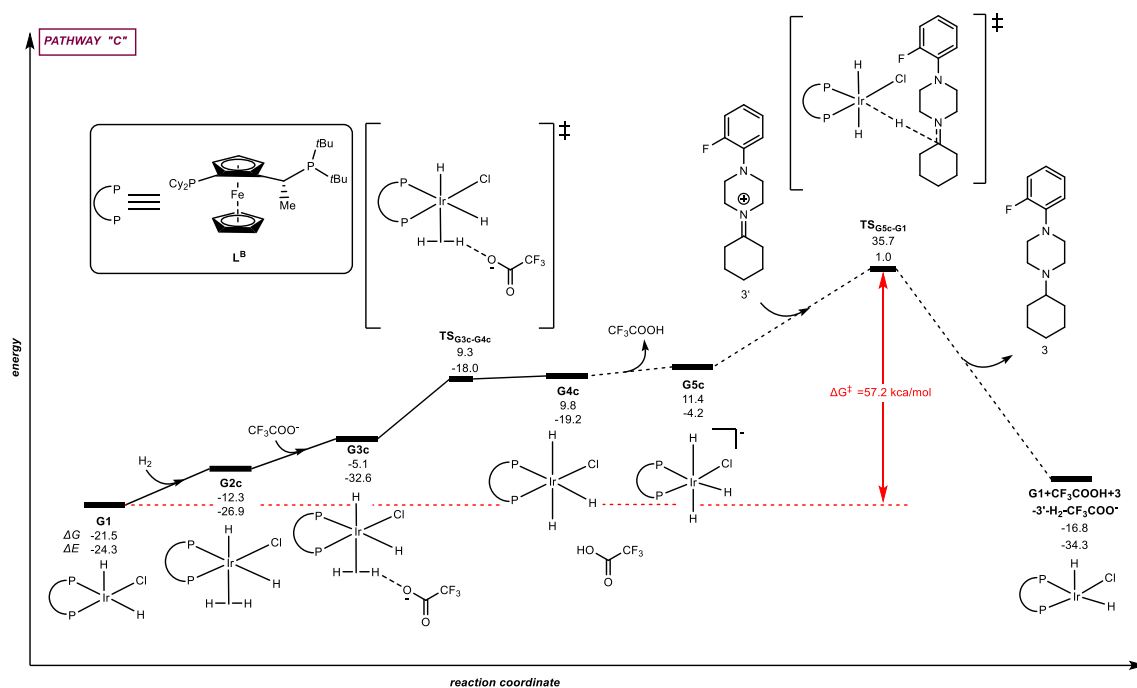


Fig. S16. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **G2c** with initial H₂ activation. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^B**. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

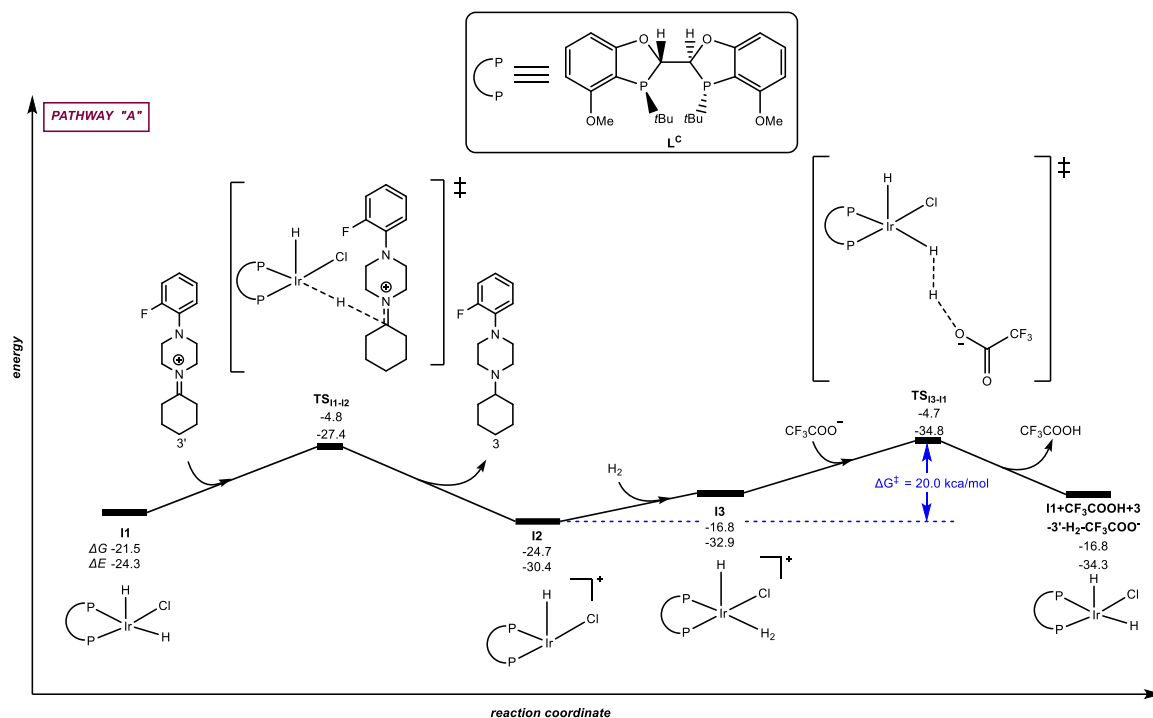


Fig. S17. Pathway "A": reaction coordinate for the hydride/hydrogen transfer pathway occurring in a penta-coordinated iridium complex **I1**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^c**. Computational method: (SMD:methanol) ω B97X-D/def2-TZVP// ω B97X-D/def2-SVP.

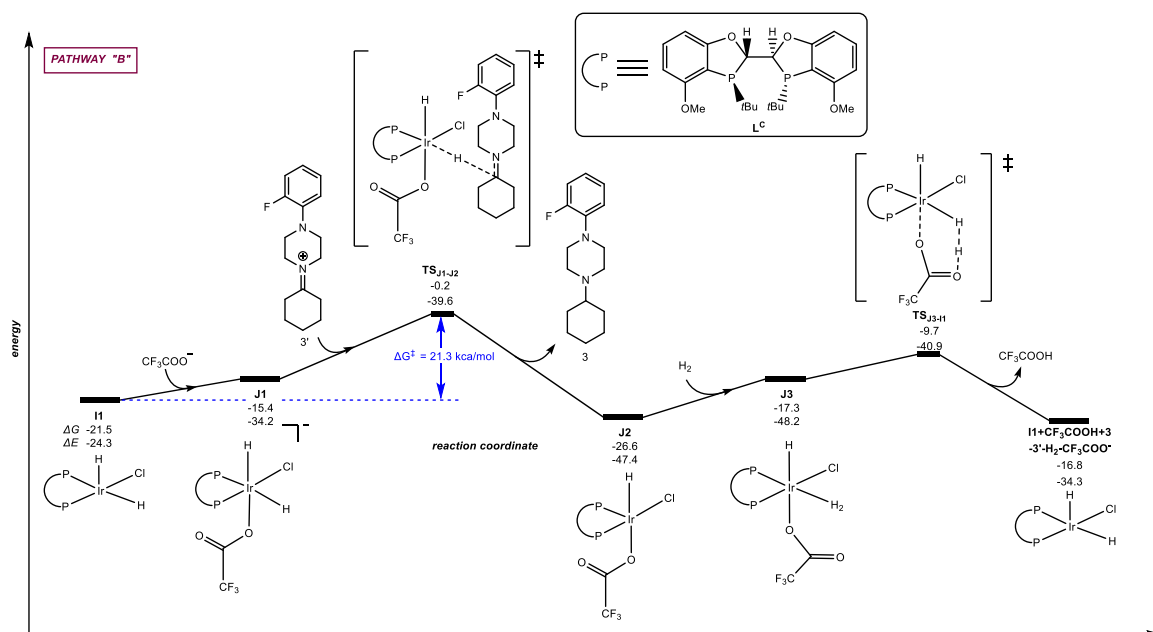


Fig. S18. Pathway "B": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **J1**. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^c**. Computational method: (SMD:methanol) ω B97X-D/def2-TZVP// ω B97X-D/def2-SVP.

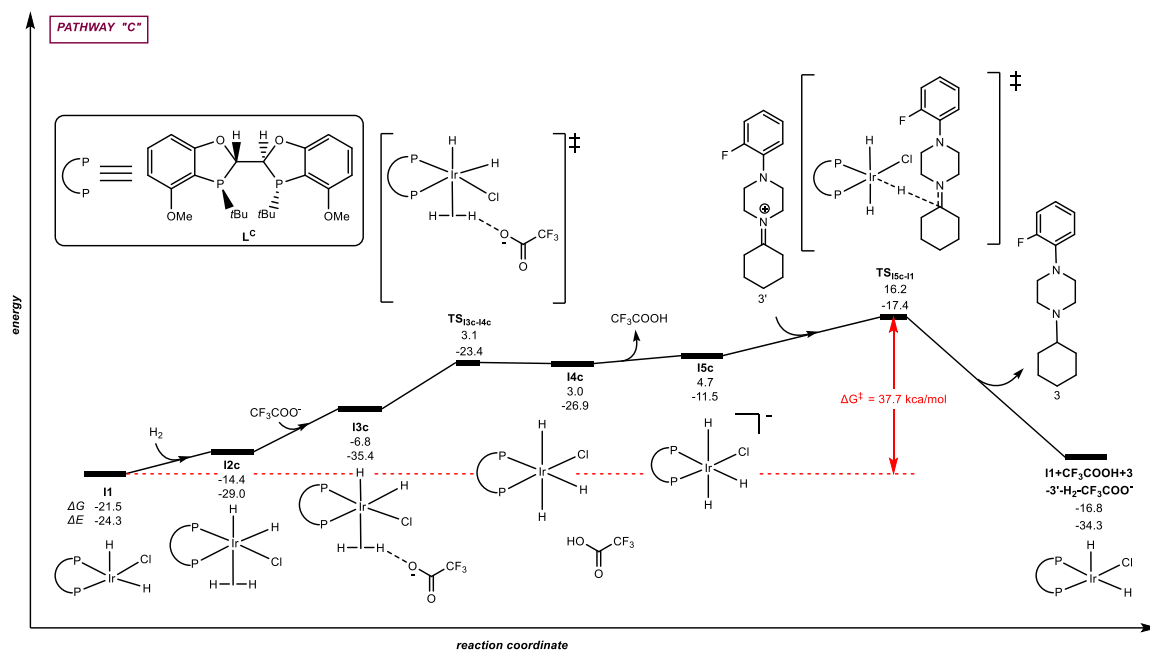


Fig. S19. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **I2c** with initial H_2 activation. The relative Gibbs free energy (ΔG) and potential energy (ΔE) are reported in kcal/mol. P-P: diphosphane ligand **L^c**. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

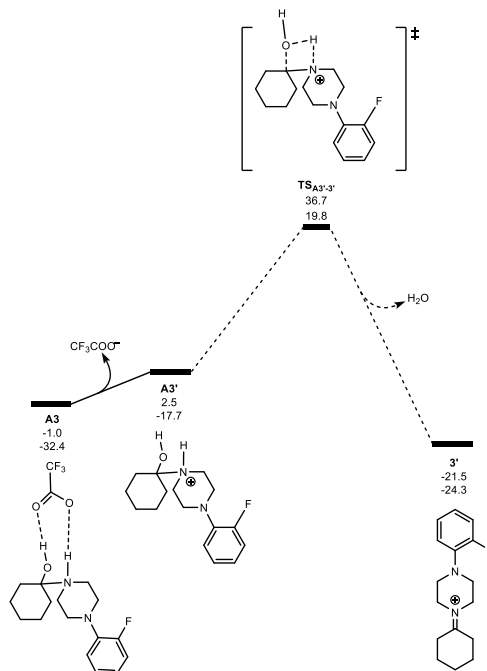


Fig. S20. Alternative formation of iminium **3'** without involving TFA in the transition state. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

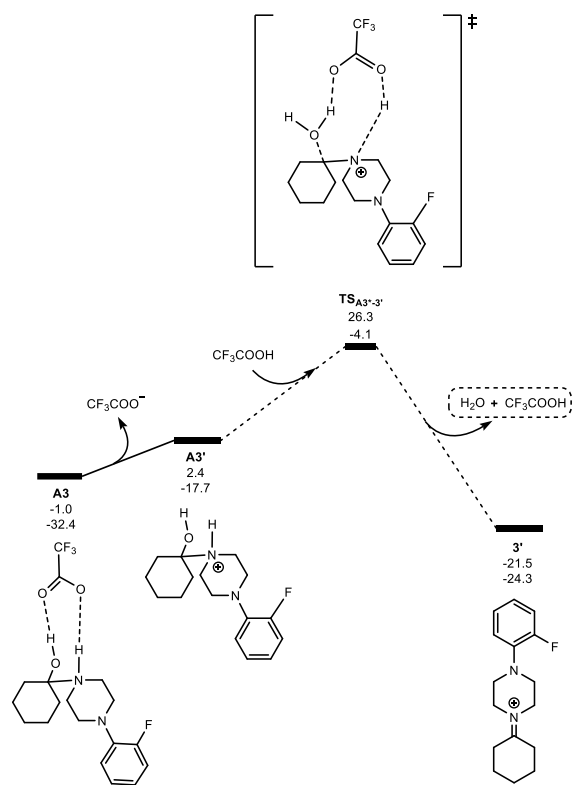


Fig. S21 Alternative formation of iminium **3'** involving a cationic, protonated aminoalcohol. Computational method: (SMD:methanol) ω B97X-D/def2-TZVPP// ω B97X-D/def2-SVP.

4. The pathway computed at 298.15 K and 50 atm

The geometric structures in methanol solution were optimized using BS-I base sets, in which 6-311G(d, p) basis sets were used for non-metallic atoms, and SDD basis sets with effective core potential were used for the iridium and Fe atoms. The BS-II basis sets were further used for single point energy optimization, in which 6-311++G(2d, p) basis sets were used for non-metallic atoms, and SDD basis sets with effective core potential were used for the iridium and Fe atoms. The contribution of thermal corrections and entropy to Gibbs free energies were obtained by using ω B97X-D/BS-I methods. The refined energies were then corrected to Gibbs energies at 298.15 K and 50 atm by using the ω B97X-D/BS-I harmonic frequencies.

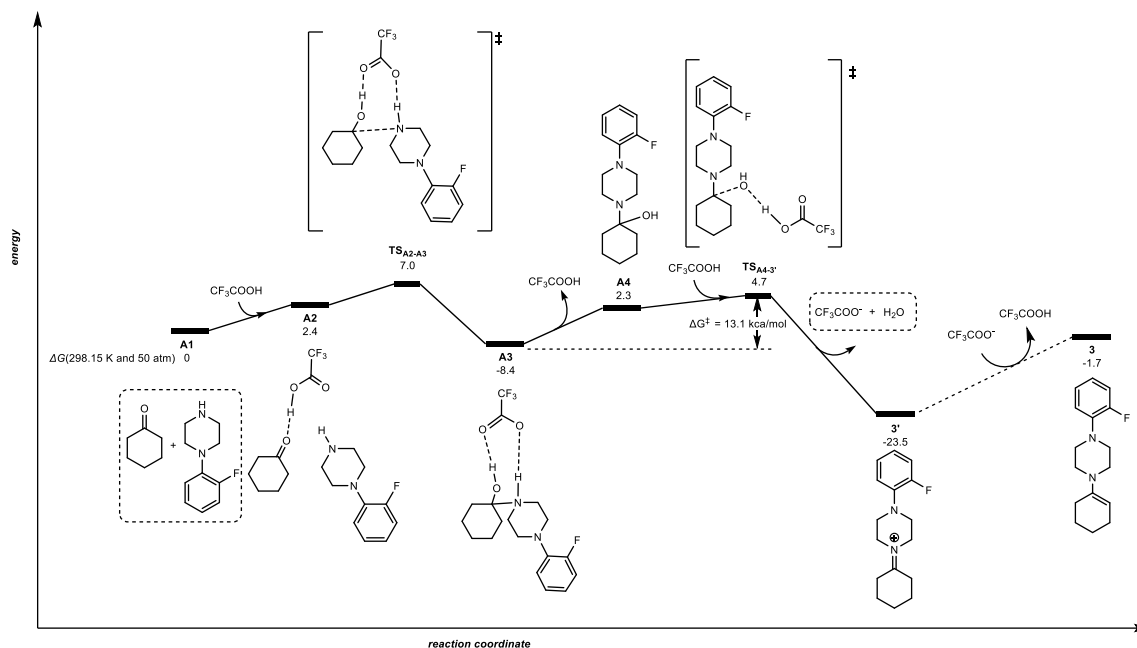


Fig. S22. Reaction pathway for the TFA-mediated condensation of ketone **1** and amine **2**. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm.

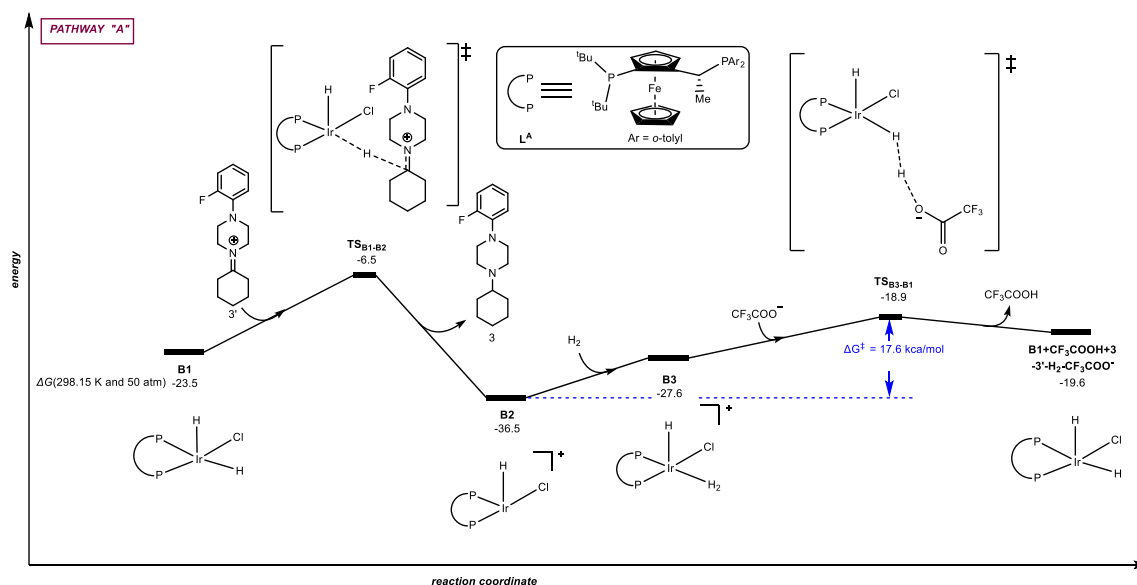


Fig. S23. Pathway "A": reaction coordinate for the hydride/hydrogen transfer pathway occurring in a penta-coordinated iridium complex **B1**. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand L^A .

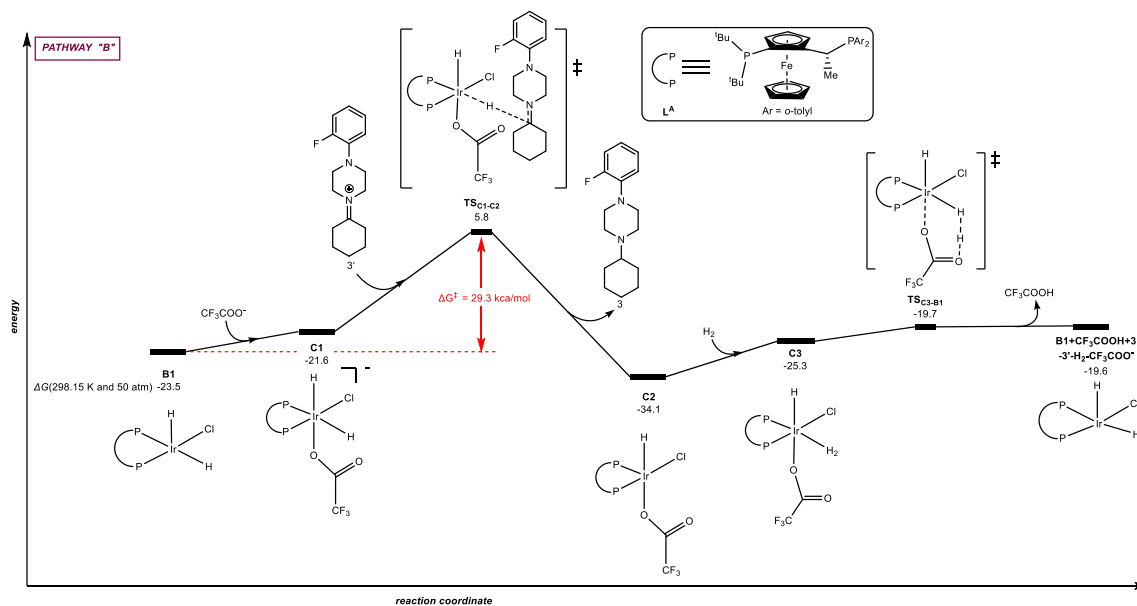


Fig. S24. Pathway “B”: reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **C1**. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand L^A .

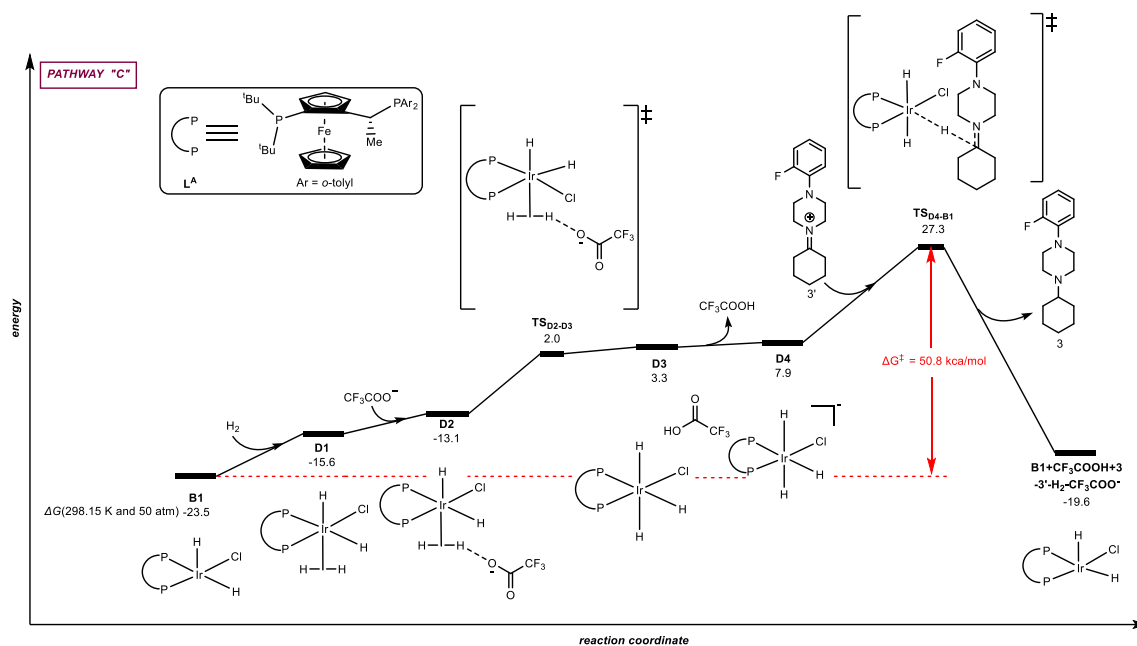


Fig. S25. Pathway “C”: reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **D1** with initial H_2 activation. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand L^A .

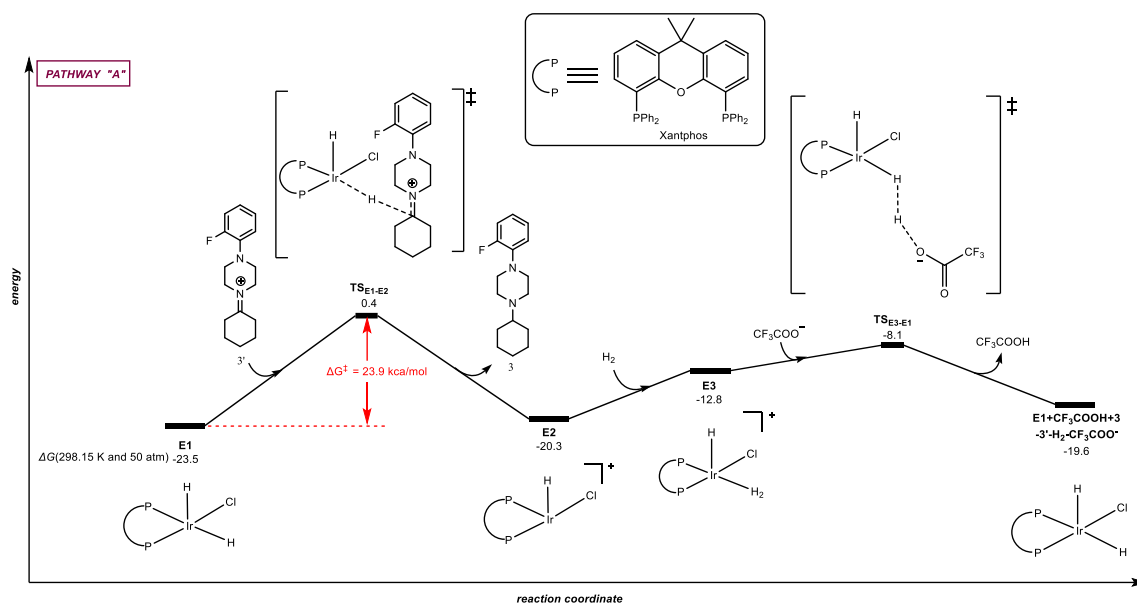


Fig. S26. Pathway "A": reaction coordinate for the hydride/hydrogen transfer pathway occurring in a penta-coordinated iridium complex E1. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand Xantphos.

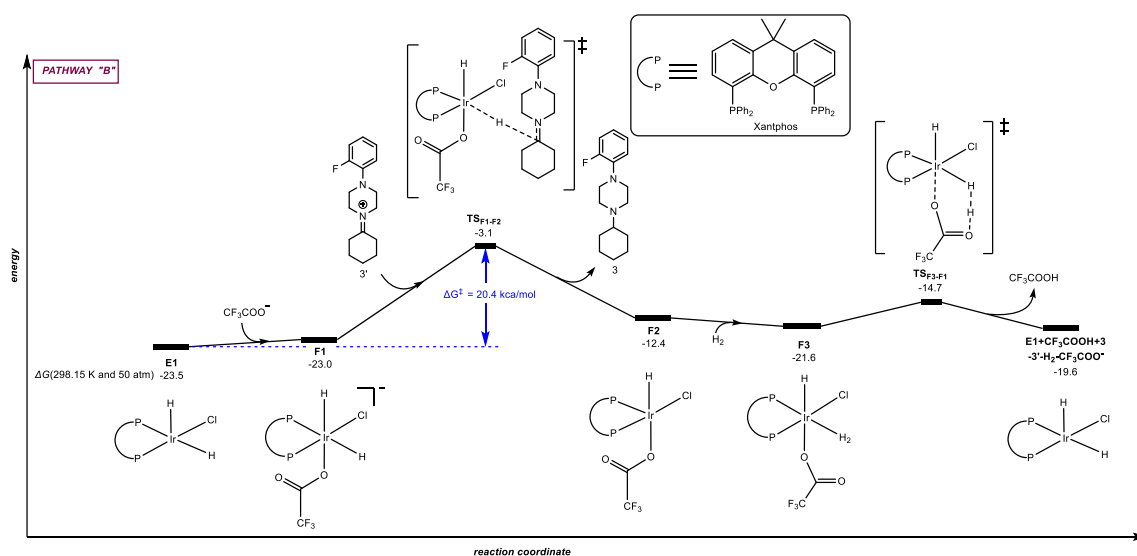


Fig. S27. Pathway "B": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex F1. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand Xantphos.

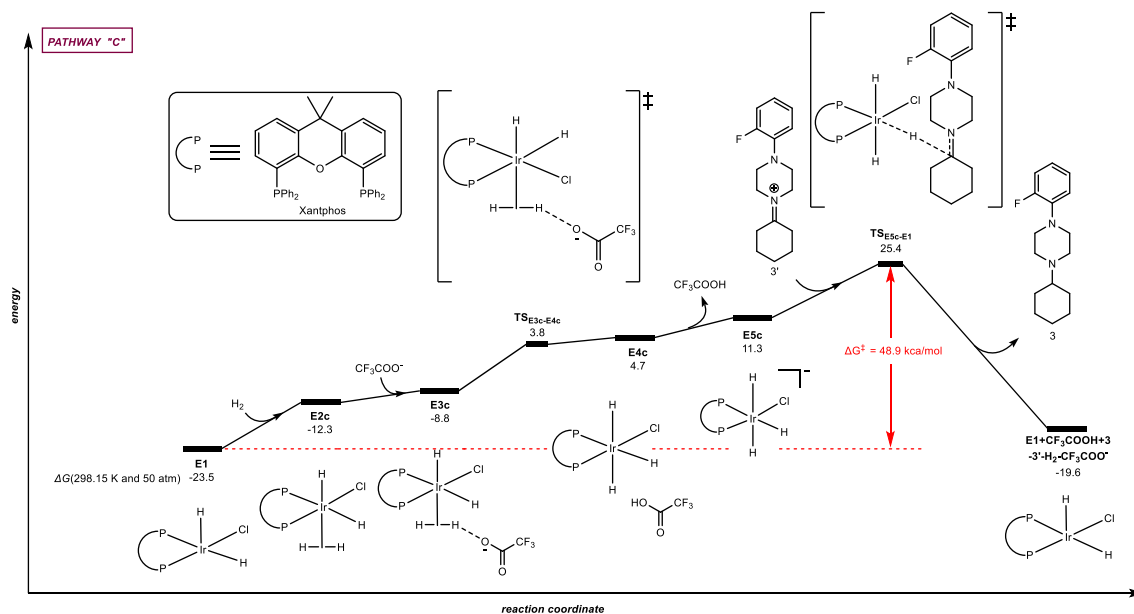


Fig. S28. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **E2c** with initial H_2 activation. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand Xantphos.

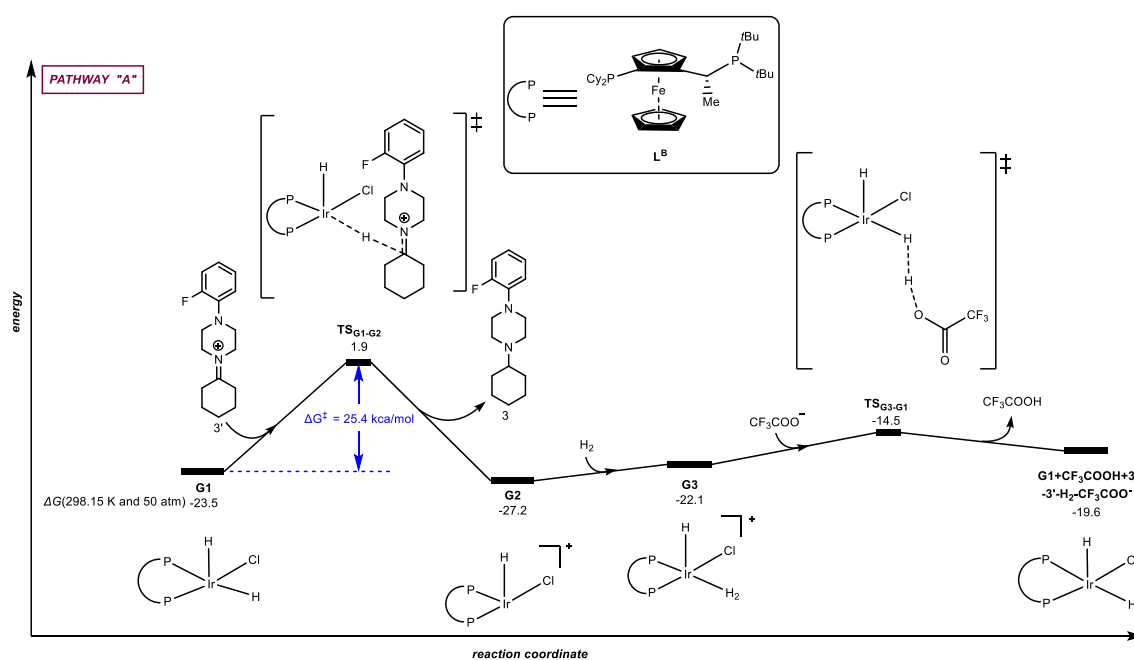


Fig. S29. Pathway "A": reaction coordinate for the hydride/hydrogen transfer pathway occurring in a penta-coordinated iridium complex **G1**. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand **L^B**.

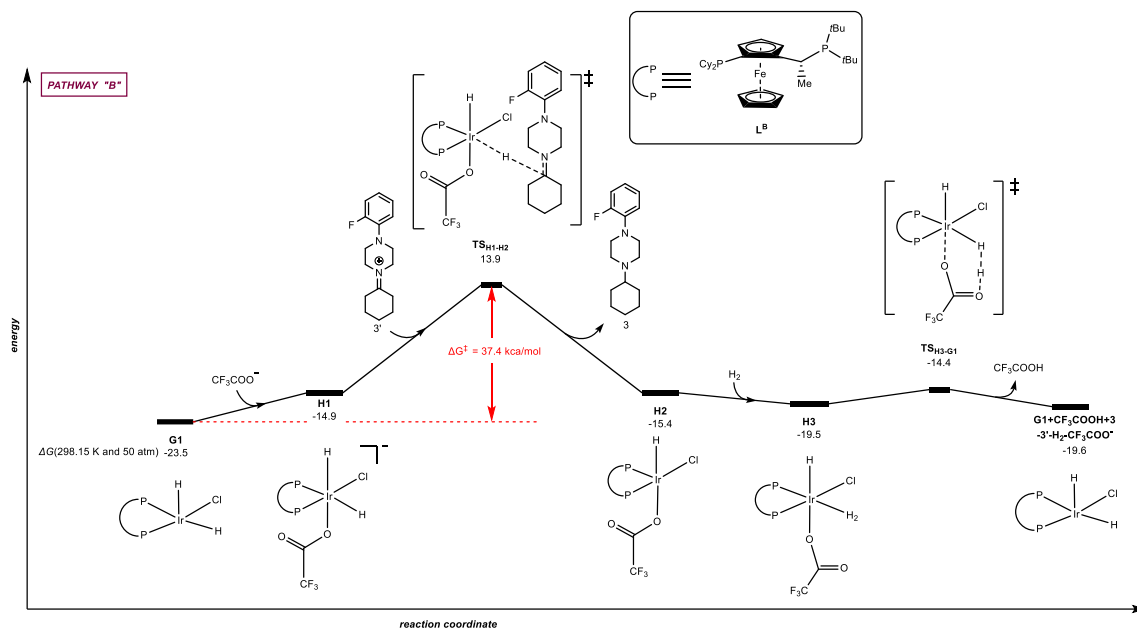


Fig. S30. Pathway “B”: reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **H1**. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand **L^B**.

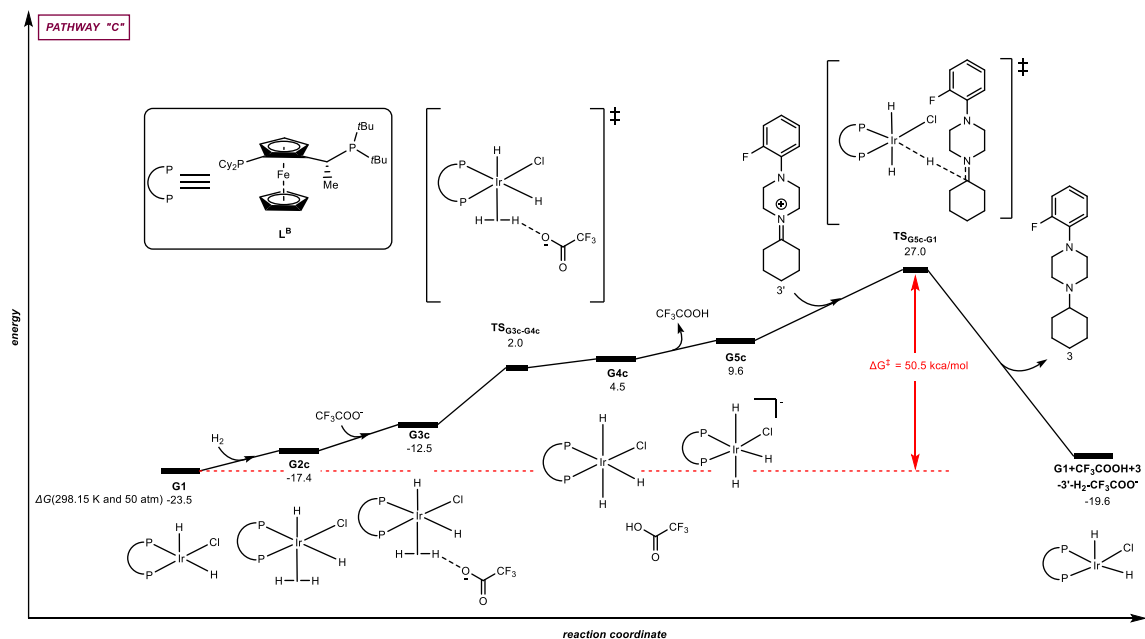


Fig. S31. Pathway “C”: reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **G2c** with initial H_2 activation. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand **L^B**.

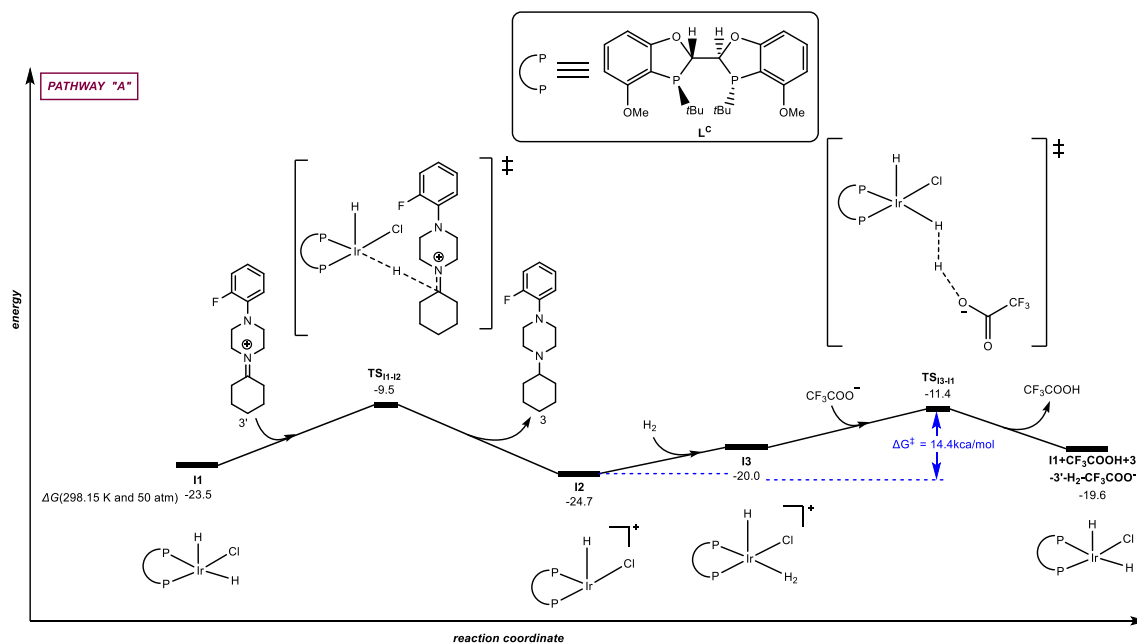


Fig. S32. Pathway "A": reaction coordinate for the hydride/hydrogen transfer pathway occurring in a penta-coordinated iridium complex **I1**. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand **L^C**.

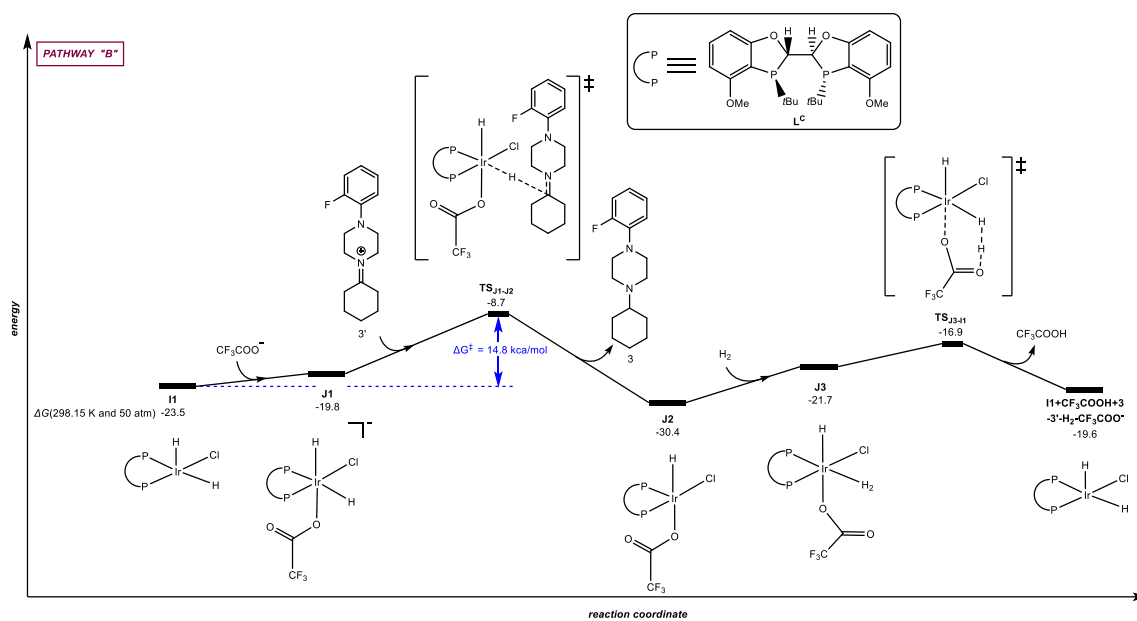


Fig. S33. Pathway "B": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **J1**. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand **L^C**.

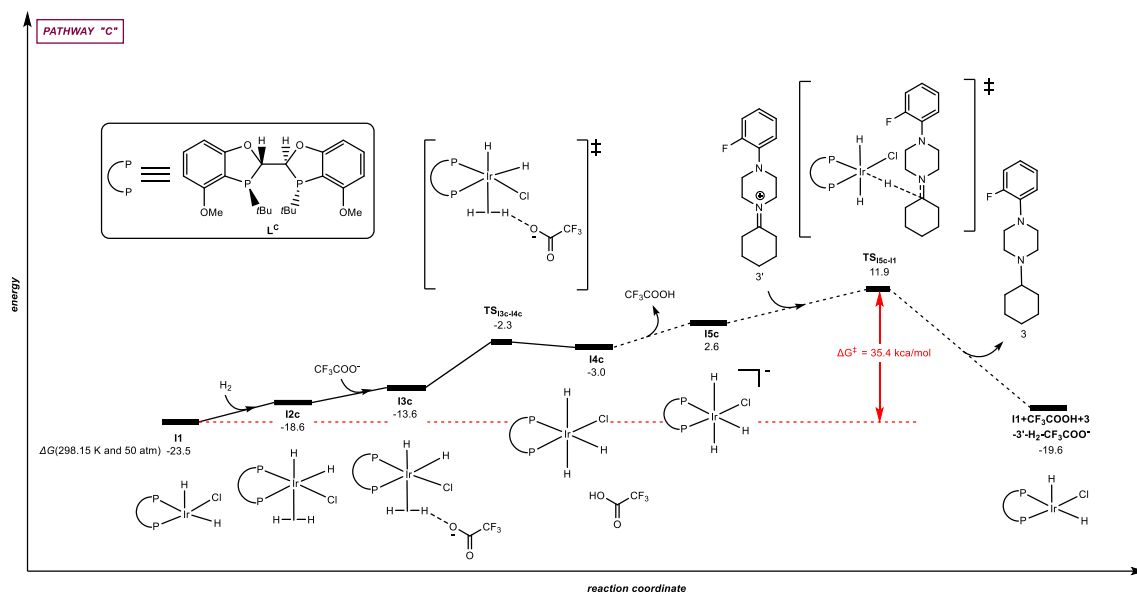


Fig. S34. Pathway "C": reaction coordinate for the trifluoroacetate-mediated, hydride/hydrogen transfer pathway occurring in a hexa-coordinated iridium complex **I2c** with initial H₂ activation. The relative Gibbs free energy (ΔG) are reported in kcal/mol at 298.15 K and 50 atm. P-P: diphosphane ligand **L^c**.

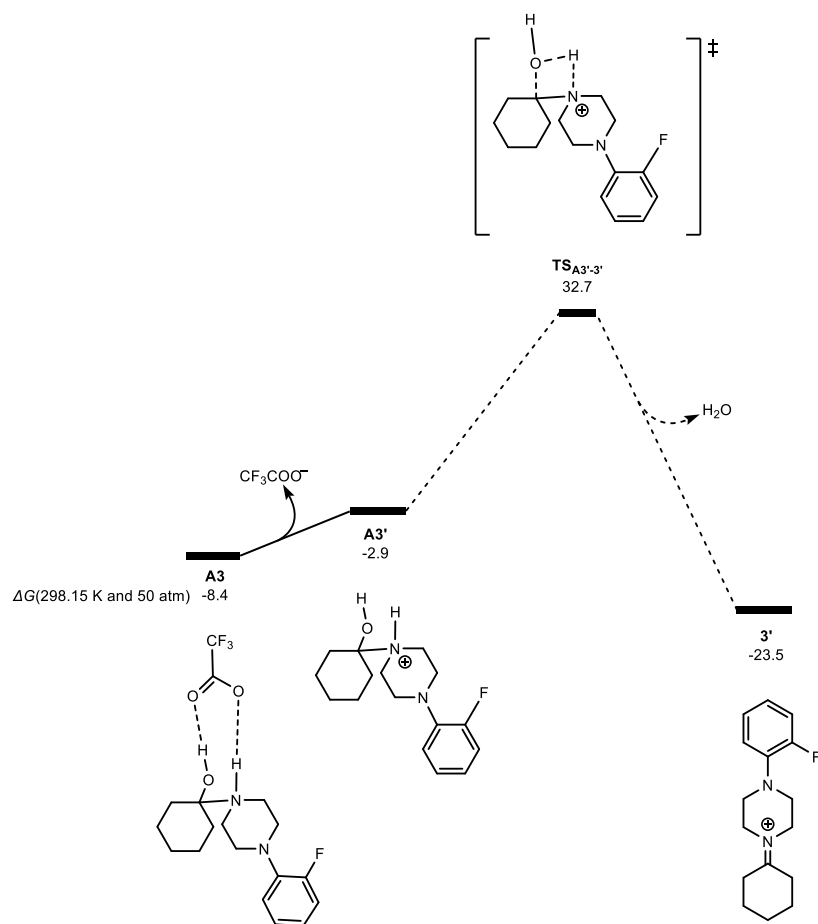


Fig. S35. Alternative formation of iminium **3'** without involving TFA in the transition state. Compute at 298.15 K and 50 atm

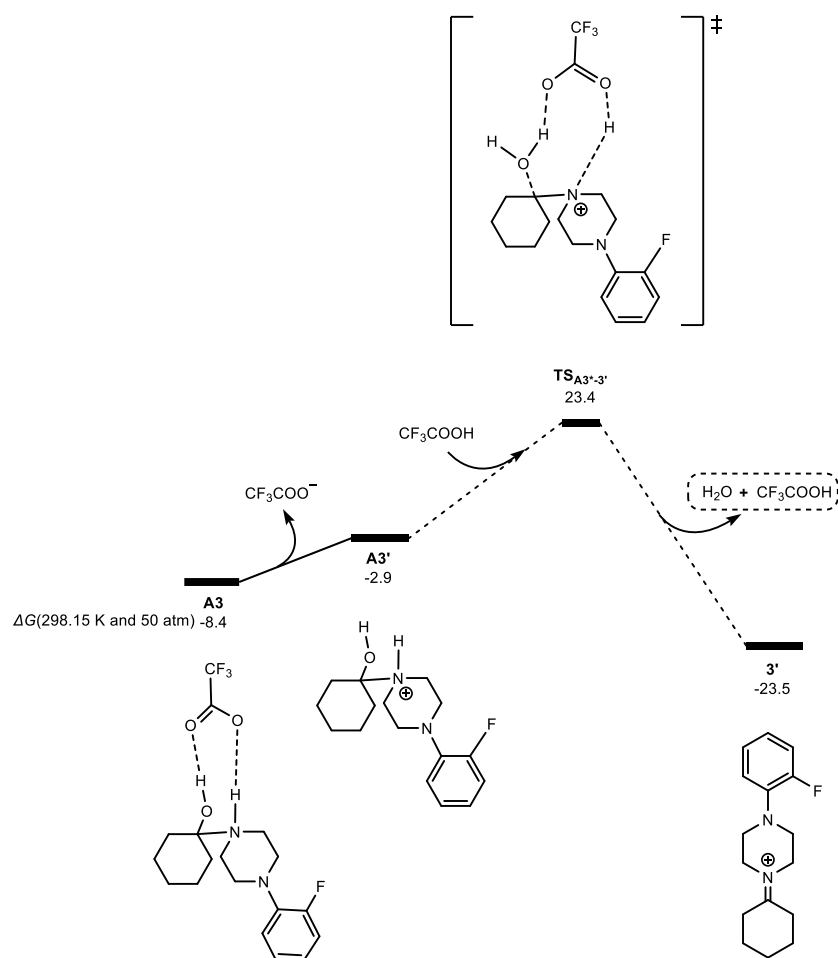


Fig. S36. Alternative formation of iminium **3'** involving a cationic, protonated aminoalcohol. Compute at 298.15 K and 50 atm.

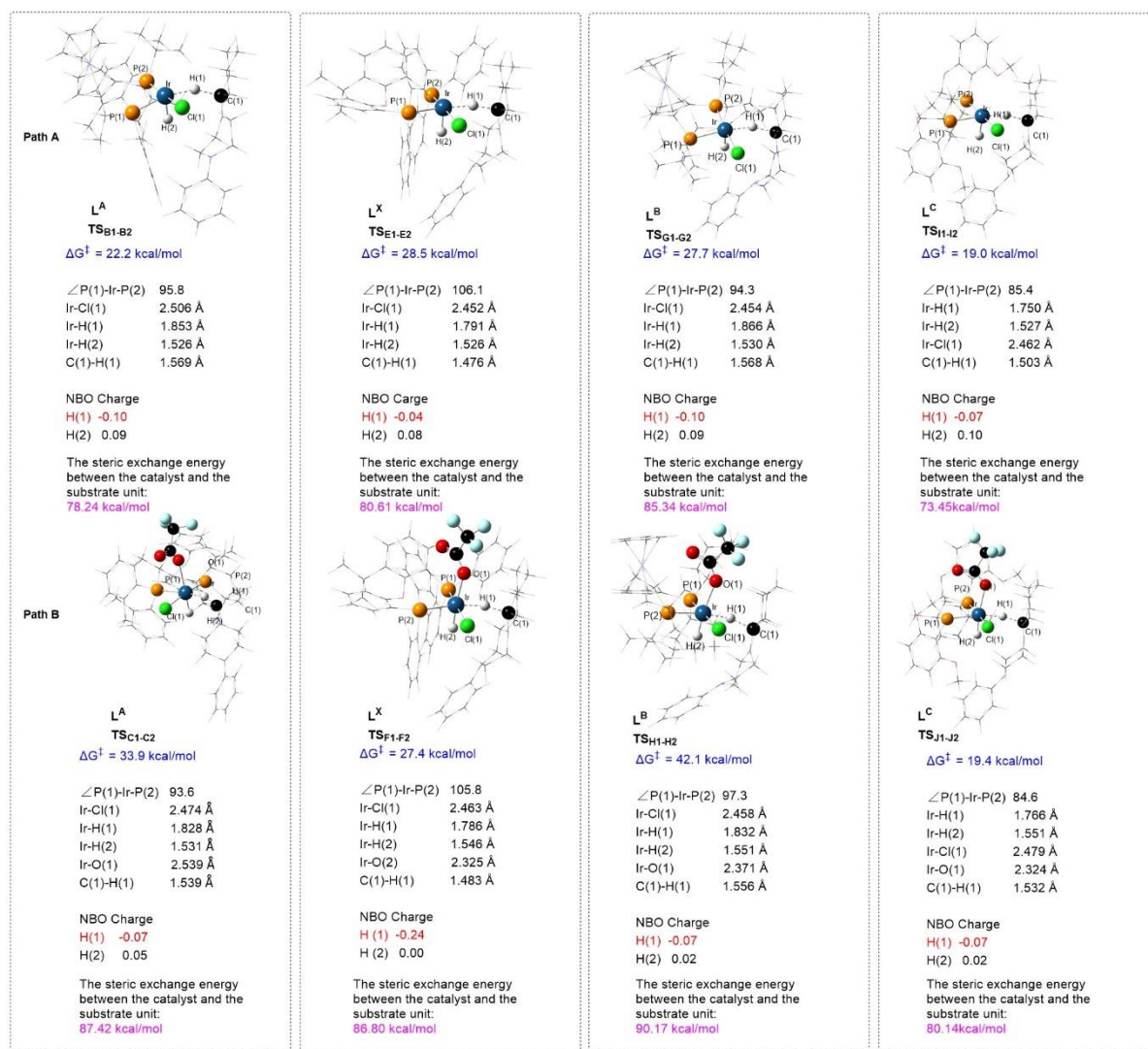


Fig. S37. The structures and NBO analysis for rationalizing the computed energy barrier results for the rate-determining hydride transfer transition states. The internuclear separations are given in Å. The substituents of diphosphine ligands and imine substrates are sketched in wireframe only for clarity.

The bite-angle of chelated ligands can strongly influence reactivity with adjusting the electronic and steric effects of ligands (*Chem. Rev.* **1977**, *77*, 313-348; *Coord. Chem. Rev.* **2002**, *233-234*, 41-51). The NBO analysis is performed to rationalize the computed energy barrier results for the rate-determining hydride transfer transition states. In this regard, the NPA charge is utilized to quantify the electronegativities of hydrides, and the steric exchange energy between the catalyst and the substrate unit is utilized to quantify the corresponding steric hindrance. It is found that the electronegativities of hydrides and the steric hindrance can well account for the computed energy barriers.

As for the ligand L^A, the transition state TS_{B1-B2} owns the lower Gibbs energy barrier compared with TS_{E1-E2}, which could be due to that TS_{E1-E2} has the more negative hydride and the lower steric hindrance between the catalyst and the substrate unit. As for the ligand Xantphos, the transition state TS_{F1-F2} has the larger steric hindrance but much more negative hydride compared with TS_{E1-E2}, which lead to the little lower Gibbs energy barrier of TS_{F1-F2} compared with TS_{E1-E2}. As for the ligand L^B, the transition state TS_{G1-G2}, with the more negative hydride and the lower steric hindrance, is more favorable with a Gibbs energy barrier of 27.7 kcal/mol. The ligand L^C has lowest steric hindrance and the lowest Gibbs energy barrier.

The experimental activity results must take into account both the computed energy barriers and the byproducts. In particular, the ligands L^B and L^C give non-negligible amounts of alcohol side-product, in contrast to the high selectivity observed for L^A and Xantphos. As a result, the ligands L^B and L^C have low experimental activities.

Table S3. Cartesian coordinates of all stationary points optimized at ω B97X-D/6-311G(d,p) level in methanol solvent.**1**

Coordinates (Angstroms)			
	X	Y	Z
C	-0.991466000	1.227224000	-0.368454000
C	-1.847193000	-0.000107000	-0.000718000
C	-0.991616000	-1.226818000	0.368971000
C	0.357801000	-1.225680000	-0.352482000
C	0.357898000	1.225391000	0.353177000
H	-0.803856000	1.238343000	-1.447190000
H	-2.502124000	0.242370000	0.841199000
H	-0.804210000	-1.236376000	1.447770000
H	0.952206000	-2.115553000	-0.134258000
H	0.204323000	1.195404000	1.440732000
H	-1.530334000	2.149362000	-0.139255000
H	-2.499737000	-0.243104000	-0.844361000
H	-1.530433000	-2.149288000	0.140989000
H	0.204324000	-1.196242000	-1.440079000
C	1.164882000	-0.000084000	0.000055000
O	2.381955000	0.000024000	-0.000533000
H	0.952362000	2.115337000	0.135429000

2

Coordinates (Angstroms)			
	X	Y	Z
C	1.458612000	-1.437369000	-0.135730000
C	0.722018000	-0.248834000	-0.044319000
C	1.475406000	0.924828000	0.125244000
C	2.851326000	0.944894000	0.155635000
C	3.555388000	-0.252525000	0.050911000
C	2.849998000	-1.438740000	-0.082320000

H	0.936084000	-2.377895000	-0.254469000
H	3.356634000	1.894784000	0.288496000
H	4.638486000	-0.248584000	0.084449000
H	3.378961000	-2.382410000	-0.157828000
C	-1.392406000	-1.466779000	0.108728000
C	-1.372882000	0.700325000	-0.942363000
C	-2.907995000	-1.176703000	0.170030000
H	-1.191641000	-2.163044000	-0.721676000
C	-2.659714000	1.174462000	-0.247293000
H	-0.746465000	1.549834000	-1.201046000
H	-3.390325000	-1.921628000	0.806100000
H	-3.401749000	1.434806000	-1.010533000
F	0.820064000	2.100269000	0.294333000
N	-0.669445000	-0.209367000	-0.039766000
N	-3.216451000	0.162438000	0.660132000
H	-2.765807000	0.271338000	1.562324000
H	-1.606965000	0.175099000	-1.880882000
H	-1.059922000	-1.946396000	1.034148000
H	-3.348880000	-1.277765000	-0.826314000
H	-2.456219000	2.076592000	0.334539000

3

Coordinates (Angstroms)			
	X	Y	Z
C	0.817361000	1.136625000	0.641291000
C	-0.635970000	0.885860000	1.013059000
C	-0.809591000	-0.819024000	-0.639763000
C	0.648409000	-0.611788000	-1.016480000
C	2.796321000	-0.243368000	0.063635000
C	3.714309000	0.806070000	-0.032037000
C	5.084582000	0.610184000	-0.049148000
C	5.593415000	-0.679413000	-0.014552000

C	4.712484000	-1.755175000	0.050285000
C	3.345604000	-1.533760000	0.100901000
H	1.369477000	1.453468000	1.528125000
H	-1.074619000	1.821159000	1.372043000
H	-0.860413000	-1.621010000	0.116702000
H	0.711229000	0.093029000	-1.862250000
H	5.732536000	1.477069000	-0.112843000
H	6.664884000	-0.839841000	-0.038833000
H	5.091891000	-2.770320000	0.082987000
H	2.661929000	-2.371671000	0.185950000
N	1.397750000	-0.100890000	0.131717000
N	-1.383275000	0.428968000	-0.151470000
H	1.077273000	-1.562484000	-1.336297000
H	-1.354294000	-1.156406000	-1.524035000
H	-0.668813000	0.157177000	1.841706000
H	0.854774000	1.946155000	-0.100698000
C	-2.834415000	0.405482000	0.070364000
C	-3.607514000	0.365430000	-1.250231000
C	-3.344678000	-0.696234000	1.013762000
C	-5.112665000	0.510068000	-1.013293000
H	-3.242759000	1.162420000	-1.905741000
C	-4.847706000	-0.547767000	1.261988000
H	-3.151659000	-1.678364000	0.564902000
C	-5.633095000	-0.558270000	-0.050144000
H	-5.316776000	1.503417000	-0.593060000
H	-5.033296000	0.399710000	1.784765000
H	-6.699684000	-0.405715000	0.143761000
H	-2.802595000	-0.663622000	1.964137000
H	-3.421083000	-0.586407000	-1.762475000
H	-5.646755000	0.454006000	-1.967073000
H	-5.532361000	-1.545138000	-0.520675000
H	-5.199838000	-1.346523000	1.922628000

H	-3.065990000	1.369030000	0.543608000
F	3.276057000	2.084978000	-0.120766000

3'

Coordinates (Angstroms)			
	X	Y	Z
C	0.325659000	0.674279000	1.214586000
C	-0.846933000	-0.055094000	1.853997000
C	-0.710486000	-1.756602000	0.150931000
C	0.468445000	-1.029932000	-0.473604000
C	2.453375000	0.218406000	0.124584000
C	2.763413000	1.577295000	0.030943000
C	4.029822000	2.002891000	-0.360417000
C	5.013792000	1.080802000	-0.685288000
C	4.731707000	-0.279574000	-0.601052000
C	3.478848000	-0.680113000	-0.191210000
H	0.874985000	1.180581000	2.009898000
H	-1.479693000	0.653718000	2.372842000
H	-0.367434000	-2.443893000	0.926346000
H	0.104419000	-0.361606000	-1.269534000
H	2.007664000	2.316387000	0.265315000
H	4.236790000	3.065381000	-0.420085000
H	5.998341000	1.408540000	-0.997759000
H	5.476496000	-1.032777000	-0.830120000
N	1.200555000	-0.275871000	0.545026000
N	-1.597567000	-0.778122000	0.809366000
H	1.117784000	-1.776943000	-0.926014000
H	-1.241755000	-2.320200000	-0.605458000
H	-0.493248000	-0.801404000	2.567158000
H	-0.068479000	1.437725000	0.525243000
C	-2.812377000	-0.515907000	0.449118000
C	-3.485312000	-1.162317000	-0.718763000

C	-3.652667000	0.547690000	1.079585000
C	-3.731539000	-0.077376000	-1.790876000
H	-2.937265000	-1.996675000	-1.143478000
C	-3.905627000	1.653472000	0.031813000
H	-4.607279000	0.079103000	1.338315000
C	-4.546430000	1.085181000	-1.230973000
H	-2.764641000	0.283961000	-2.157753000
H	-2.952087000	2.134080000	-0.212195000
H	-4.641268000	1.870098000	-1.986139000
H	-3.233861000	0.970858000	1.986489000
H	-4.449535000	-1.538710000	-0.364598000
H	-4.244719000	-0.544459000	-2.634114000
H	-5.558728000	0.736113000	-0.996424000
H	-4.546027000	2.412468000	0.486128000
F	3.234054000	-2.005889000	-0.079451000

3”

Coordinates (Angstroms)			
	X	Y	Z
C	-0.669959000	1.412219000	-0.004700000
C	0.765980000	1.268094000	-0.480597000
C	0.720071000	-1.056892000	0.118946000
C	-0.714737000	-0.903986000	0.584121000
C	-2.784622000	0.209207000	-0.003645000
C	-3.464301000	1.296499000	0.554482000
C	-4.852387000	1.306502000	0.662746000
C	-5.601697000	0.221716000	0.232075000
C	-4.952886000	-0.874634000	-0.329371000
C	-3.580466000	-0.855551000	-0.446891000
H	-1.155239000	2.188782000	-0.599682000
H	1.275011000	2.215339000	-0.292305000
H	0.725817000	-1.411846000	-0.925351000

H	-0.728167000	-0.668573000	1.660961000
H	-2.902666000	2.150081000	0.912203000
H	-5.342744000	2.169600000	1.098871000
H	-6.681577000	0.222017000	0.322782000
H	-5.499007000	-1.736162000	-0.696079000
N	-1.388615000	0.156797000	-0.170619000
N	1.451860000	0.205284000	0.236235000
H	-1.230409000	-1.851619000	0.438186000
H	1.193597000	-1.820538000	0.734811000
H	0.775398000	1.089749000	-1.569343000
H	-0.665704000	1.739460000	1.048192000
C	2.848073000	0.111581000	0.051252000
C	3.529144000	-0.978751000	0.852890000
C	3.557459000	0.949181000	-0.723000000
C	5.020476000	-0.714121000	1.047966000
H	3.033241000	-1.067467000	1.824656000
C	5.060146000	0.923139000	-0.842472000
C	5.677593000	-0.355169000	-0.280388000
H	5.155756000	0.113310000	1.755467000
H	5.482986000	1.794542000	-0.322320000
H	6.757808000	-0.231495000	-0.159193000
H	3.054910000	1.725013000	-1.289937000
H	3.398798000	-1.943925000	0.348352000
H	5.492469000	-1.595702000	1.491477000
H	5.524027000	-1.178701000	-0.988770000
H	5.339540000	1.044732000	-1.894980000
F	-2.977097000	-1.915042000	-1.035311000

A2

Coordinates (Angstroms)			
	X	Y	Z
C	0.420194000	3.241451000	1.208830000

C	-1.091622000	3.005289000	1.386093000
C	-1.645462000	1.964038000	0.396696000
C	-0.865482000	1.937592000	-0.916321000
C	1.140824000	2.009791000	0.652628000
H	0.587409000	4.074645000	0.518697000
H	-1.297789000	2.666255000	2.405406000
H	-1.577888000	0.965536000	0.834438000
H	-1.270651000	1.218971000	-1.630705000
H	0.877348000	3.528252000	2.158098000
H	-1.613903000	3.958173000	1.260971000
H	-2.702388000	2.149103000	0.192889000
H	-0.891420000	2.924609000	-1.400120000
C	0.582493000	1.628316000	-0.688430000
O	1.270049000	1.129553000	-1.577084000
C	-3.475447000	-0.403300000	-1.532364000
C	-3.441862000	-0.990174000	-0.258022000
C	-4.414529000	-0.524871000	0.643098000
C	-5.307938000	0.481272000	0.349318000
C	-5.297688000	1.059783000	-0.916575000
C	-4.386130000	0.596265000	-1.854769000
H	-2.762182000	-0.718278000	-2.282509000
H	-6.020361000	0.782703000	1.108835000
H	-6.000231000	1.847503000	-1.160910000
H	-4.363072000	1.025892000	-2.850302000
C	-1.891313000	-1.933254000	1.414033000
C	-1.728804000	-2.619288000	-0.916950000
C	-0.368331000	-1.982714000	1.243482000
H	-2.152872000	-0.990466000	1.893288000
C	-0.420870000	-1.848605000	-1.165254000
H	-1.493747000	-3.627799000	-0.565707000
H	-0.019941000	-3.026109000	1.173567000
H	-0.550681000	-1.085955000	-1.939888000

F	-4.506194000	-1.112250000	1.864200000
N	-2.564527000	-2.004089000	0.103385000
N	-0.008119000	-1.190740000	0.077083000
H	0.991639000	-1.025870000	0.063594000
H	-2.293050000	-2.742441000	-1.841561000
H	-2.222911000	-2.747019000	2.068627000
H	0.097714000	-1.549936000	2.131770000
H	0.329492000	-2.565163000	-1.532468000
C	5.430286000	-0.445546000	0.099202000
F	5.630920000	-1.427106000	0.972312000
F	5.949841000	0.679296000	0.607910000
F	6.099972000	-0.735886000	-1.020299000
C	3.924034000	-0.256295000	-0.182928000
O	3.741057000	0.616813000	-1.124634000
H	2.751865000	0.798078000	-1.287540000
O	3.096614000	-0.866222000	0.445805000
H	0.980550000	1.144358000	1.308274000
H	2.218868000	2.162636000	0.569581000

A3

Coordinates (Angstroms)			
	X	Y	Z
C	1.126526000	3.711887000	-0.202994000
C	-0.290942000	4.225167000	0.116847000
C	-1.303458000	3.073181000	0.235741000
C	-0.960516000	1.937768000	-0.727231000
C	1.335555000	2.292751000	0.321720000
H	1.290319000	3.706334000	-1.285130000
H	-0.281993000	4.791337000	1.052944000
H	-1.315658000	2.698034000	1.263450000
H	-1.733946000	1.166876000	-0.732893000
H	1.880210000	4.377817000	0.222907000

H	-0.609092000	4.918105000	-0.667749000
H	-2.314737000	3.430979000	0.028385000
H	-0.919463000	2.334234000	-1.744965000
C	0.425240000	1.331346000	-0.456665000
O	0.991378000	1.008939000	-1.688706000
C	-3.469208000	-1.581632000	-1.295275000
C	-3.365778000	-1.236862000	0.060110000
C	-4.541432000	-0.757307000	0.656298000
C	-5.725966000	-0.583616000	-0.025504000
C	-5.794007000	-0.925430000	-1.371919000
C	-4.662836000	-1.434715000	-1.993521000
H	-2.606903000	-1.967474000	-1.822904000
H	-6.587261000	-0.204377000	0.512419000
H	-6.722032000	-0.800424000	-1.916808000
H	-4.695342000	-1.711337000	-3.041435000
C	-1.824576000	-0.230874000	1.668397000
C	-1.062317000	-2.071022000	0.251283000
C	-0.322289000	0.007218000	1.671064000
H	-2.344392000	0.665796000	1.327951000
C	-0.172306000	-1.133412000	-0.545722000
H	-0.496933000	-2.548974000	1.054616000
H	0.186709000	-0.764798000	2.247312000
H	-0.722278000	-0.702027000	-1.378769000
F	-4.525871000	-0.470452000	1.981367000
N	-2.204316000	-1.377773000	0.825647000
N	0.329632000	-0.003250000	0.321145000
H	1.331432000	-0.246282000	0.517068000
H	-1.401230000	-2.876150000	-0.398756000
H	-2.109044000	-0.391258000	2.711713000
H	-0.116219000	0.956681000	2.157887000
H	0.698823000	-1.653691000	-0.942121000
C	5.106352000	-1.172334000	0.034055000

F	5.067997000	-2.499847000	0.241370000
F	5.668100000	-0.618572000	1.123152000
F	5.928638000	-0.952006000	-0.995474000
C	3.678922000	-0.606829000	-0.193811000
O	3.481539000	-0.017818000	-1.266011000
H	1.909713000	0.681972000	-1.554941000
O	2.901323000	-0.820828000	0.756027000
H	1.126022000	2.269391000	1.393291000
H	2.370593000	1.970241000	0.187534000

A4

Coordinates (Angstroms)			
	X	Y	Z
C	0.949930000	1.153192000	0.414813000
C	-0.496683000	0.930093000	0.821196000
C	-0.622979000	-1.036814000	-0.515039000
C	0.842193000	-0.870148000	-0.889601000
C	2.969370000	-0.258794000	0.113604000
C	3.865006000	0.782107000	-0.146884000
C	5.239387000	0.618024000	-0.123757000
C	5.776637000	-0.636072000	0.124195000
C	4.918915000	-1.706714000	0.360276000
C	3.547160000	-1.512414000	0.365601000
H	1.481372000	1.643776000	1.232211000
H	-0.962427000	1.894576000	1.024307000
H	-0.694914000	-1.704985000	0.360686000
H	0.908202000	-0.336482000	-1.852419000
H	5.867682000	1.477737000	-0.327484000
H	6.851505000	-0.773608000	0.132581000
H	5.320440000	-2.693908000	0.559405000
H	2.882785000	-2.341255000	0.585141000
N	1.567807000	-0.140322000	0.148167000

N	-1.226523000	0.265728000	-0.257497000
H	1.287989000	-1.856792000	-1.021427000
H	-1.116382000	-1.525297000	-1.354125000
H	-0.509583000	0.338206000	1.751140000
H	0.973799000	1.814246000	-0.462795000
C	-2.688396000	0.308597000	-0.093862000
C	-3.390236000	-0.428256000	-1.244707000
C	-3.195192000	-0.230717000	1.251315000
C	-4.911069000	-0.309929000	-1.142983000
H	-3.023075000	-0.024617000	-2.194901000
C	-4.721372000	-0.179448000	1.367662000
H	-2.850121000	-1.266437000	1.349551000
C	-5.409518000	-0.868934000	0.189769000
H	-5.206686000	0.740384000	-1.236372000
H	-5.041629000	0.867230000	1.412343000
H	-6.495182000	-0.754429000	0.269255000
H	-2.744461000	0.339971000	2.067121000
H	-3.132069000	-1.490428000	-1.216375000
H	-5.372269000	-0.846652000	-1.977617000
H	-5.198132000	-1.945734000	0.227434000
H	-5.028702000	-0.643718000	2.310068000
O	-3.061369000	1.684299000	-0.125432000
H	-2.736305000	2.043060000	-0.957673000
F	3.400135000	2.018919000	-0.446764000

TS_{A2-A3}

Coordinates (Angstroms)			
	X	Y	Z
C	0.451547000	3.207003000	0.936880000
C	-1.088402000	3.279778000	0.999467000
C	-1.759742000	2.074167000	0.319505000
C	-0.978696000	1.615070000	-0.902521000

C	0.957901000	1.762759000	0.747821000
H	0.826707000	3.816243000	0.109256000
H	-1.419039000	3.326281000	2.040446000
H	-1.818281000	1.242925000	1.024880000
H	-1.438690000	0.762596000	-1.403498000
H	0.896721000	3.609809000	1.848308000
H	-1.420186000	4.205626000	0.521446000
H	-2.786128000	2.312069000	0.032249000
H	-0.920627000	2.416423000	-1.651909000
C	0.435990000	1.290807000	-0.569146000
O	1.190387000	0.967990000	-1.531807000
C	-3.538342000	-0.673745000	-1.530254000
C	-3.399164000	-1.019305000	-0.176401000
C	-4.366560000	-0.474124000	0.684776000
C	-5.350303000	0.397083000	0.271959000
C	-5.442487000	0.741846000	-1.072935000
C	-4.538977000	0.185950000	-1.967982000
H	-2.836251000	-1.065843000	-2.254684000
H	-6.050918000	0.775667000	1.007656000
H	-6.215281000	1.422773000	-1.408868000
H	-4.597724000	0.428309000	-3.023410000
C	-1.732864000	-1.565095000	1.564900000
C	-1.578570000	-2.613828000	-0.629054000
C	-0.214210000	-1.625835000	1.390731000
H	-2.011526000	-0.561701000	1.882611000
C	-0.323715000	-1.833247000	-1.035237000
H	-1.284874000	-3.542261000	-0.131103000
H	0.142131000	-2.660587000	1.495073000
H	-0.542875000	-1.146010000	-1.860013000
F	-4.357847000	-0.838989000	1.992849000
N	-2.419604000	-1.877392000	0.301195000
N	0.182078000	-1.053361000	0.106283000

H	1.199650000	-1.044788000	0.071329000
H	-2.152304000	-2.908558000	-1.507525000
H	-2.032978000	-2.257982000	2.358474000
H	0.254535000	-1.050984000	2.193328000
H	0.427331000	-2.545346000	-1.398685000
C	5.416042000	-0.345701000	0.034171000
F	5.874533000	-1.597095000	-0.111344000
F	5.629654000	0.011053000	1.313528000
F	6.164434000	0.450197000	-0.733866000
C	3.902229000	-0.266202000	-0.289581000
O	3.574770000	0.681393000	-1.050200000
H	2.226642000	0.826367000	-1.278442000
O	3.198974000	-1.115977000	0.250676000
H	0.551050000	1.130804000	1.539543000
H	2.045505000	1.705431000	0.778755000

TS_{A4-3'}

Coordinates (Angstroms)			
	X	Y	Z
C	2.238814000	-0.810927000	1.306178000
C	1.472471000	-2.122941000	1.399268000
C	1.644165000	-2.458774000	-0.962412000
C	2.415384000	-1.150392000	-1.108188000
C	3.969937000	0.306382000	0.040458000
C	3.492224000	1.599735000	-0.178781000
C	4.320564000	2.701601000	-0.268086000
C	5.692404000	2.520696000	-0.135081000
C	6.207375000	1.248357000	0.082571000
C	5.349167000	0.157555000	0.168090000
H	2.853463000	-0.693185000	2.202350000
H	0.820574000	-2.110871000	2.268011000
H	2.354136000	-3.276464000	-0.798614000

H	1.722141000	-0.352187000	-1.403100000
H	3.885926000	3.679870000	-0.437488000
H	6.354068000	3.376790000	-0.201398000
H	7.276229000	1.102774000	0.188158000
H	5.737535000	-0.840563000	0.337629000
N	3.122863000	-0.837380000	0.138433000
N	0.727336000	-2.429177000	0.177629000
H	3.158030000	-1.263586000	-1.902297000
H	1.112808000	-2.666998000	-1.887389000
H	2.191094000	-2.936599000	1.545425000
H	1.530896000	0.032353000	1.282815000
C	-0.613654000	-2.099772000	0.007209000
C	-1.298467000	-2.888541000	-1.109314000
C	-1.409575000	-2.072701000	1.311085000
C	-2.808953000	-2.681127000	-1.218254000
H	-0.829801000	-2.663732000	-2.067222000
C	-2.920873000	-1.908191000	1.149823000
H	-1.209143000	-3.026860000	1.810112000
C	-3.499466000	-2.877637000	0.126310000
H	-3.027403000	-1.677395000	-1.596487000
H	-3.157860000	-0.886127000	0.846323000
H	-4.577339000	-2.720984000	0.025992000
H	-1.027647000	-1.278677000	1.955274000
H	-1.098159000	-3.941619000	-0.886714000
H	-3.194344000	-3.386744000	-1.959488000
H	-3.351560000	-3.909994000	0.468250000
H	-3.380780000	-2.057820000	2.130526000
O	-0.677772000	-0.569119000	-0.579264000
H	-0.166942000	0.001646000	0.010717000
F	2.159667000	1.794691000	-0.309260000
C	-2.751126000	1.615993000	0.042980000
C	-4.056288000	2.448439000	0.003815000

O	-2.675529000	0.786959000	-0.910796000
H	-1.614116000	-0.028819000	-0.737267000
O	-1.966657000	1.806571000	0.962271000
F	-5.120901000	1.657723000	0.229571000
F	-4.236783000	3.025980000	-1.193266000
F	-4.070667000	3.413813000	0.925146000

B1

Coordinates (Angstroms)			
	X	Y	Z
C	-3.824941000	3.313385000	0.052514000
C	-2.687755000	3.948230000	0.625350000
H	-2.688872000	4.576942000	1.504144000
C	-1.543209000	3.561795000	-0.123573000
C	-3.384654000	2.535376000	-1.051821000
H	-4.006346000	1.922477000	-1.687563000
C	-1.974426000	2.689514000	-1.158785000
H	-1.342294000	2.227779000	-1.898660000
H	-4.838968000	3.378960000	0.420031000
C	-3.275111000	1.189683000	2.432234000
C	-1.918217000	1.540772000	2.614764000
C	-1.106166000	0.761102000	1.739378000
C	-3.326716000	0.197804000	1.430213000
H	-4.233649000	-0.248469000	1.064478000
C	-1.993365000	-0.096349000	0.981091000
H	-4.125978000	1.642310000	2.920280000
Fe	-2.467548000	1.910766000	0.686762000
C	0.399089000	0.893592000	1.899882000
H	0.566833000	1.968259000	1.957489000
P	-1.529635000	-1.536838000	-0.051380000
C	-1.820314000	-2.965113000	1.176208000
C	-1.090954000	-2.601259000	2.476468000

H	-0.029899000	-2.414070000	2.296947000
H	-1.524462000	-1.726186000	2.964831000
H	-1.167879000	-3.445251000	3.169978000
C	-3.303394000	-3.188965000	1.495173000
H	-3.860700000	-3.561516000	0.634285000
H	-3.374015000	-3.947249000	2.282617000
H	-3.792480000	-2.287583000	1.867381000
C	-1.222932000	-4.284826000	0.664838000
H	-1.415825000	-5.056959000	1.417690000
H	-1.665499000	-4.620396000	-0.272146000
H	-0.143495000	-4.213451000	0.527170000
C	-2.760718000	-1.661864000	-1.506341000
C	-2.776283000	-3.092514000	-2.066005000
H	-3.307769000	-3.784815000	-1.410809000
H	-3.308335000	-3.073702000	-3.023172000
H	-1.773389000	-3.480094000	-2.251065000
C	-4.210866000	-1.257116000	-1.215227000
H	-4.799922000	-1.463719000	-2.115567000
H	-4.660113000	-1.821095000	-0.397365000
H	-4.302182000	-0.191806000	-1.008067000
C	-2.226561000	-0.728404000	-2.601396000
H	-2.125309000	0.295869000	-2.244037000
H	-1.258146000	-1.065578000	-2.981418000
H	-2.931790000	-0.724528000	-3.439441000
H	-0.523873000	3.856746000	0.075883000
C	0.820613000	0.359067000	3.276746000
H	0.233889000	0.879518000	4.037694000
H	0.641982000	-0.707901000	3.399513000
H	1.872908000	0.565066000	3.475484000
P	1.414101000	0.381039000	0.392636000
C	3.096885000	-0.092363000	1.016777000
C	4.336564000	0.364780000	0.525250000

C	3.094354000	-1.133217000	1.955115000
C	5.503797000	-0.154463000	1.100074000
C	4.261467000	-1.642657000	2.499781000
H	2.155086000	-1.577879000	2.256113000
C	5.482080000	-1.126235000	2.087003000
H	6.459810000	0.205005000	0.731964000
H	4.213265000	-2.440894000	3.232124000
H	6.410931000	-1.502129000	2.502299000
C	1.632531000	2.061332000	-0.352207000
C	1.370371000	2.344615000	-1.700379000
C	2.093562000	3.085885000	0.483392000
C	1.553045000	3.655255000	-2.153518000
C	2.278063000	4.376985000	0.016669000
H	2.342693000	2.872485000	1.517917000
C	1.998420000	4.664322000	-1.314355000
H	1.339693000	3.879727000	-3.193802000
H	2.641195000	5.148878000	0.685861000
H	2.129932000	5.669794000	-1.699422000
C	0.934878000	1.305729000	-2.695336000
H	1.774423000	0.667912000	-2.986374000
H	0.162350000	0.655004000	-2.279592000
H	0.531876000	1.775486000	-3.594987000
C	4.524735000	1.307015000	-0.639003000
H	3.830191000	1.081829000	-1.448389000
H	4.390376000	2.354663000	-0.361822000
H	5.537635000	1.194681000	-1.031542000
Ir	0.584438000	-1.473065000	-0.882681000
H	0.144397000	-2.824439000	-1.654025000
Cl	2.802951000	-1.779823000	-2.021270000
H	-1.542578000	2.301490000	3.284696000
H	0.998445000	-2.386460000	0.279875000

B2

Coordinates (Angstroms)			
	X	Y	Z
C	-4.189323000	2.940290000	0.150340000
C	-3.091764000	3.659178000	0.700361000
H	-3.115159000	4.262966000	1.596044000
C	-1.946269000	3.392519000	-0.098124000
C	-3.724366000	2.229892000	-0.989701000
H	-4.313382000	1.577952000	-1.618071000
C	-2.339322000	2.513495000	-1.142120000
H	-1.689284000	2.134908000	-1.913033000
H	-5.190257000	2.905603000	0.555563000
C	-3.409764000	0.808132000	2.434545000
C	-2.095504000	1.299668000	2.620735000
C	-1.215920000	0.629730000	1.722101000
C	-3.368648000	-0.159167000	1.407672000
H	-4.220344000	-0.699173000	1.030291000
C	-2.012706000	-0.290380000	0.952402000
H	-4.297831000	1.156217000	2.941328000
Fe	-2.696598000	1.650095000	0.701656000
C	0.270796000	0.896588000	1.824803000
H	0.351678000	1.980904000	1.764449000
P	-1.380281000	-1.646742000	-0.054807000
C	-1.482527000	-3.126906000	1.121273000
C	-0.847896000	-2.682900000	2.445653000
H	0.181860000	-2.351429000	2.298423000
H	-1.409788000	-1.882288000	2.930678000
H	-0.827465000	-3.540132000	3.125725000
C	-2.927306000	-3.567015000	1.381037000
H	-3.394597000	-3.987905000	0.489220000
H	-2.912754000	-4.349687000	2.146729000
H	-3.551159000	-2.753997000	1.756870000

C	-0.680082000	-4.324822000	0.592321000
H	-0.712695000	-5.112616000	1.352033000
H	-1.090066000	-4.740633000	-0.326987000
H	0.369541000	-4.075053000	0.422475000
C	-2.462759000	-1.876044000	-1.588330000
C	-2.166623000	-3.253190000	-2.197480000
H	-2.609741000	-4.062700000	-1.615412000
H	-2.605382000	-3.286396000	-3.199778000
H	-1.093515000	-3.442070000	-2.299871000
C	-3.970113000	-1.729189000	-1.363668000
H	-4.475258000	-1.979126000	-2.302946000
H	-4.357130000	-2.396170000	-0.593406000
H	-4.237506000	-0.702360000	-1.112539000
C	-2.021808000	-0.795931000	-2.586624000
H	-2.123834000	0.200191000	-2.161541000
H	-0.983628000	-0.933906000	-2.914605000
H	-2.656884000	-0.853924000	-3.476358000
H	-0.948987000	3.771284000	0.069481000
C	0.784762000	0.526627000	3.223087000
H	0.208489000	1.095869000	3.955202000
H	0.661269000	-0.531129000	3.452657000
H	1.832815000	0.799049000	3.349379000
P	1.327371000	0.390689000	0.356944000
C	3.026980000	0.027101000	0.987568000
C	4.239519000	0.574741000	0.524888000
C	3.065106000	-1.005373000	1.934128000
C	5.425333000	0.112516000	1.109219000
C	4.251349000	-1.452857000	2.487620000
H	2.147953000	-1.488533000	2.242014000
C	5.445489000	-0.872278000	2.082409000
H	6.363468000	0.533892000	0.762862000
H	4.238678000	-2.249523000	3.222462000

H	6.389470000	-1.201380000	2.502754000
C	1.322270000	1.944611000	-0.623622000
C	1.704233000	3.196934000	-0.105195000
C	0.902237000	1.846844000	-1.952597000
C	1.648413000	4.302144000	-0.955430000
C	0.855586000	2.958831000	-2.779184000
H	0.600119000	0.888529000	-2.360273000
C	1.231651000	4.195289000	-2.274265000
H	1.952232000	5.269098000	-0.567267000
H	0.524507000	2.855122000	-3.806079000
H	1.206458000	5.076373000	-2.906090000
C	2.191104000	3.435804000	1.303274000
H	1.379340000	3.806073000	1.938393000
H	2.607330000	2.546896000	1.778457000
H	2.968174000	4.202847000	1.298489000
C	4.389437000	1.587858000	-0.580614000
H	3.692075000	1.414017000	-1.397710000
H	4.244021000	2.608202000	-0.217768000
H	5.400934000	1.527570000	-0.986697000
Ir	0.729488000	-1.335433000	-0.930194000
Cl	2.937729000	-1.339475000	-2.145755000
H	-1.801523000	2.081627000	3.305918000
H	1.281569000	-2.193780000	0.205267000

B3

Coordinates (Angstroms)			
	X	Y	Z
C	-4.082334000	3.059245000	0.078495000
C	-3.020474000	3.778779000	0.694006000
H	-3.095941000	4.373083000	1.593102000
C	-1.830997000	3.525861000	-0.043082000
C	-3.550833000	2.363031000	-1.039511000

H	-4.101467000	1.719263000	-1.709193000
C	-2.160708000	2.651722000	-1.113091000
H	-1.469569000	2.274499000	-1.848114000
H	-5.104123000	3.015454000	0.426955000
C	-3.330732000	0.980435000	2.457133000
C	-1.998301000	1.425326000	2.618282000
C	-1.154903000	0.708975000	1.721121000
C	-3.336791000	-0.000008000	1.443930000
H	-4.215835000	-0.508978000	1.090366000
C	-1.991203000	-0.193725000	0.971080000
H	-4.200685000	1.369033000	2.965844000
Fe	-2.608448000	1.772438000	0.702252000
C	0.337956000	0.929671000	1.826557000
H	0.452538000	2.010937000	1.789388000
P	-1.461543000	-1.606403000	-0.034176000
C	-1.669717000	-3.057418000	1.162172000
C	-0.979467000	-2.658651000	2.473677000
H	0.072493000	-2.411581000	2.309304000
H	-1.469514000	-1.814742000	2.963365000
H	-1.016141000	-3.512390000	3.157849000
C	-3.143927000	-3.371190000	1.442147000
H	-3.660761000	-3.743635000	0.556220000
H	-3.185890000	-4.156372000	2.203983000
H	-3.687355000	-2.509845000	1.832139000
C	-0.979275000	-4.322523000	0.632362000
H	-1.171630000	-5.133939000	1.341419000
H	-1.354505000	-4.640666000	-0.340900000
H	0.103234000	-4.194845000	0.566925000
C	-2.594408000	-1.733234000	-1.549097000
C	-2.549189000	-3.140804000	-2.161128000
H	-3.049946000	-3.875603000	-1.528179000
H	-3.087229000	-3.105458000	-3.113812000

H	-1.540182000	-3.492338000	-2.374752000
C	-4.065707000	-1.387756000	-1.296132000
H	-4.606914000	-1.542979000	-2.235331000
H	-4.525071000	-2.028504000	-0.542181000
H	-4.201073000	-0.346536000	-1.011426000
C	-2.015036000	-0.723794000	-2.552596000
H	-1.970273000	0.278233000	-2.127876000
H	-1.008112000	-1.012514000	-2.879360000
H	-2.653701000	-0.691734000	-3.441083000
H	-0.846318000	3.905703000	0.184988000
C	0.834810000	0.513241000	3.218078000
H	0.267829000	1.075519000	3.962653000
H	0.686166000	-0.547110000	3.419370000
H	1.888374000	0.756868000	3.356388000
P	1.364317000	0.391192000	0.355557000
C	3.055295000	-0.006725000	0.990766000
C	4.281101000	0.537328000	0.561207000
C	3.066580000	-1.050448000	1.926327000
C	5.450841000	0.063413000	1.169278000
C	4.237261000	-1.509725000	2.502959000
H	2.138870000	-1.530603000	2.209763000
C	5.443379000	-0.930114000	2.133437000
H	6.398971000	0.483457000	0.849401000
H	4.203396000	-2.313646000	3.229251000
H	6.375474000	-1.267144000	2.573560000
C	1.395392000	1.916640000	-0.659370000
C	1.770994000	3.187605000	-0.184956000
C	1.016495000	1.762092000	-1.994206000
C	1.741695000	4.253868000	-1.084864000
C	1.004591000	2.832335000	-2.874386000
H	0.721991000	0.782576000	-2.349320000
C	1.367855000	4.089005000	-2.411132000

H	2.035754000	5.237220000	-0.731682000
H	0.709118000	2.683229000	-3.906477000
H	1.366577000	4.941296000	-3.081812000
C	2.228520000	3.481546000	1.222207000
H	1.402464000	3.869284000	1.827782000
H	2.640672000	2.610932000	1.734241000
H	3.001045000	4.252900000	1.204361000
C	4.464183000	1.556838000	-0.533975000
H	3.783374000	1.393933000	-1.367135000
H	4.320759000	2.576050000	-0.167676000
H	5.483957000	1.490348000	-0.917877000
Ir	0.689700000	-1.460011000	-0.904680000
H	0.274643000	-3.145100000	-1.386258000
Cl	2.906424000	-1.372157000	-2.100254000
H	-1.664883000	2.206472000	3.286294000
H	1.253928000	-2.227440000	0.294507000
H	0.609749000	-2.845345000	-2.069766000

TS_{B1-B2}

Coordinates (Angstroms)			
	X	Y	Z
C	5.959496000	-1.017192000	-2.131920000
C	5.942678000	0.358058000	-1.768706000
H	6.333972000	1.173859000	-2.359214000
C	5.268697000	0.476659000	-0.523078000
C	5.297089000	-1.749576000	-1.110540000
H	5.139343000	-2.817582000	-1.094014000
C	4.869899000	-0.825376000	-0.118167000
H	4.337893000	-1.063219000	0.787593000
H	6.368516000	-1.427663000	-3.043829000
C	3.375219000	-0.208467000	-3.883580000
C	3.151200000	1.005087000	-3.193066000

C	2.285877000	0.758036000	-2.088700000
C	2.668871000	-1.223375000	-3.204137000
H	2.663729000	-2.257286000	-3.496599000
C	1.976718000	-0.648647000	-2.081012000
H	4.017867000	-0.349445000	-4.740232000
Fe	4.029583000	-0.346435000	-1.941909000
C	1.800179000	1.943930000	-1.288155000
H	2.706694000	2.498336000	-1.053924000
P	0.655657000	-1.498789000	-1.148604000
C	-0.707304000	-1.563501000	-2.463922000
C	-0.901589000	-0.130503000	-2.977542000
H	-1.152856000	0.552582000	-2.164210000
H	-0.018430000	0.247905000	-3.495190000
H	-1.735402000	-0.125602000	-3.686244000
C	-0.371898000	-2.466025000	-3.655685000
H	-0.241329000	-3.511035000	-3.371289000
H	-1.208647000	-2.421141000	-4.361320000
H	0.520386000	-2.134393000	-4.188053000
C	-2.028495000	-2.014111000	-1.837187000
H	-2.835679000	-1.834408000	-2.554725000
H	-2.037076000	-3.075329000	-1.591101000
H	-2.247868000	-1.445710000	-0.934873000
C	1.290196000	-3.235922000	-0.713908000
C	0.083480000	-4.158870000	-0.540186000
H	-0.329370000	-4.469572000	-1.500954000
H	0.400093000	-5.060764000	-0.007801000
H	-0.702594000	-3.682714000	0.035433000
C	2.245885000	-3.912135000	-1.699576000
H	2.468870000	-4.909275000	-1.303724000
H	1.802938000	-4.048359000	-2.687661000
H	3.189896000	-3.381069000	-1.798016000
C	2.019636000	-3.078449000	0.630301000

H	2.893641000	-2.435436000	0.531982000
H	1.370073000	-2.664986000	1.409306000
H	2.361281000	-4.061261000	0.971856000
H	5.071086000	1.395731000	0.006981000
C	0.969931000	2.881796000	-2.175793000
H	1.577003000	3.157168000	-3.041343000
H	0.055908000	2.420510000	-2.546253000
H	0.713225000	3.801456000	-1.648913000
P	1.132776000	1.548798000	0.418775000
C	-0.101533000	2.884151000	0.801575000
C	-0.112852000	3.780895000	1.888518000
C	-1.193526000	2.880487000	-0.075909000
C	-1.183692000	4.679281000	1.981771000
C	-2.247861000	3.768839000	0.043536000
H	-1.229914000	2.152717000	-0.874498000
C	-2.233207000	4.693510000	1.078292000
H	-1.192975000	5.377402000	2.813060000
H	-3.069472000	3.727053000	-0.661752000
H	-3.041960000	5.406660000	1.195675000
C	2.656604000	1.783085000	1.421859000
C	3.456355000	2.942987000	1.404390000
C	3.032480000	0.702206000	2.221510000
C	4.592766000	2.968177000	2.214105000
C	4.170487000	0.744542000	3.012727000
H	2.422132000	-0.193996000	2.225185000
C	4.953250000	1.890233000	3.010778000
H	5.206837000	3.863400000	2.218056000
H	4.440788000	-0.111418000	3.620670000
H	5.844500000	1.947134000	3.626233000
C	3.174983000	4.171977000	0.575000000
H	3.760599000	4.156468000	-0.350449000
H	2.125306000	4.283735000	0.302314000

H	3.473620000	5.066768000	1.125212000
C	0.903017000	3.849394000	3.000879000
H	1.320189000	2.876209000	3.244496000
H	1.723840000	4.527020000	2.752184000
H	0.422610000	4.242723000	3.899287000
Ir	0.045449000	-0.480473000	0.847034000
H	-1.147060000	-1.781668000	1.412844000
Cl	-0.300146000	0.594315000	3.084281000
H	3.584024000	1.965865000	-3.432902000
H	-1.129312000	0.177341000	0.128366000
C	-7.186713000	0.543435000	-1.381740000
C	-7.963179000	1.360891000	-2.196655000
C	-7.378098000	2.347032000	-2.978322000
C	-5.994406000	2.495425000	-2.955532000
C	-5.239720000	1.661294000	-2.161217000
C	-5.791769000	0.672546000	-1.333198000
H	-7.675120000	-0.199798000	-0.764109000
H	-9.039259000	1.227222000	-2.204051000
H	-7.982293000	2.991188000	-3.605881000
H	-5.489063000	3.234868000	-3.566385000
C	-4.442585000	-2.267811000	0.502803000
C	-5.544950000	-1.317027000	0.066736000
N	-4.972376000	-0.132960000	-0.549099000
C	-3.927435000	0.528544000	0.245402000
C	-3.712479000	-0.161222000	1.585491000
N	-3.504227000	-1.593615000	1.405969000
H	-4.908205000	-3.110999000	1.020543000
H	-6.151694000	-1.846865000	-0.669394000
H	-2.986804000	0.540864000	-0.308336000
H	-2.821828000	0.277098000	2.032807000
C	-1.280263000	-4.436760000	2.516983000
C	-2.448190000	-3.743993000	1.816169000

C	-2.505702000	-2.246971000	2.044193000
C	-2.288465000	-1.876644000	3.501002000
C	-1.124048000	-2.590033000	4.173655000
C	-1.224292000	-4.101374000	4.002293000
H	-1.373244000	-5.514653000	2.357756000
H	-2.472690000	-3.978570000	0.751745000
H	-2.203773000	-0.804113000	3.638545000
H	-0.183632000	-2.231336000	3.742788000
H	-2.124634000	-4.474323000	4.506152000
H	-3.383804000	-4.136745000	2.236762000
H	-3.226296000	-2.192993000	3.979279000
H	-1.111985000	-2.314668000	5.232298000
H	-0.365937000	-4.596809000	4.465543000
H	-0.337821000	-4.126317000	2.061005000
F	-3.888325000	1.787599000	-2.211659000
H	-6.198540000	-1.075706000	0.917901000
H	-3.932312000	-2.658123000	-0.378798000
H	-4.554574000	0.024257000	2.260396000
H	-4.199461000	1.568609000	0.450105000

TS_{B3-B1}

Coordinates (Angstroms)			
	X	Y	Z
C	4.018380000	-2.971069000	2.128157000
C	4.718135000	-1.732394000	2.110300000
H	5.762761000	-1.597138000	1.869461000
C	3.788537000	-0.696985000	2.404653000
C	2.658873000	-2.701546000	2.433865000
H	1.868307000	-3.432423000	2.513410000
C	2.516200000	-1.296601000	2.601307000
H	1.600749000	-0.776165000	2.830167000
H	4.440949000	-3.940560000	1.906620000

C	4.121769000	-2.230110000	-1.066184000
C	4.084950000	-0.824868000	-0.918335000
C	2.727559000	-0.400611000	-0.817646000
C	2.790729000	-2.697475000	-1.038397000
H	2.506575000	-3.732777000	-1.106249000
C	1.898519000	-1.577064000	-0.901970000
H	5.008339000	-2.845096000	-1.119331000
Fe	3.229678000	-1.707984000	0.706840000
C	2.462280000	1.091266000	-0.799307000
H	3.135413000	1.481855000	-0.039611000
P	0.104764000	-1.654691000	-1.220861000
C	0.056970000	-2.088906000	-3.068036000
C	1.009044000	-1.119757000	-3.784465000
H	0.760135000	-0.077338000	-3.568916000
H	2.054250000	-1.291866000	-3.517902000
H	0.907658000	-1.269889000	-4.864282000
C	0.501152000	-3.528012000	-3.357649000
H	-0.195684000	-4.263635000	-2.952920000
H	0.527231000	-3.664667000	-4.444000000
H	1.500769000	-3.745622000	-2.981515000
C	-1.350867000	-1.887681000	-3.649572000
H	-1.336611000	-2.222842000	-4.691870000
H	-2.115881000	-2.463059000	-3.127070000
H	-1.645147000	-0.837574000	-3.641548000
C	-0.611675000	-3.039968000	-0.145194000
C	-1.966603000	-3.513780000	-0.688650000
H	-1.857203000	-4.091749000	-1.608038000
H	-2.416787000	-4.172242000	0.061898000
H	-2.668387000	-2.701264000	-0.867724000
C	0.276146000	-4.276099000	0.031702000
H	-0.268814000	-4.986568000	0.662825000
H	0.495013000	-4.777796000	-0.912223000

H	1.211837000	-4.043819000	0.535116000
C	-0.825516000	-2.379998000	1.223747000
H	0.110607000	-2.007807000	1.641887000
H	-1.524172000	-1.542801000	1.149213000
H	-1.246223000	-3.111364000	1.921745000
H	4.005696000	0.360187000	2.438942000
C	2.939216000	1.699593000	-2.127067000
H	3.985564000	1.424989000	-2.274221000
H	2.376848000	1.327372000	-2.984108000
H	2.885914000	2.787986000	-2.112702000
P	0.770200000	1.620721000	-0.195222000
C	0.475973000	3.310568000	-0.895018000
C	0.179564000	4.498296000	-0.199974000
C	0.409048000	3.316117000	-2.295147000
C	-0.064645000	5.653558000	-0.954357000
C	0.152403000	4.466785000	-3.019330000
H	0.541336000	2.390667000	-2.840555000
C	-0.066411000	5.656903000	-2.339136000
H	-0.285690000	6.574584000	-0.424312000
H	0.113251000	4.426551000	-4.102101000
H	-0.267116000	6.575670000	-2.879547000
C	0.972635000	1.706952000	1.626449000
C	2.016199000	2.361459000	2.305080000
C	-0.029777000	1.065217000	2.362179000
C	2.021250000	2.315259000	3.700855000
C	-0.021123000	1.054468000	3.747990000
H	-0.835620000	0.554638000	1.848239000
C	1.020997000	1.677877000	4.420781000
H	2.824614000	2.815629000	4.232494000
H	-0.815455000	0.553995000	4.289755000
H	1.054722000	1.675593000	5.504865000
C	3.112282000	3.152003000	1.634703000

H	4.017516000	2.548108000	1.511553000
H	2.826810000	3.536850000	0.654262000
H	3.383714000	4.006250000	2.258928000
C	0.028615000	4.632346000	1.294119000
H	-0.529686000	3.802129000	1.725653000
H	0.992522000	4.691401000	1.803206000
H	-0.513041000	5.552947000	1.519282000
Ir	-1.081368000	0.277404000	-0.762895000
H	-2.354677000	-0.554842000	-1.479955000
Cl	-2.589235000	2.238559000	-0.374618000
H	4.940939000	-0.168127000	-0.853937000
H	-0.847693000	0.720957000	-2.209396000
H	-2.947501000	-0.559185000	-0.722840000
C	-4.277915000	-0.745645000	1.093847000
O	-4.135541000	-0.873297000	-0.157429000
C	-5.708051000	-1.134243000	1.551001000
O	-3.474997000	-0.395292000	1.945298000
F	-5.897790000	-0.925956000	2.855289000
F	-5.940082000	-2.436807000	1.311319000
F	-6.640704000	-0.434467000	0.887555000

c1

Coordinates (Angstroms)			
	X	Y	Z
C	-3.289846000	-0.486314000	-3.322221000
C	-4.177640000	0.624398000	-3.266919000
H	-4.017330000	1.590894000	-3.722287000
C	-5.291009000	0.258082000	-2.460014000
H	-6.119045000	0.899719000	-2.195459000
C	-3.860961000	-1.537133000	-2.556818000
H	-3.428469000	-2.512383000	-2.407567000
C	-5.091827000	-1.079244000	-2.015121000

H	-5.750203000	-1.641599000	-1.368853000
H	-2.340104000	-0.520515000	-3.836336000
C	-1.793058000	0.924696000	-0.654898000
C	-2.807384000	1.923507000	-0.719411000
C	-3.891839000	1.523395000	0.097688000
H	-4.829173000	2.046719000	0.217422000
C	-2.236118000	-0.096358000	0.265624000
C	-3.559303000	0.274869000	0.673631000
H	-4.203663000	-0.282714000	1.331412000
Fe	-3.558919000	0.144712000	-1.379529000
P	-1.128369000	-1.311582000	1.115576000
H	-2.781067000	2.815319000	-1.326119000
C	-0.473882000	1.023621000	-1.382404000
H	-0.176930000	0.027378000	-1.716086000
C	-0.566989000	1.943319000	-2.598316000
H	-1.312457000	1.548260000	-3.292923000
H	-0.870093000	2.954859000	-2.327833000
H	0.382880000	2.009259000	-3.128519000
P	0.795374000	1.434188000	-0.062534000
Ir	1.029807000	-0.544736000	1.322330000
Cl	3.379351000	0.048918000	2.034508000
H	0.504690000	0.165747000	2.598522000
O	3.130831000	-3.325862000	0.457921000
C	2.821572000	-2.578867000	-0.470764000
C	3.323681000	-3.026194000	-1.871641000
O	2.116812000	-1.546651000	-0.498925000
F	2.480392000	-3.955965000	-2.372837000
F	4.539269000	-3.587013000	-1.820616000
F	3.382336000	-2.033043000	-2.768766000
H	1.242475000	-1.867774000	2.206178000
C	2.370135000	1.838604000	-0.915567000
C	3.355892000	2.648313000	-0.320079000

C	2.646131000	1.200884000	-2.128150000
C	4.556890000	2.837895000	-1.006022000
C	3.851155000	1.395543000	-2.788581000
H	1.918942000	0.527093000	-2.563745000
C	4.807653000	2.231936000	-2.229921000
H	5.318094000	3.468822000	-0.556916000
H	4.039156000	0.891187000	-3.729841000
H	5.753953000	2.398525000	-2.733517000
C	0.090044000	3.007190000	0.606691000
C	0.105492000	4.273920000	-0.008738000
C	-0.625076000	2.842303000	1.797887000
C	-0.607798000	5.311017000	0.603838000
C	-1.327973000	3.881062000	2.386371000
H	-0.630461000	1.868529000	2.267077000
C	-1.319474000	5.130063000	1.779642000
H	-0.596981000	6.290065000	0.133920000
H	-1.872874000	3.712866000	3.308880000
H	-1.859701000	5.961699000	2.219354000
C	0.868349000	4.640675000	-1.259065000
H	1.209982000	3.786985000	-1.834519000
H	0.245221000	5.262205000	-1.907235000
H	1.751799000	5.231872000	-0.995588000
C	3.183045000	3.328717000	1.013332000
H	2.694884000	4.301892000	0.905595000
H	2.594260000	2.726131000	1.704398000
H	4.159855000	3.498109000	1.471569000
C	-1.919798000	-1.543092000	2.852425000
C	-3.239521000	-2.336147000	2.845530000
H	-3.737605000	-2.179970000	3.808124000
H	-3.940494000	-2.054300000	2.062349000
H	-3.048851000	-3.405772000	2.753603000
C	-0.962723000	-2.308931000	3.783944000

H	-0.624908000	-3.256541000	3.363705000
H	-0.083349000	-1.720239000	4.040570000
H	-1.504976000	-2.530103000	4.710139000
C	-2.153590000	-0.171002000	3.509756000
H	-1.217140000	0.371883000	3.641690000
H	-2.848956000	0.466690000	2.965384000
H	-2.572140000	-0.342878000	4.507144000
C	-1.288967000	-2.918569000	0.114307000
C	-2.725461000	-3.451238000	-0.002334000
H	-2.779215000	-4.112722000	-0.873842000
H	-3.012097000	-4.043659000	0.864500000
H	-3.463965000	-2.661221000	-0.140212000
C	-0.410272000	-4.020395000	0.715880000
H	-0.416422000	-4.878548000	0.033744000
H	0.625281000	-3.704175000	0.847166000
H	-0.794921000	-4.367561000	1.677020000
C	-0.772685000	-2.591479000	-1.296198000
H	0.259096000	-2.247422000	-1.280307000
H	-0.821497000	-3.500318000	-1.905972000
H	-1.382950000	-1.830856000	-1.781867000

C2

Coordinates (Angstroms)			
	X	Y	Z
C	-3.677571000	-0.483842000	-3.197865000
C	-4.735089000	0.414036000	-2.881780000
H	-4.815772000	1.441794000	-3.204865000
C	-5.641328000	-0.261406000	-2.017157000
H	-6.527721000	0.165984000	-1.571312000
C	-3.935981000	-1.710772000	-2.533605000
H	-3.315174000	-2.590233000	-2.576771000
C	-5.143510000	-1.576187000	-1.796809000

H	-5.592472000	-2.330445000	-1.166786000
H	-2.819151000	-0.267938000	-3.817063000
C	-2.072950000	0.768267000	-0.511713000
C	-3.192206000	1.637766000	-0.390468000
C	-4.144091000	1.028188000	0.466976000
H	-5.119249000	1.422471000	0.712251000
C	-2.316773000	-0.378183000	0.324236000
C	-3.622333000	-0.219134000	0.887406000
H	-4.123720000	-0.922430000	1.533450000
Fe	-3.787335000	-0.158286000	-1.161825000
P	-0.988602000	-1.481227000	0.898448000
H	-3.322293000	2.579805000	-0.900726000
C	-0.827797000	1.041960000	-1.311438000
H	-0.489902000	0.114179000	-1.773503000
C	-1.062168000	2.081040000	-2.405244000
H	-1.812466000	1.694971000	-3.098779000
H	-1.435579000	3.022254000	-2.002899000
H	-0.153223000	2.284982000	-2.971188000
P	0.515545000	1.439070000	-0.079210000
Ir	1.058266000	-0.382464000	1.112656000
Cl	3.265570000	0.354099000	1.985695000
H	0.419897000	0.302028000	2.335348000
O	3.322898000	-2.958962000	0.628263000
C	3.158487000	-2.231740000	-0.349216000
C	4.141464000	-2.391951000	-1.538953000
O	2.310157000	-1.334474000	-0.560587000
F	4.841663000	-3.528762000	-1.478736000
F	5.025810000	-1.376221000	-1.554860000
F	3.504925000	-2.375896000	-2.721808000
C	2.019011000	1.904916000	-1.012488000
C	3.019216000	2.751798000	-0.501708000
C	2.209424000	1.258008000	-2.238010000

C	4.164358000	2.945037000	-1.276266000
C	3.358563000	1.462623000	-2.984990000
H	1.463167000	0.569190000	-2.614267000
C	4.339212000	2.318314000	-2.501711000
H	4.941845000	3.600291000	-0.896269000
H	3.488102000	0.948102000	-3.930104000
H	5.247305000	2.488458000	-3.069894000
C	-0.213630000	2.909015000	0.766768000
C	-0.268377000	4.207464000	0.219725000
C	-0.896564000	2.648481000	1.960853000
C	-0.978817000	5.185158000	0.926204000
C	-1.599542000	3.631220000	2.635833000
H	-0.893934000	1.648850000	2.367106000
C	-1.635199000	4.917557000	2.115085000
H	-1.014277000	6.188172000	0.512030000
H	-2.115724000	3.388106000	3.557631000
H	-2.174822000	5.707089000	2.626640000
C	0.370524000	4.681885000	-1.064825000
H	0.845516000	3.901484000	-1.648666000
H	-0.386327000	5.156115000	-1.694861000
H	1.125860000	5.441808000	-0.844866000
C	2.930364000	3.479702000	0.813599000
H	2.493394000	4.473367000	0.679800000
H	2.339861000	2.944877000	1.554336000
H	3.931901000	3.614547000	1.226753000
C	-1.379972000	-2.005207000	2.691977000
C	-2.455762000	-3.091730000	2.804688000
H	-2.690275000	-3.230062000	3.865213000
H	-3.383236000	-2.835501000	2.289591000
H	-2.100535000	-4.049603000	2.425402000
C	-0.073312000	-2.545195000	3.308803000
H	0.289095000	-3.446654000	2.815795000

H	0.724933000	-1.793277000	3.291653000
H	-0.265204000	-2.793797000	4.357802000
C	-1.813379000	-0.795236000	3.536610000
H	-1.025272000	-0.046376000	3.614624000
H	-2.718908000	-0.312527000	3.171005000
H	-2.015852000	-1.155468000	4.550318000
C	-0.986679000	-2.995306000	-0.232291000
C	-2.367699000	-3.667831000	-0.312815000
H	-2.428457000	-4.227999000	-1.251419000
H	-2.519359000	-4.379875000	0.496270000
H	-3.189932000	-2.952567000	-0.299186000
C	0.044318000	-4.028699000	0.234315000
H	0.139649000	-4.794428000	-0.543371000
H	1.032203000	-3.595567000	0.396129000
H	-0.271675000	-4.532930000	1.148965000
C	-0.577626000	-2.493639000	-1.626300000
H	0.416010000	-2.043070000	-1.616275000
H	-0.555613000	-3.349124000	-2.309273000
H	-1.292787000	-1.774108000	-2.025516000

C3

Coordinates (Angstroms)			
	X	Y	Z
C	3.245860000	-0.405465000	3.379231000
C	4.049272000	0.768492000	3.370508000
H	3.799771000	1.714196000	3.829341000
C	5.213617000	0.497975000	2.599445000
H	5.998779000	1.204288000	2.372035000
C	3.922867000	-1.400363000	2.625309000
H	3.570080000	-2.402961000	2.449385000
C	5.133603000	-0.844906000	2.133830000
H	5.854514000	-1.345907000	1.504057000

H	2.284258000	-0.517901000	3.858901000
C	1.756805000	0.966086000	0.690704000
C	2.712913000	2.016899000	0.787612000
C	3.836561000	1.682760000	-0.006345000
H	4.746963000	2.256941000	-0.095208000
C	2.280567000	-0.018601000	-0.225747000
C	3.589665000	0.424908000	-0.603017000
H	4.276939000	-0.093391000	-1.250472000
Fe	3.535414000	0.272345000	1.453836000
P	1.279513000	-1.287737000	-1.087637000
H	2.626243000	2.899773000	1.401466000
C	0.412869000	0.972722000	1.376513000
H	0.161510000	-0.040763000	1.694806000
C	0.408241000	1.887285000	2.600118000
H	1.147438000	1.516529000	3.313653000
H	0.670547000	2.915138000	2.351693000
H	-0.560982000	1.898363000	3.096723000
P	-0.828491000	1.332646000	0.025078000
Ir	-0.983944000	-0.638564000	-1.290102000
Cl	-3.341573000	-0.186131000	-1.942093000
H	-0.509630000	0.135450000	-2.546864000
O	-2.791464000	-3.400827000	-0.269190000
C	-2.646842000	-2.551741000	0.606147000
C	-3.448387000	-2.755134000	1.918877000
O	-1.957227000	-1.503308000	0.621956000
F	-3.737443000	-4.042478000	2.140229000
F	-4.616568000	-2.088434000	1.855606000
F	-2.793608000	-2.303364000	2.999310000
H	-1.179229000	-1.766924000	-2.590651000
C	-2.457358000	1.688867000	0.778419000
C	-3.428953000	2.477058000	0.135255000
C	-2.755469000	1.070797000	1.995240000

C	-4.651904000	2.661989000	0.782508000
C	-3.981888000	1.261029000	2.613418000
H	-2.034975000	0.413731000	2.463121000
C	-4.930641000	2.073869000	2.008313000
H	-5.407738000	3.272745000	0.298533000
H	-4.192499000	0.769686000	3.556436000
H	-5.894227000	2.235898000	2.479322000
C	-0.159843000	2.887259000	-0.693313000
C	-0.240256000	4.157695000	-0.089319000
C	0.598162000	2.731279000	-1.856284000
C	0.453297000	5.210628000	-0.696523000
C	1.279277000	3.787006000	-2.437404000
H	0.663333000	1.754566000	-2.307890000
C	1.204948000	5.041955000	-1.848232000
H	0.392976000	6.193435000	-0.239172000
H	1.859786000	3.625605000	-3.338777000
H	1.727522000	5.887589000	-2.281970000
C	-1.041121000	4.519948000	1.138458000
H	-1.386400000	3.670109000	1.716883000
H	-0.441521000	5.155929000	1.794226000
H	-1.924592000	5.096839000	0.846259000
C	-3.232746000	3.135310000	-1.206088000
H	-2.799566000	4.134141000	-1.099092000
H	-2.587382000	2.554710000	-1.864105000
H	-4.198142000	3.246984000	-1.703830000
C	2.031076000	-1.453512000	-2.844156000
C	3.375533000	-2.201378000	-2.857784000
H	3.842161000	-2.039557000	-3.834438000
H	4.082745000	-1.876142000	-2.096642000
H	3.225226000	-3.275163000	-2.747225000
C	1.080591000	-2.235535000	-3.770656000
H	0.729211000	-3.174380000	-3.342208000

H	0.216027000	-1.638932000	-4.063669000
H	1.632428000	-2.475863000	-4.684910000
C	2.213955000	-0.067050000	-3.483442000
H	1.256228000	0.430454000	-3.637957000
H	2.868594000	0.597378000	-2.920780000
H	2.659206000	-0.214134000	-4.472577000
C	1.514197000	-2.898043000	-0.113426000
C	2.988983000	-3.315857000	0.009671000
H	3.084920000	-3.976083000	0.877434000
H	3.326066000	-3.879430000	-0.857320000
H	3.663068000	-2.472379000	0.158845000
C	0.733483000	-4.056920000	-0.741966000
H	0.840683000	-4.929941000	-0.088868000
H	-0.334294000	-3.847673000	-0.828850000
H	1.127178000	-4.335105000	-1.720925000
C	0.954617000	-2.637804000	1.293537000
H	-0.108080000	-2.408111000	1.273900000
H	1.097001000	-3.542695000	1.893114000
H	1.475553000	-1.821508000	1.792583000
H	-1.238614000	-2.261974000	-1.911169000

TS_{c1-c2}

Coordinates (Angstroms)			
	X	Y	Z
C	-5.001784000	-2.784083000	-1.570755000
C	-4.972599000	-4.063924000	-0.950901000
H	-5.413868000	-4.318241000	0.001975000
C	-4.211089000	-4.935922000	-1.778279000
H	-3.976898000	-5.968419000	-1.563002000
C	-4.267423000	-2.871185000	-2.783116000
H	-4.115254000	-2.066381000	-3.483148000
C	-3.769050000	-4.195284000	-2.910760000

H	-3.153304000	-4.569216000	-3.716118000
H	-5.479059000	-1.896928000	-1.180495000
C	-2.229011000	-2.101775000	0.244083000
C	-2.390698000	-3.415395000	0.767690000
C	-1.638924000	-4.309278000	-0.028052000
H	-1.590365000	-5.382010000	0.088395000
C	-1.340046000	-2.171538000	-0.885705000
C	-1.013727000	-3.561424000	-1.051140000
H	-0.383427000	-3.995615000	-1.805565000
Fe	-3.062273000	-3.361114000	-1.158510000
P	-0.456206000	-0.723028000	-1.618527000
H	-3.004014000	-3.692789000	1.610347000
C	-2.734280000	-0.861106000	0.919045000
H	-2.965957000	-0.098498000	0.177146000
C	-3.997015000	-1.124952000	1.736549000
H	-4.797095000	-1.400339000	1.044065000
H	-3.877717000	-1.940300000	2.446254000
H	-4.322899000	-0.244471000	2.288517000
P	-1.192485000	-0.173292000	1.745664000
Ir	0.161597000	0.859257000	0.076989000
Cl	1.051990000	2.253507000	1.916852000
H	1.338346000	-0.071511000	0.382181000
O	-2.003199000	4.395392000	0.826801000
C	-2.296349000	3.553772000	-0.023341000
C	-3.581158000	3.832123000	-0.859730000
O	-1.747635000	2.480417000	-0.342146000
F	-4.130733000	5.023106000	-0.600876000
F	-4.526438000	2.900039000	-0.611605000
F	-3.333197000	3.789315000	-2.182367000
H	1.297073000	1.852890000	-0.956581000
C	-1.767045000	1.053645000	2.986672000
C	-1.128063000	1.318916000	4.212929000

C	-2.888698000	1.801461000	2.620768000
C	-1.684436000	2.295216000	5.041208000
C	-3.415884000	2.776495000	3.453958000
H	-3.357797000	1.634536000	1.659628000
C	-2.814842000	3.015714000	4.680962000
H	-1.201044000	2.502958000	5.990962000
H	-4.282477000	3.345392000	3.136912000
H	-3.211536000	3.770819000	5.351121000
C	-0.516439000	-1.641718000	2.638780000
C	-1.116130000	-2.268032000	3.748475000
C	0.622131000	-2.220886000	2.069827000
C	-0.540640000	-3.449885000	4.226725000
C	1.172558000	-3.395223000	2.555823000
H	1.080944000	-1.744617000	1.217164000
C	0.581705000	-4.018261000	3.646701000
H	-0.998704000	-3.931704000	5.085406000
H	2.053498000	-3.815653000	2.083500000
H	0.993447000	-4.938023000	4.047960000
C	-2.327094000	-1.781462000	4.506966000
H	-2.766547000	-0.871319000	4.112831000
H	-3.098835000	-2.555999000	4.511342000
H	-2.057016000	-1.593574000	5.550474000
C	0.116456000	0.624131000	4.702281000
H	-0.131465000	-0.247515000	5.315126000
H	0.760508000	0.297627000	3.888928000
H	0.693942000	1.309088000	5.327301000
C	1.043812000	-1.558732000	-2.447938000
C	0.711721000	-2.615751000	-3.533527000
H	1.438501000	-3.430647000	-3.469316000
H	-0.279009000	-3.055443000	-3.470837000
H	0.802212000	-2.180945000	-4.529683000
C	1.880485000	-0.469585000	-3.112830000

H	1.359597000	-0.005971000	-3.949936000
H	2.153682000	0.290945000	-2.386790000
H	2.797316000	-0.917808000	-3.508334000
C	1.920457000	-2.202322000	-1.358306000
H	2.304391000	-1.457221000	-0.661013000
H	1.404215000	-2.975175000	-0.788454000
H	2.782902000	-2.668206000	-1.845410000
C	-1.583331000	0.002257000	-2.970370000
C	-1.769306000	-0.919994000	-4.177655000
H	-2.583123000	-0.520392000	-4.793105000
H	-0.874994000	-0.949936000	-4.800144000
H	-2.031469000	-1.939707000	-3.898541000
C	-1.016108000	1.338454000	-3.465278000
H	-1.803709000	1.876355000	-4.003026000
H	-0.684516000	1.964097000	-2.640070000
H	-0.184944000	1.205816000	-4.158010000
C	-2.945453000	0.286512000	-2.322741000
H	-2.851600000	1.048290000	-1.552011000
H	-3.623819000	0.668126000	-3.093101000
H	-3.394946000	-0.607472000	-1.895502000
C	5.030712000	0.046642000	-1.763365000
C	4.498209000	1.418066000	-2.149634000
C	4.149134000	1.908839000	0.210718000
C	4.654776000	0.517712000	0.536914000
C	6.373142000	-1.066816000	-0.075938000
C	6.306098000	-2.286635000	-0.755284000
C	7.073463000	-3.378606000	-0.358555000
C	7.917820000	-3.285977000	0.737939000
C	8.003653000	-2.083306000	1.434217000
C	7.249649000	-1.009554000	1.014619000
H	5.773782000	-0.242042000	-2.509799000
H	3.996923000	1.322380000	-3.107716000

H	4.969189000	2.631597000	0.314307000
H	3.807367000	-0.186893000	0.557490000
H	5.645506000	-2.388111000	-1.607206000
H	6.997543000	-4.308787000	-0.910379000
H	8.512813000	-4.135064000	1.053099000
H	8.663259000	-1.962554000	2.285808000
N	5.650207000	0.083975000	-0.446605000
N	3.601605000	1.981655000	-1.140642000
H	5.096534000	0.543784000	1.531616000
H	3.370606000	2.148085000	0.929595000
H	5.343481000	2.107648000	-2.276627000
H	4.213251000	-0.683801000	-1.791832000
F	7.374397000	0.160752000	1.682351000
C	2.488771000	2.718401000	-1.403287000
C	2.306602000	3.969924000	-0.564526000
C	2.159297000	2.979865000	-2.874737000
C	0.954604000	4.670381000	-0.677548000
H	2.532007000	3.804512000	0.483113000
C	1.362084000	4.268817000	-3.128202000
H	3.105075000	3.069820000	-3.412839000
C	0.309978000	4.543941000	-2.062853000
H	0.286455000	4.272609000	0.084476000
H	0.900118000	4.192324000	-4.116444000
H	-0.421592000	3.736985000	-2.055435000
H	3.099119000	4.621793000	-0.960660000
H	1.641236000	2.124573000	-3.298372000
H	1.116769000	5.724860000	-0.433123000
H	-0.241828000	5.455689000	-2.309223000
H	2.055448000	5.116187000	-3.170655000

TS_{C3-B1}

Coordinates (Angstroms)

	X	Y	Z
C	-3.473335000	-0.785955000	-3.250386000
C	-4.598324000	0.047988000	-2.997213000
H	-4.732547000	1.059788000	-3.351472000
C	-5.491436000	-0.663691000	-2.148900000
H	-6.419449000	-0.283988000	-1.746729000
C	-3.677506000	-2.010463000	-2.563450000
H	-2.999151000	-2.847208000	-2.560258000
C	-4.917299000	-1.936166000	-1.873339000
H	-5.340591000	-2.702478000	-1.240150000
H	-2.608294000	-0.530644000	-3.845035000
C	-2.062126000	0.663604000	-0.563218000
C	-3.255292000	1.435656000	-0.490327000
C	-4.172536000	0.771614000	0.360397000
H	-5.184396000	1.083520000	0.573370000
C	-2.221787000	-0.480992000	0.302818000
C	-3.556306000	-0.414610000	0.822524000
H	-4.022995000	-1.132063000	1.476461000
Fe	-3.678170000	-0.417870000	-1.230296000
P	-0.842864000	-1.500552000	0.973540000
H	-3.453632000	2.348254000	-1.030555000
C	-0.845828000	1.053500000	-1.361613000
H	-0.404839000	0.153532000	-1.792992000
C	-1.178411000	2.032231000	-2.484210000
H	-1.880527000	1.560112000	-3.174863000
H	-1.643715000	2.942781000	-2.108863000
H	-0.289273000	2.314597000	-3.048239000
P	0.414537000	1.609555000	-0.102405000
Ir	1.169421000	-0.318176000	1.072288000
Cl	3.353540000	0.729178000	1.644636000
H	0.621230000	0.235184000	2.400383000
O	3.388495000	-2.486747000	0.761421000

C	3.275523000	-2.037140000	-0.409219000
C	4.221147000	-2.655231000	-1.456161000
O	2.462318000	-1.203755000	-0.815025000
F	5.375707000	-3.053351000	-0.922086000
F	4.492947000	-1.796171000	-2.439547000
F	3.628849000	-3.729821000	-2.004214000
H	1.683041000	-1.610301000	2.027326000
C	1.845534000	2.297266000	-1.020667000
C	2.718383000	3.264417000	-0.489863000
C	2.145007000	1.692092000	-2.244775000
C	3.834212000	3.625162000	-1.247582000
C	3.265837000	2.058747000	-2.974592000
H	1.506776000	0.909870000	-2.638307000
C	4.110489000	3.040906000	-2.475907000
H	4.511933000	4.373975000	-0.849191000
H	3.476267000	1.573873000	-3.921181000
H	4.991932000	3.341698000	-3.031950000
C	-0.498806000	2.951131000	0.767084000
C	-0.769062000	4.236652000	0.259555000
C	-1.083615000	2.560921000	1.976415000
C	-1.609457000	5.070424000	1.006085000
C	-1.920479000	3.398707000	2.693414000
H	-0.887308000	1.569793000	2.355391000
C	-2.184444000	4.670114000	2.201252000
H	-1.814007000	6.065659000	0.622793000
H	-2.360749000	3.056900000	3.623421000
H	-2.834381000	5.347658000	2.744344000
C	-0.220716000	4.826885000	-1.017095000
H	0.377831000	4.138409000	-1.604687000
H	-1.041981000	5.180590000	-1.646068000
H	0.401710000	5.696309000	-0.785116000
C	2.520562000	3.933746000	0.845073000

H	1.889322000	4.822423000	0.755446000
H	2.066759000	3.267841000	1.577792000
H	3.485330000	4.255013000	1.243054000
C	-1.373382000	-1.965893000	2.757888000
C	-2.484834000	-3.027985000	2.801873000
H	-2.885063000	-3.060384000	3.820070000
H	-3.317352000	-2.839518000	2.126201000
H	-2.084057000	-4.017710000	2.579996000
C	-0.183455000	-2.542489000	3.548194000
H	0.332233000	-3.350935000	3.029056000
H	0.546640000	-1.775191000	3.804259000
H	-0.577532000	-2.951019000	4.484831000
C	-1.831368000	-0.713700000	3.524844000
H	-1.021599000	0.009147000	3.632383000
H	-2.690729000	-0.212231000	3.081316000
H	-2.114790000	-1.027004000	4.535051000
C	-0.786012000	-3.060299000	-0.105262000
C	-2.139246000	-3.785542000	-0.199547000
H	-2.145580000	-4.386794000	-1.114475000
H	-2.291342000	-4.470498000	0.632048000
H	-2.986496000	-3.102519000	-0.244718000
C	0.255910000	-4.060455000	0.406024000
H	0.339294000	-4.870714000	-0.326867000
H	1.246472000	-3.622460000	0.524770000
H	-0.045291000	-4.509605000	1.354168000
C	-0.372749000	-2.588269000	-1.508421000
H	0.617413000	-2.134648000	-1.511055000
H	-0.347832000	-3.456896000	-2.174843000
H	-1.085664000	-1.874884000	-1.922169000
H	2.425910000	-1.883345000	1.432849000

D1

Coordinates (Angstroms)			
	X	Y	Z
C	-3.338451000	3.709297000	-0.076207000
C	-2.091003000	4.202163000	0.396884000
H	-1.952162000	4.902105000	1.208249000
C	-1.057152000	3.570265000	-0.346834000
C	-3.077715000	2.772315000	-1.112272000
H	-3.821110000	2.212682000	-1.660805000
C	-1.665382000	2.686110000	-1.278637000
H	-1.140815000	2.058465000	-1.982401000
H	-4.312201000	3.970850000	0.312376000
C	-2.987948000	1.684366000	2.479274000
C	-1.588552000	1.852745000	2.562891000
C	-0.944580000	0.918937000	1.697760000
C	-3.236800000	0.650087000	1.553585000
H	-4.217517000	0.309048000	1.279665000
C	-1.988234000	0.153946000	1.042062000
H	-3.737524000	2.273532000	2.987359000
Fe	-2.189111000	2.167473000	0.642929000
C	0.574225000	0.885414000	1.776817000
H	0.846522000	1.937973000	1.740940000
P	-1.792293000	-1.341250000	0.003641000
C	-2.046955000	-2.712213000	1.307300000
C	-1.164688000	-2.364759000	2.512000000
H	-0.126438000	-2.224911000	2.213176000
H	-1.507550000	-1.466440000	3.028190000
H	-1.198665000	-3.196553000	3.222855000
C	-3.495776000	-2.796689000	1.804956000
H	-4.183449000	-3.174256000	1.047918000
H	-3.523172000	-3.497564000	2.646256000
H	-3.865398000	-1.836337000	2.170474000
C	-1.607390000	-4.091511000	0.793853000

H	-1.803228000	-4.823797000	1.584600000
H	-2.146998000	-4.415296000	-0.094458000
H	-0.539836000	-4.117198000	0.573275000
C	-3.234271000	-1.437292000	-1.267498000
C	-3.406398000	-2.892366000	-1.731805000
H	-3.867203000	-3.526078000	-0.973702000
H	-4.074405000	-2.886772000	-2.599635000
H	-2.462342000	-3.341608000	-2.046040000
C	-4.596439000	-0.928183000	-0.769649000
H	-5.343974000	-1.207219000	-1.519421000
H	-4.912619000	-1.360530000	0.177698000
H	-4.610341000	0.159283000	-0.691947000
C	-2.892277000	-0.610173000	-2.516541000
H	-2.554697000	0.396585000	-2.275936000
H	-2.136122000	-1.096388000	-3.131661000
H	-3.801970000	-0.521178000	-3.119019000
H	0.003862000	3.712418000	-0.204301000
C	1.013627000	0.407501000	3.170034000
H	0.582785000	1.082195000	3.913855000
H	0.673051000	-0.598995000	3.405208000
H	2.097078000	0.443839000	3.286525000
P	1.473464000	0.192993000	0.274192000
C	3.023958000	-0.637073000	0.875318000
C	4.331994000	-0.434425000	0.389350000
C	2.810254000	-1.660320000	1.806336000
C	5.363310000	-1.208592000	0.935916000
C	3.844116000	-2.419203000	2.328975000
H	1.803372000	-1.889252000	2.124451000
C	5.141823000	-2.177454000	1.901137000
H	6.372060000	-1.051650000	0.566771000
H	3.630855000	-3.195827000	3.054908000
H	5.972176000	-2.754553000	2.293469000

C	1.986761000	1.788102000	-0.514969000
C	2.639201000	2.832258000	0.173590000
C	1.678542000	1.963113000	-1.864700000
C	2.889839000	4.023663000	-0.510058000
C	1.944405000	3.150826000	-2.530392000
H	1.233579000	1.149901000	-2.418086000
C	2.539969000	4.197013000	-1.841582000
H	3.390415000	4.829067000	0.018743000
H	1.687836000	3.252721000	-3.578906000
H	2.748815000	5.137736000	-2.339448000
C	3.139181000	2.743128000	1.594861000
H	2.428471000	3.183357000	2.301824000
H	3.334896000	1.719053000	1.910549000
H	4.073009000	3.301643000	1.688820000
C	4.723335000	0.516717000	-0.713711000
H	4.012246000	0.495411000	-1.538285000
H	4.800647000	1.547737000	-0.360196000
H	5.701088000	0.230435000	-1.106666000
Ir	0.250243000	-1.419149000	-1.040227000
H	-0.401109000	-2.682377000	-1.810743000
Cl	2.399435000	-1.935129000	-2.284142000
H	-1.070717000	2.591317000	3.158744000
H	0.677547000	-2.475357000	0.047544000
H	-0.112209000	-0.531463000	-2.611737000
H	-0.353503000	-0.010797000	-2.025017000

D2

Coordinates (Angstroms)			
	X	Y	Z
C	2.499308000	1.385979000	3.942338000
C	1.256581000	0.905259000	4.440439000
H	0.732600000	1.282863000	5.306806000

C	0.796591000	-0.115494000	3.563563000
C	2.808020000	0.662468000	2.758987000
H	3.681964000	0.804838000	2.140712000
C	1.753682000	-0.265282000	2.523873000
H	1.688463000	-0.964300000	1.704301000
H	3.084987000	2.188912000	4.366686000
C	0.549776000	3.661805000	2.599724000
C	-0.616344000	2.867262000	2.664214000
C	-0.702185000	2.053769000	1.494886000
C	1.212248000	3.347054000	1.395131000
H	2.139189000	3.789981000	1.081451000
C	0.463677000	2.347090000	0.684194000
H	0.903908000	4.345641000	3.357387000
Fe	1.017244000	1.655740000	2.546080000
C	-1.977940000	1.238863000	1.343265000
H	-2.108065000	0.792978000	2.327171000
P	0.800165000	1.799310000	-1.028520000
C	0.171327000	3.311364000	-2.011897000
C	-1.215566000	3.672601000	-1.465102000
H	-1.895878000	2.822539000	-1.514429000
H	-1.173497000	4.032461000	-0.435277000
H	-1.636225000	4.471523000	-2.084436000
C	1.070600000	4.543855000	-1.846851000
H	2.035520000	4.429642000	-2.341181000
H	0.566298000	5.397431000	-2.312357000
H	1.239696000	4.798340000	-0.798753000
C	0.010307000	3.007709000	-3.509060000
H	-0.332030000	3.923149000	-4.003771000
H	0.936648000	2.700161000	-3.991154000
H	-0.737352000	2.233742000	-3.683798000
C	2.698671000	1.649716000	-1.295908000
C	3.013638000	1.749416000	-2.797627000

H	2.920097000	2.764661000	-3.184617000
H	4.055049000	1.441646000	-2.938955000
H	2.390176000	1.081588000	-3.395206000
C	3.564770000	2.680682000	-0.555455000
H	4.589299000	2.571967000	-0.926835000
H	3.268397000	3.714277000	-0.725844000
H	3.590477000	2.485691000	0.516678000
C	3.178424000	0.264576000	-0.838377000
H	2.824491000	-0.001063000	0.155709000
H	2.873333000	-0.511971000	-1.537777000
H	4.271916000	0.279755000	-0.812753000
H	-0.134182000	-0.656205000	3.652989000
H	-4.450277000	-3.843786000	-0.419526000
Ir	-0.273057000	-0.150156000	-1.566574000
H	0.594791000	-0.020995000	-2.922974000
Cl	-1.321763000	-2.207047000	-2.588302000
H	-1.326355000	2.842446000	3.478928000
H	-1.345001000	0.754268000	-2.298775000
H	0.967646000	-1.407373000	-1.201815000
H	0.867033000	-1.012900000	-0.479459000
C	2.950879000	-3.154668000	-0.523869000
C	4.469294000	-3.044108000	-0.861913000
O	2.219166000	-3.409268000	-1.492947000
O	2.674499000	-3.009638000	0.676158000
F	4.699673000	-2.551439000	-2.090280000
F	5.142365000	-2.268134000	0.003413000
F	5.044609000	-4.264571000	-0.818554000

D3

Coordinates (Angstroms)

	X	Y	Z
C	1.711668000	2.752908000	3.749087000

C	0.573620000	2.066848000	4.257591000
H	-0.107252000	2.437604000	5.010383000
C	0.457326000	0.832402000	3.561655000
C	2.298737000	1.942427000	2.739024000
H	3.166885000	2.196449000	2.148991000
C	1.519714000	0.756571000	2.620645000
H	1.677386000	-0.045555000	1.916533000
H	2.048365000	3.734590000	4.050609000
C	-0.574552000	4.201362000	1.863089000
C	-1.522116000	3.165291000	2.018245000
C	-1.288633000	2.157256000	1.034623000
C	0.268411000	3.845887000	0.788982000
H	1.093864000	4.443416000	0.451254000
C	-0.143040000	2.577347000	0.251960000
H	-0.474193000	5.079636000	2.484339000
Fe	0.353770000	2.404143000	2.246073000
C	-2.314181000	1.035809000	0.973046000
H	-2.438218000	0.750432000	2.015179000
P	0.487716000	1.816097000	-1.299149000
C	-0.364924000	2.963255000	-2.584103000
C	-1.855112000	3.008609000	-2.220651000
H	-2.280854000	2.006089000	-2.173642000
H	-2.029887000	3.511672000	-1.267767000
H	-2.390660000	3.564620000	-2.997467000
C	0.155861000	4.406430000	-2.573114000
H	1.171121000	4.492217000	-2.961885000
H	-0.489191000	5.006043000	-3.225304000
H	0.118364000	4.858047000	-1.580126000
C	-0.258504000	2.418714000	-4.016512000
H	-0.834878000	3.079912000	-4.673512000
H	0.762602000	2.394909000	-4.393649000
H	-0.678285000	1.416460000	-4.099665000

C	2.390213000	2.138434000	-1.419238000
C	2.823206000	2.066896000	-2.892723000
H	2.542616000	2.956536000	-3.457457000
H	3.916279000	1.997885000	-2.918535000
H	2.427558000	1.183313000	-3.397419000
C	2.889520000	3.475155000	-0.846915000
H	3.940081000	3.585044000	-1.136840000
H	2.360470000	4.348074000	-1.224137000
H	2.857037000	3.479390000	0.242695000
C	3.167465000	1.039244000	-0.678158000
H	2.772785000	0.839288000	0.314692000
H	3.174201000	0.109561000	-1.241882000
H	4.206139000	1.371265000	-0.571110000
H	-0.321075000	0.096188000	3.698054000
C	-3.675128000	1.611203000	0.551303000
H	-3.952892000	2.395183000	1.260238000
H	-3.658196000	2.057713000	-0.441640000
H	-4.457760000	0.852760000	0.578583000
P	-1.733335000	-0.569998000	0.168112000
C	-3.241262000	-1.385576000	-0.568927000
C	-3.667462000	-2.717103000	-0.381709000
C	-3.922744000	-0.600785000	-1.507607000
C	-4.807716000	-3.149425000	-1.071796000
C	-5.046277000	-1.048030000	-2.182604000
H	-3.553779000	0.388739000	-1.735971000
C	-5.507978000	-2.335468000	-1.946851000
H	-5.138135000	-4.172851000	-0.922517000
H	-5.545029000	-0.397421000	-2.892578000
H	-6.386215000	-2.714152000	-2.458695000
C	-1.364936000	-1.520163000	1.722247000
C	-2.266701000	-1.661118000	2.798372000
C	-0.102069000	-2.103376000	1.824892000

C	-1.838048000	-2.341907000	3.940049000
C	0.304076000	-2.784273000	2.963862000
H	0.581625000	-2.012725000	0.992269000
C	-0.568560000	-2.894772000	4.036518000
H	-2.532381000	-2.451989000	4.767794000
H	1.297159000	-3.217733000	3.007992000
H	-0.271479000	-3.416584000	4.940055000
C	-3.692568000	-1.163353000	2.804078000
H	-3.776931000	-0.198211000	3.314510000
H	-4.110604000	-1.049069000	1.805064000
H	-4.324568000	-1.868460000	3.348947000
C	-2.974180000	-3.752772000	0.468510000
H	-1.891508000	-3.694322000	0.371354000
H	-3.225778000	-3.653392000	1.527051000
H	-3.287652000	-4.748999000	0.148687000
Ir	-0.045857000	-0.380316000	-1.499155000
H	1.042196000	-0.359046000	-2.707259000
Cl	-0.366212000	-2.871669000	-1.988334000
H	-2.289576000	3.113443000	2.777843000
H	-1.211814000	-0.071838000	-2.635615000
H	1.970997000	-1.772003000	-0.864136000
H	1.148238000	-0.726709000	-0.389594000
C	3.525309000	-2.408797000	0.082424000
C	4.856075000	-3.136223000	-0.207842000
O	2.779985000	-2.385270000	-0.980012000
O	3.306903000	-1.934424000	1.167420000
F	5.605465000	-2.401036000	-1.041269000
F	5.548820000	-3.325428000	0.911132000
F	4.652774000	-4.325517000	-0.781910000

D4

Coordinates (Angstroms)

	X	Y	Z
C	-3.294488000	3.750070000	-0.055675000
C	-2.036295000	4.222136000	0.410857000
H	-1.881820000	4.921417000	1.220114000
C	-1.017191000	3.571084000	-0.336900000
C	-3.054217000	2.807455000	-1.092201000
H	-3.809303000	2.258984000	-1.635704000
C	-1.644612000	2.694994000	-1.264175000
H	-1.133465000	2.040750000	-1.953469000
H	-4.261933000	4.030512000	0.335826000
C	-2.965323000	1.693065000	2.485818000
C	-1.563898000	1.847279000	2.570406000
C	-0.931102000	0.914051000	1.694816000
C	-3.222264000	0.670740000	1.547435000
H	-4.206815000	0.345847000	1.268413000
C	-1.978915000	0.165157000	1.032055000
H	-3.709840000	2.282975000	3.000838000
Fe	-2.166304000	2.188734000	0.657266000
C	0.586892000	0.853283000	1.770267000
H	0.881220000	1.899907000	1.738903000
P	-1.778660000	-1.328961000	-0.021896000
C	-2.129157000	-2.688763000	1.292620000
C	-1.225558000	-2.391316000	2.496492000
H	-0.178790000	-2.327181000	2.196234000
H	-1.505815000	-1.465949000	3.003356000
H	-1.317638000	-3.209989000	3.218327000
C	-3.578355000	-2.714072000	1.795074000
H	-4.280606000	-3.059696000	1.035659000
H	-3.636364000	-3.419654000	2.631684000
H	-3.910714000	-1.743271000	2.167668000
C	-1.766871000	-4.093036000	0.785505000
H	-1.944003000	-4.805106000	1.599602000

H	-2.368800000	-4.412459000	-0.063723000
H	-0.716062000	-4.158608000	0.504313000
C	-3.234740000	-1.380131000	-1.294658000
C	-3.447588000	-2.827632000	-1.766930000
H	-3.955103000	-3.441945000	-1.022104000
H	-4.089382000	-2.800690000	-2.654500000
H	-2.512142000	-3.312632000	-2.052138000
C	-4.589047000	-0.845401000	-0.799465000
H	-5.339884000	-1.101792000	-1.554726000
H	-4.921410000	-1.277284000	0.142254000
H	-4.580974000	0.241313000	-0.712706000
C	-2.884955000	-0.553484000	-2.541731000
H	-2.542537000	0.449200000	-2.294441000
H	-2.116388000	-1.033736000	-3.144772000
H	-3.791716000	-0.463270000	-3.150531000
H	0.046933000	3.691818000	-0.198533000
C	1.006308000	0.360232000	3.164025000
H	0.568309000	1.025764000	3.912096000
H	0.658600000	-0.649067000	3.379197000
H	2.088572000	0.390592000	3.294171000
P	1.460213000	0.126334000	0.261343000
C	3.055796000	-0.627270000	0.874023000
C	4.354172000	-0.401336000	0.371156000
C	2.889133000	-1.619001000	1.849105000
C	5.418104000	-1.110794000	0.944679000
C	3.953709000	-2.311435000	2.401513000
H	1.891587000	-1.874879000	2.177221000
C	5.240134000	-2.040234000	1.956015000
H	6.417743000	-0.933789000	0.559430000
H	3.773776000	-3.063369000	3.161982000
H	6.094295000	-2.565189000	2.370207000
C	1.951712000	1.730473000	-0.541606000

C	2.628581000	2.776863000	0.119479000
C	1.594801000	1.901652000	-1.879364000
C	2.872269000	3.959967000	-0.581618000
C	1.853514000	3.080942000	-2.563590000
H	1.094072000	1.085914000	-2.386242000
C	2.487174000	4.124689000	-1.904784000
H	3.391650000	4.766944000	-0.073146000
H	1.556708000	3.181370000	-3.601975000
H	2.691700000	5.059046000	-2.416811000
C	3.152256000	2.710193000	1.534611000
H	2.469223000	3.201514000	2.235582000
H	3.312749000	1.691801000	1.884534000
H	4.107657000	3.236435000	1.597447000
C	4.709866000	0.512045000	-0.776168000
H	3.969792000	0.469559000	-1.572903000
H	4.808691000	1.553056000	-0.458277000
H	5.671176000	0.205007000	-1.194293000
Ir	0.254571000	-1.478596000	-1.005024000
H	-0.455145000	-2.629169000	-1.906039000
Cl	2.382314000	-1.838774000	-2.418260000
H	-1.038213000	2.573736000	3.174375000
H	0.793539000	-2.691271000	0.013724000
H	-0.222902000	-0.374869000	-2.141969000

TS_{D2-D3}

Coordinates (Angstroms)			
	X	Y	Z
C	1.973647000	2.537767000	3.754499000
C	0.784934000	1.945907000	4.264777000
H	0.143216000	2.366754000	5.025657000
C	0.556583000	0.735352000	3.555046000
C	2.480593000	1.692174000	2.730153000

H	3.364541000	1.876568000	2.137836000
C	1.601032000	0.579543000	2.603457000
H	1.694212000	-0.233793000	1.900222000
H	2.396447000	3.483056000	4.063792000
C	-0.200679000	4.198458000	1.914007000
C	-1.229014000	3.242135000	2.066728000
C	-1.091795000	2.233350000	1.065599000
C	0.597065000	3.791975000	0.823489000
H	1.465080000	4.323554000	0.481720000
C	0.075053000	2.570344000	0.273966000
H	-0.018990000	5.053788000	2.548613000
Fe	0.578478000	2.324386000	2.258294000
C	-2.208599000	1.202095000	1.004428000
H	-2.347067000	0.921734000	2.046400000
P	0.629991000	1.777522000	-1.287109000
C	-0.145926000	2.979755000	-2.561420000
C	-1.619338000	3.162443000	-2.175503000
H	-2.132749000	2.202975000	-2.111470000
H	-1.734133000	3.690061000	-1.226611000
H	-2.114377000	3.754704000	-2.952262000
C	0.505659000	4.369230000	-2.563047000
H	1.512483000	4.361823000	-2.981416000
H	-0.101238000	5.028488000	-3.193574000
H	0.540815000	4.816920000	-1.568082000
C	-0.115173000	2.420043000	-3.991921000
H	-0.578666000	3.160285000	-4.653887000
H	0.890931000	2.234413000	-4.363829000
H	-0.685221000	1.494457000	-4.074021000
C	2.547759000	1.943253000	-1.426982000
C	2.959999000	1.839669000	-2.904562000
H	2.741792000	2.747661000	-3.467793000
H	4.044250000	1.688143000	-2.938791000

H	2.494303000	0.988256000	-3.404513000
C	3.163949000	3.228561000	-0.852621000
H	4.216218000	3.251477000	-1.156337000
H	2.705513000	4.146032000	-1.217204000
H	3.147585000	3.227247000	0.237415000
C	3.225243000	0.773839000	-0.699282000
H	2.838092000	0.622622000	0.305452000
H	3.115334000	-0.153727000	-1.255648000
H	4.295745000	0.993559000	-0.621458000
H	-0.284044000	0.070839000	3.688186000
C	-3.520641000	1.889536000	0.595724000
H	-3.723364000	2.695432000	1.305480000
H	-3.478544000	2.331817000	-0.398163000
H	-4.364026000	1.199467000	0.633702000
P	-1.773035000	-0.443529000	0.190497000
C	-3.338858000	-1.112893000	-0.568761000
C	-3.884464000	-2.401893000	-0.393732000
C	-3.929031000	-0.268244000	-1.516776000
C	-5.045467000	-2.729526000	-1.106099000
C	-5.072929000	-0.614180000	-2.216943000
H	-3.470747000	0.685670000	-1.734035000
C	-5.651392000	-1.855783000	-1.994134000
H	-5.468828000	-3.719552000	-0.967384000
H	-5.495563000	0.077557000	-2.937286000
H	-6.547591000	-2.155304000	-2.526827000
C	-1.485451000	-1.439430000	1.731387000
C	-2.387622000	-1.500161000	2.814381000
C	-0.285197000	-2.145185000	1.817740000
C	-2.014798000	-2.222431000	3.950132000
C	0.065106000	-2.865510000	2.950623000
H	0.395004000	-2.128090000	0.979286000
C	-0.802229000	-2.893061000	4.032570000

H	-2.708244000	-2.269956000	4.784490000
H	1.011641000	-3.393712000	2.980490000
H	-0.547728000	-3.443241000	4.932216000
C	-3.763363000	-0.877712000	2.826604000
H	-3.765246000	0.081477000	3.354631000
H	-4.164322000	-0.710382000	1.828144000
H	-4.457351000	-1.535443000	3.355022000
C	-3.296759000	-3.498623000	0.459578000
H	-2.214326000	-3.555001000	0.352685000
H	-3.526971000	-3.368739000	1.519467000
H	-3.715229000	-4.458517000	0.149295000
Ir	-0.071418000	-0.379669000	-1.490724000
H	0.963376000	-0.408818000	-2.735186000
Cl	-0.650613000	-2.793914000	-2.047671000
H	-1.988522000	3.240530000	2.836021000
H	-1.184073000	0.098405000	-2.560947000
H	1.637471000	-1.651211000	-0.720066000
H	1.091061000	-0.854922000	-0.319795000
C	3.280471000	-2.618548000	0.103564000
C	4.556017000	-3.404269000	-0.286600000
O	2.485205000	-2.497071000	-0.885504000
O	3.170742000	-2.196033000	1.239195000
F	5.281044000	-2.702044000	-1.173508000
F	5.333886000	-3.648373000	0.768192000
F	4.254292000	-4.579723000	-0.854673000

TS_{D4-B1}

Coordinates (Angstroms)			
	X	Y	Z
C	5.915763000	-1.420915000	-1.793696000
C	5.962243000	-0.012626000	-1.597662000
H	6.451576000	0.701548000	-2.244347000

C	5.207557000	0.295139000	-0.432801000
C	5.131640000	-1.984284000	-0.750190000
H	4.894756000	-3.031106000	-0.630154000
C	4.691013000	-0.921635000	0.089106000
H	4.050744000	-1.008291000	0.953680000
H	6.365575000	-1.962016000	-2.613783000
C	3.443734000	-0.643013000	-3.804830000
C	3.221296000	0.624893000	-3.224231000
C	2.316252000	0.485081000	-2.130765000
C	2.694439000	-1.584653000	-3.067752000
H	2.683203000	-2.636097000	-3.279363000
C	1.985234000	-0.913764000	-2.010599000
H	4.110579000	-0.868068000	-4.624564000
Fe	4.020727000	-0.629130000	-1.829770000
C	1.831172000	1.759146000	-1.478178000
H	2.746015000	2.321652000	-1.312278000
P	0.675618000	-1.667555000	-0.968058000
C	-0.720662000	-1.788014000	-2.280708000
C	-0.866959000	-0.400798000	-2.919142000
H	-1.067982000	0.359205000	-2.165005000
H	0.017463000	-0.112739000	-3.490037000
H	-1.718490000	-0.421052000	-3.606859000
C	-0.457643000	-2.789647000	-3.411587000
H	-0.475807000	-3.826230000	-3.074248000
H	-1.257217000	-2.679458000	-4.152869000
H	0.487368000	-2.603561000	-3.925315000
C	-2.059522000	-2.121575000	-1.616842000
H	-2.860253000	-1.985795000	-2.352260000
H	-2.111062000	-3.149949000	-1.262117000
H	-2.253093000	-1.453068000	-0.779800000
C	1.233515000	-3.469137000	-0.559680000
C	-0.029149000	-4.284642000	-0.263967000

H	-0.539311000	-4.602374000	-1.173601000
H	0.252824000	-5.186804000	0.288388000
H	-0.726106000	-3.720987000	0.346860000
C	2.030897000	-4.223619000	-1.634942000
H	2.099253000	-5.267580000	-1.309496000
H	1.559441000	-4.225353000	-2.615660000
H	3.050438000	-3.849093000	-1.723316000
C	2.110101000	-3.479725000	0.700230000
H	2.951027000	-2.793914000	0.617951000
H	1.552008000	-3.214458000	1.595248000
H	2.507571000	-4.492672000	0.828559000
H	5.030632000	1.282468000	-0.033748000
C	1.025259000	2.590778000	-2.488195000
H	1.648041000	2.754666000	-3.370899000
H	0.112203000	2.098029000	-2.816126000
H	0.766042000	3.569423000	-2.084106000
P	1.155855000	1.581005000	0.266091000
C	-0.085406000	2.972184000	0.456310000
C	-0.098048000	4.006949000	1.414606000
C	-1.164152000	2.885004000	-0.432676000
C	-1.155404000	4.927334000	1.377694000
C	-2.201567000	3.800581000	-0.449299000
H	-1.210225000	2.059655000	-1.126643000
C	-2.190334000	4.847431000	0.461704000
H	-1.164471000	5.721894000	2.117582000
H	-3.010286000	3.684683000	-1.161563000
H	-2.988694000	5.581723000	0.475509000
C	2.684477000	2.095263000	1.190864000
C	3.421581000	3.265889000	0.908638000
C	3.133775000	1.241989000	2.198371000
C	4.590912000	3.502666000	1.634791000
C	4.296577000	1.497538000	2.911005000

H	2.554101000	0.354378000	2.417183000
C	5.036539000	2.634346000	2.620909000
H	5.156609000	4.405105000	1.423252000
H	4.619536000	0.807687000	3.682993000
H	5.951468000	2.852067000	3.161705000
C	3.038533000	4.323454000	-0.100929000
H	3.570493000	4.182136000	-1.047502000
H	1.972009000	4.349627000	-0.318978000
H	3.321369000	5.307629000	0.279137000
C	0.905259000	4.216599000	2.522028000
H	1.314600000	3.283256000	2.897156000
H	1.733736000	4.852515000	2.198211000
H	0.414958000	4.726991000	3.354362000
Ir	0.111405000	-0.404179000	0.893002000
H	-1.115325000	-1.589555000	1.573737000
Cl	-0.264432000	0.969889000	2.984991000
H	3.675402000	1.556854000	-3.530191000
H	-1.212797000	0.223777000	0.149215000
H	1.380623000	-1.086173000	1.736004000
C	-7.290663000	0.376298000	-1.283479000
C	-8.095819000	1.088586000	-2.166484000
C	-7.540828000	1.983990000	-3.069982000
C	-6.158454000	2.146383000	-3.099311000
C	-5.375473000	1.414612000	-2.234463000
C	-5.896703000	0.522639000	-1.285359000
H	-7.754109000	-0.296096000	-0.572303000
H	-9.170297000	0.946475000	-2.130765000
H	-8.167071000	2.549089000	-3.749982000
H	-5.677063000	2.815967000	-3.802982000
C	-4.443617000	-2.189701000	0.790591000
C	-5.580587000	-1.304963000	0.307838000
N	-5.048310000	-0.177789000	-0.435236000

C	-4.013921000	0.591579000	0.275961000
C	-3.727865000	0.020219000	1.659097000
N	-3.493272000	-1.418632000	1.599081000
H	-4.872580000	-2.992472000	1.396595000
H	-6.200358000	-1.912120000	-0.354268000
H	-3.088013000	0.599643000	-0.299128000
H	-2.826916000	0.511028000	2.025164000
C	-1.224516000	-4.123954000	2.927826000
C	-2.417323000	-3.510492000	2.198998000
C	-2.480590000	-2.000017000	2.279541000
C	-2.221575000	-1.476799000	3.679859000
C	-1.035019000	-2.115745000	4.387679000
C	-1.124273000	-3.637494000	4.369267000
H	-1.314190000	-5.213126000	2.883242000
H	-2.468863000	-3.847453000	1.163639000
H	-2.125207000	-0.396310000	3.692678000
H	-0.113374000	-1.791852000	3.894753000
H	-2.003945000	-3.966287000	4.937301000
H	-3.337966000	-3.864652000	2.682753000
H	-3.146003000	-1.731526000	4.218365000
H	-0.998921000	-1.738114000	5.414059000
H	-0.246114000	-4.077615000	4.851137000
H	-0.302484000	-3.854870000	2.408630000
F	-4.027688000	1.544782000	-2.331208000
H	-6.210841000	-0.996048000	1.155159000
H	-3.951136000	-2.644404000	-0.070053000
H	-4.544572000	0.244820000	2.353640000
H	-4.334250000	1.630431000	0.410985000

E1

Coordinates (Angstroms)

X	Y	Z
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P	1.872872000	-0.530238000	-0.236895000
P	-1.887584000	-0.091072000	-0.106449000
O	0.292950000	1.822716000	0.244761000
C	0.602381000	4.531918000	-0.218548000
C	1.642618000	3.532816000	-0.722025000
C	-0.758897000	3.861650000	-0.395334000
C	1.429291000	2.192891000	-0.423457000
C	-0.834103000	2.493723000	-0.151423000
C	0.843831000	4.769032000	1.289737000
C	0.685834000	5.867717000	-0.954867000
C	2.310010000	1.173223000	-0.752020000
C	-1.988049000	1.737858000	-0.300284000
C	2.808987000	3.846481000	-1.412289000
C	-1.935802000	4.504483000	-0.760138000
C	3.479041000	1.523257000	-1.427682000
C	-3.156231000	2.421390000	-0.647626000
C	3.716759000	2.850825000	-1.760237000
C	-3.126077000	3.791552000	-0.867034000
C	1.923453000	-0.467130000	1.593900000
C	3.408478000	-1.424962000	-0.695603000
C	-3.532123000	-0.553630000	-0.763376000
C	-2.006206000	-0.353452000	1.706427000
C	2.421003000	0.611146000	2.322732000
C	4.473101000	-1.534823000	0.197230000
C	-4.661417000	-0.707215000	0.037189000
C	-2.247931000	-1.655381000	2.159352000
C	1.404725000	-1.573968000	2.270719000
C	3.537413000	-1.948738000	-1.983716000
C	-3.650579000	-0.676249000	-2.149146000
C	-1.755129000	0.654287000	2.635963000
C	2.390636000	0.584262000	3.712938000
C	5.647508000	-2.172885000	-0.189284000

C	-5.895803000	-0.985492000	-0.542401000
C	-2.262412000	-1.934963000	3.518417000
C	1.383578000	-1.601962000	3.658074000
C	4.715197000	-2.573450000	-2.371219000
C	-4.884229000	-0.940754000	-2.726447000
C	-1.753787000	0.365968000	3.997332000
C	1.872410000	-0.518837000	4.381085000
C	5.771270000	-2.690959000	-1.472178000
C	-6.009717000	-1.099581000	-1.922348000
C	-2.012033000	-0.924532000	4.441550000
H	0.089308000	5.456013000	1.683434000
H	0.790549000	3.836940000	1.858272000
H	1.832179000	5.211130000	1.444748000
H	1.665328000	6.326690000	-0.802451000
H	0.521107000	5.747330000	-2.029105000
H	-0.057116000	6.567135000	-0.565327000
H	3.024066000	4.875131000	-1.675327000
H	-1.935558000	5.569539000	-0.958327000
H	4.202339000	0.765719000	-1.702459000
H	-4.089609000	1.885793000	-0.766706000
H	4.623554000	3.113853000	-2.292534000
H	-4.039009000	4.308927000	-1.138804000
H	2.835048000	1.475778000	1.815731000
H	4.393522000	-1.126188000	1.198206000
H	-4.588796000	-0.601620000	1.113683000
H	-2.432511000	-2.451376000	1.444528000
H	1.016651000	-2.419018000	1.708483000
H	2.714639000	-1.870223000	-2.685883000
H	-2.773210000	-0.564963000	-2.778080000
H	-1.564558000	1.671169000	2.311948000
H	2.774320000	1.429685000	4.273217000
H	6.465310000	-2.262600000	0.517217000

H	-6.769846000	-1.105560000	0.088353000
H	-2.460609000	-2.946357000	3.856025000
H	0.975266000	-2.464319000	4.172479000
H	4.806303000	-2.975792000	-3.374115000
H	-4.967984000	-1.032173000	-3.803792000
H	-1.552405000	1.157023000	4.711249000
H	1.846897000	-0.534838000	5.465217000
H	6.687405000	-3.187787000	-1.772286000
H	-6.973212000	-1.311072000	-2.373233000
H	-2.012439000	-1.144342000	5.503533000
Ir	-0.036717000	-1.621500000	-0.795883000
H	0.090703000	-1.135616000	-2.255175000
Cl	-1.729775000	-3.397307000	-1.200759000
H	0.990874000	-2.769470000	-1.188513000

E2

Coordinates (Angstroms)			
	X	Y	Z
P	-1.722377000	-0.264514000	0.046852000
P	1.783790000	-0.325611000	-0.102561000
O	0.067405000	1.908275000	-1.012147000
C	0.101348000	4.617563000	-0.645183000
C	-1.152016000	3.802956000	-0.298646000
C	1.305919000	3.763854000	-0.226688000
C	-1.076699000	2.426112000	-0.484913000
C	1.199712000	2.390980000	-0.428575000
C	0.150595000	4.835418000	-2.173372000
C	0.103194000	5.974787000	0.056497000
C	-2.064020000	1.530448000	-0.110702000
C	2.145826000	1.465298000	-0.027555000
C	-2.348549000	4.301256000	0.200123000
C	2.488822000	4.219471000	0.339213000

C	-3.265450000	2.067217000	0.366728000
C	3.337395000	1.957650000	0.515089000
C	-3.404628000	3.440400000	0.499504000
C	3.504084000	3.323520000	0.680882000
C	-3.383031000	-0.960518000	-0.283274000
C	-1.443899000	-0.515819000	1.832564000
C	2.097425000	-0.920693000	1.593340000
C	3.165525000	-1.013651000	-1.087275000
C	-3.999654000	-1.854470000	0.587345000
C	-1.107356000	-1.806454000	2.255036000
C	2.344476000	-2.284765000	1.772173000
C	2.937723000	-1.294711000	-2.436000000
C	-4.037702000	-0.574816000	-1.456140000
C	-1.572770000	0.504439000	2.772674000
C	2.040994000	-0.079014000	2.702134000
C	4.428872000	-1.244971000	-0.538336000
C	-5.258843000	-2.364137000	0.284285000
C	-0.947347000	-2.078759000	3.604504000
C	2.566758000	-2.791859000	3.044043000
C	3.961251000	-1.801734000	-3.228301000
C	-5.294465000	-1.079205000	-1.750336000
C	-1.396213000	0.228389000	4.124228000
C	2.260987000	-0.593624000	3.974836000
C	5.449730000	-1.745412000	-1.334971000
C	-5.906332000	-1.979276000	-0.881419000
C	-1.095598000	-1.061225000	4.541718000
C	2.531959000	-1.944708000	4.147224000
C	5.217473000	-2.025016000	-2.678304000
H	1.057602000	5.384283000	-2.441481000
H	0.148188000	3.887993000	-2.717430000
H	-0.717548000	5.418266000	-2.493494000
H	-0.754999000	6.570910000	-0.261498000

H	0.067950000	5.866717000	1.144077000
H	0.999774000	6.539682000	-0.208622000
H	-2.474033000	5.365104000	0.362168000
H	2.637524000	5.277147000	0.521166000
H	-4.075631000	1.413751000	0.667933000
H	4.116753000	1.276623000	0.837086000
H	-4.336131000	3.847687000	0.874439000
H	4.425740000	3.700859000	1.108036000
H	-3.517635000	-2.157107000	1.508532000
H	-0.979174000	-2.602778000	1.528270000
H	2.374848000	-2.953076000	0.917652000
H	1.958285000	-1.111164000	-2.870218000
H	-3.566205000	0.120650000	-2.142182000
H	-1.807229000	1.516047000	2.465134000
H	1.827827000	0.976942000	2.583533000
H	4.617866000	-1.041640000	0.509620000
H	-5.732587000	-3.058663000	0.968925000
H	-0.695856000	-3.083522000	3.923644000
H	2.766440000	-3.849479000	3.174417000
H	3.774962000	-2.018717000	-4.273949000
H	-5.796543000	-0.773441000	-2.661326000
H	-1.494491000	1.027255000	4.850555000
H	2.217076000	0.067893000	4.832701000
H	6.429049000	-1.919346000	-0.903485000
H	-6.888575000	-2.376100000	-1.113321000
H	-0.960914000	-1.272340000	5.596740000
H	2.705612000	-2.341638000	5.141272000
H	6.017457000	-2.418475000	-3.295702000
Ir	-0.092391000	-1.304592000	-1.113357000
Cl	-1.607338000	-2.542139000	-2.583842000
H	-0.176246000	-0.114386000	-2.063581000

E3

Coordinates (Angstroms)			
	X	Y	Z
P	-1.827950000	-0.130003000	-0.001028000
P	1.806510000	-0.446124000	-0.101379000
O	0.143462000	1.925765000	-0.791792000
C	0.338421000	4.620331000	-0.299306000
C	-0.982126000	3.881919000	-0.061978000
C	1.452785000	3.665511000	0.146351000
C	-0.989113000	2.513799000	-0.311903000
C	1.275657000	2.313263000	-0.138595000
C	0.495228000	4.894422000	-1.811324000
C	0.387385000	5.945480000	0.459152000
C	-2.058287000	1.680084000	-0.039523000
C	2.162038000	1.318200000	0.228929000
C	-2.167179000	4.438730000	0.402142000
C	2.627240000	4.018523000	0.796179000
C	-3.243322000	2.271622000	0.409552000
C	3.352052000	1.710669000	0.852254000
C	-3.293966000	3.642805000	0.608569000
C	3.575171000	3.049425000	1.129101000
C	-3.512314000	-0.698577000	-0.426704000
C	-1.598772000	-0.529870000	1.764020000
C	1.983126000	-1.292974000	1.501472000
C	3.307746000	-0.883572000	-1.061223000
C	-4.259596000	-1.529639000	0.402138000
C	-1.375378000	-1.871972000	2.093236000
C	2.053175000	-2.690027000	1.485430000
C	3.351688000	-0.506258000	-2.406200000
C	-4.054524000	-0.256681000	-1.636098000
C	-1.620871000	0.433285000	2.769825000
C	2.012078000	-0.613816000	2.717146000

C	4.417586000	-1.491541000	-0.479096000
C	-5.540139000	-1.920936000	0.020577000
C	-1.219408000	-2.246566000	3.418961000
C	2.186413000	-3.393671000	2.673218000
C	4.490356000	-0.747862000	-3.161093000
C	-5.332774000	-0.642112000	-2.007932000
C	-1.446885000	0.052661000	4.096796000
C	2.140369000	-1.325627000	3.904538000
C	5.556010000	-1.734396000	-1.241693000
C	-6.077529000	-1.478584000	-1.180527000
C	-1.257325000	-1.283519000	4.422683000
C	2.237100000	-2.710915000	3.884440000
C	5.594048000	-1.365644000	-2.579990000
H	1.451747000	5.388937000	-2.001661000
H	0.462212000	3.971675000	-2.395530000
H	-0.310232000	5.549200000	-2.155306000
H	-0.405781000	6.612100000	0.113401000
H	0.273618000	5.798575000	1.536706000
H	1.335090000	6.456182000	0.275320000
H	-2.227059000	5.500133000	0.610813000
H	2.824496000	5.054731000	1.043204000
H	-4.110594000	1.661806000	0.633950000
H	4.091591000	0.970918000	1.137796000
H	-4.212437000	4.097283000	0.960715000
H	4.493430000	3.347104000	1.621494000
H	-3.860504000	-1.873572000	1.348621000
H	-1.337903000	-2.629426000	1.316389000
H	2.020234000	-3.228302000	0.543033000
H	2.495771000	-0.022614000	-2.866695000
H	-3.478326000	0.391238000	-2.288264000
H	-1.772778000	1.479639000	2.532643000
H	1.932818000	0.466206000	2.749483000

H	4.407280000	-1.775928000	0.566288000
H	-6.118292000	-2.566871000	0.671835000
H	-1.055248000	-3.288817000	3.666440000
H	2.253471000	-4.475517000	2.652148000
H	4.515927000	-0.453932000	-4.204365000
H	-5.748731000	-0.291942000	-2.945914000
H	-1.462266000	0.807060000	4.875204000
H	2.161572000	-0.791480000	4.847595000
H	6.415060000	-2.210492000	-0.782503000
H	-7.077374000	-1.780884000	-1.472248000
H	-1.124303000	-1.575228000	5.458531000
H	2.342809000	-3.259782000	4.813555000
H	6.483171000	-1.556841000	-3.170534000
Ir	-0.108414000	-1.306194000	-1.175250000
Cl	-1.755164000	-2.518159000	-2.525207000
H	-0.060277000	-0.159874000	-2.187563000
H	1.004364000	-2.512220000	-1.851574000
H	0.959989000	-1.893463000	-2.420903000

TS_{E1-E2}

Coordinates (Angstroms)			
	X	Y	Z
P	-1.080129000	1.414912000	-1.580740000
P	0.149114000	-0.057224000	1.698604000
O	-0.454728000	2.653175000	1.116294000
C	-1.563550000	4.771710000	2.457447000
C	-1.793592000	4.610517000	0.955101000
C	-1.666157000	3.358877000	3.034347000
C	-1.236528000	3.480498000	0.355147000
C	-1.051134000	2.345066000	2.310310000
C	-0.135260000	5.306011000	2.707595000
C	-2.571631000	5.727365000	3.091663000

C	-1.509783000	3.088825000	-0.937634000
C	-0.986345000	1.019044000	2.700629000
C	-2.562703000	5.441142000	0.154554000
C	-2.288083000	2.992953000	4.221848000
C	-2.275921000	3.955847000	-1.726256000
C	-1.598219000	0.690831000	3.912243000
C	-2.774776000	5.129233000	-1.188507000
C	-2.254828000	1.668670000	4.649551000
C	-0.226956000	1.954380000	-3.107224000
C	-2.774404000	0.808916000	-1.954004000
C	0.127872000	-1.540408000	2.777396000
C	1.712250000	0.828078000	2.138139000
C	-0.880103000	2.235961000	-4.305007000
C	-3.105116000	0.079080000	-3.096328000
C	1.232065000	-1.982551000	3.504263000
C	2.608799000	1.304461000	1.185225000
C	1.142378000	2.197039000	-2.995119000
C	-3.734923000	0.978352000	-0.950451000
C	-1.083121000	-2.225530000	2.893778000
C	1.948810000	1.117403000	3.488304000
C	-0.162501000	2.734818000	-5.387107000
C	-4.382943000	-0.448849000	-3.242127000
C	1.126778000	-3.095327000	4.330230000
C	3.722744000	2.045444000	1.572093000
C	1.852844000	2.703943000	-4.074494000
C	-5.005702000	0.438407000	-1.095476000
C	-1.192182000	-3.324512000	3.734267000
C	3.065896000	1.842110000	3.873205000
C	1.202534000	2.968506000	-5.275321000
C	-5.334475000	-0.272852000	-2.244693000
C	-0.085409000	-3.764524000	4.451424000
C	3.957704000	2.310615000	2.913020000

H	0.044227000	5.395782000	3.782614000
H	0.626682000	4.645533000	2.286922000
H	-0.023383000	6.294217000	2.252759000
H	-2.463867000	6.729135000	2.669713000
H	-3.601249000	5.393253000	2.936855000
H	-2.391523000	5.811424000	4.165803000
H	-3.017331000	6.332776000	0.569171000
H	-2.792743000	3.735766000	4.828125000
H	-2.511789000	3.698923000	-2.752287000
H	-1.558493000	-0.317529000	4.300035000
H	-3.370504000	5.790842000	-1.806597000
H	-2.734984000	1.395634000	5.582211000
H	-1.945643000	2.073050000	-4.409695000
H	-2.367185000	-0.093729000	-3.867771000
H	2.185252000	-1.475910000	3.422096000
H	2.450663000	1.116530000	0.132181000
H	1.658900000	1.981388000	-2.066016000
H	-3.494561000	1.534739000	-0.049643000
H	-1.951591000	-1.894569000	2.333350000
H	1.254512000	0.781419000	4.250136000
H	-0.676654000	2.942200000	-6.319145000
H	-4.630690000	-1.003611000	-4.140395000
H	1.996159000	-3.435662000	4.881520000
H	4.406124000	2.415424000	0.816303000
H	2.917157000	2.883672000	-3.977749000
H	-5.740372000	0.577217000	-0.310140000
H	-2.141191000	-3.840990000	3.821947000
H	3.234512000	2.047764000	4.924338000
H	1.758299000	3.358309000	-6.121046000
H	-6.328252000	-0.691016000	-2.361048000
H	-0.167385000	-4.627119000	5.103428000
H	4.828171000	2.885225000	3.210149000

Ir	-0.116982000	-0.546865000	-0.587973000
H	1.294082000	0.006072000	-0.769085000
Cl	0.010650000	-1.162755000	-2.957748000
H	0.479410000	-2.224328000	-0.395526000
C	6.357594000	0.044652000	0.218109000
C	7.258223000	1.103100000	0.170085000
C	7.092619000	2.139077000	-0.738394000
C	5.995525000	2.113847000	-1.594468000
C	5.101214000	1.070074000	-1.515756000
C	5.238146000	-0.006065000	-0.626643000
H	6.527341000	-0.754882000	0.927638000
H	8.104840000	1.103377000	0.847802000
H	7.798886000	2.959422000	-0.783158000
H	5.809335000	2.908190000	-2.308365000
C	2.979309000	-2.596486000	0.746002000
C	4.330280000	-1.933816000	0.558873000
N	4.282033000	-1.006362000	-0.558103000
C	3.699129000	-1.533599000	-1.801751000
C	3.346548000	-3.002317000	-1.635886000
N	2.491815000	-3.228861000	-0.474003000
H	3.034821000	-3.312448000	1.569132000
H	4.528582000	-1.376251000	1.476606000
H	2.801340000	-0.977725000	-2.078477000
H	2.869309000	-3.356878000	-2.542828000
C	-0.934805000	-4.428608000	0.579961000
C	0.567671000	-4.189654000	0.683132000
C	1.168830000	-3.520221000	-0.546098000
C	0.670988000	-4.118126000	-1.848283000
C	-0.830512000	-4.385166000	-1.896428000
C	-1.308253000	-5.179683000	-0.689969000
H	-1.260902000	-4.971896000	1.469789000
H	0.805716000	-3.637632000	1.586954000

H	0.944663000	-3.491466000	-2.692047000
H	-1.361136000	-3.428643000	-1.936422000
H	-0.841838000	-6.172695000	-0.685751000
H	1.083960000	-5.156657000	0.751994000
H	1.210041000	-5.069276000	-1.949107000
H	-1.052932000	-4.910365000	-2.829689000
H	-2.390726000	-5.330629000	-0.737435000
H	-1.455534000	-3.464588000	0.590367000
F	4.000250000	1.121474000	-2.307508000
H	4.255024000	-3.595810000	-1.501125000
H	4.417609000	-1.452877000	-2.623656000
H	5.126596000	-2.684729000	0.454704000
H	2.253616000	-1.820085000	1.014336000

TS_{E3-E1}

Coordinates (Angstroms)			
	X	Y	Z
P	-1.838049000	-0.189348000	-0.021516000
P	1.781087000	-0.642939000	-0.172364000
O	0.177928000	1.813556000	-0.822922000
C	0.484041000	4.489248000	-0.312646000
C	-0.851957000	3.796290000	-0.031767000
C	1.582543000	3.492841000	0.077890000
C	-0.916993000	2.431967000	-0.295629000
C	1.349787000	2.149394000	-0.214225000
C	0.589215000	4.773020000	-1.827711000
C	0.609186000	5.805592000	0.452386000
C	-2.009677000	1.633904000	-0.004895000
C	2.219910000	1.120734000	0.103689000
C	-2.000953000	4.392615000	0.472077000
C	2.792551000	3.803149000	0.682207000
C	-3.158476000	2.267966000	0.478442000

C	3.444016000	1.473691000	0.683158000
C	-3.151809000	3.637484000	0.697826000
C	3.722240000	2.801281000	0.964547000
C	-3.557373000	-0.674780000	-0.435951000
C	-1.662848000	-0.625970000	1.747071000
C	1.902089000	-1.396841000	1.486341000
C	3.294424000	-1.196062000	-1.056347000
C	-4.327930000	-1.496480000	0.381219000
C	-1.439121000	-1.975174000	2.042526000
C	1.977363000	-2.790603000	1.570326000
C	3.383925000	-0.919605000	-2.422701000
C	-4.096787000	-0.193610000	-1.631584000
C	-1.739491000	0.298732000	2.785930000
C	1.891854000	-0.635152000	2.653621000
C	4.362925000	-1.816088000	-0.412458000
C	-5.625407000	-1.835886000	0.006384000
C	-1.339195000	-2.396686000	3.359855000
C	2.089778000	-3.406844000	2.808493000
C	4.517814000	-1.277434000	-3.136797000
C	-5.392170000	-0.525639000	-1.997738000
C	-1.618691000	-0.125717000	4.105648000
C	1.994563000	-1.259883000	3.891206000
C	5.496360000	-2.178256000	-1.133584000
C	-6.159428000	-1.351054000	-1.179663000
C	-1.430375000	-1.470589000	4.394326000
C	2.106238000	-2.642216000	3.970406000
C	5.574411000	-1.915075000	-2.494138000
H	1.552535000	5.239184000	-2.052477000
H	0.503493000	3.857246000	-2.417428000
H	-0.208060000	5.456021000	-2.134117000
H	-0.175092000	6.500732000	0.144627000
H	0.535142000	5.653985000	1.532819000

H	1.564477000	6.287251000	0.232703000
H	-2.013850000	5.453114000	0.693846000
H	3.030265000	4.830012000	0.933138000
H	-4.043994000	1.688777000	0.713857000
H	4.169450000	0.708899000	0.937199000
H	-4.043427000	4.121606000	1.078874000
H	4.668487000	3.063223000	1.423355000
H	-3.931934000	-1.875101000	1.315861000
H	-1.351171000	-2.702120000	1.240081000
H	1.969973000	-3.393053000	0.667476000
H	2.561281000	-0.431581000	-2.934302000
H	-3.503746000	0.445410000	-2.277541000
H	-1.890642000	1.351576000	2.579743000
H	1.806959000	0.444103000	2.607476000
H	4.319906000	-2.028478000	0.648724000
H	-6.218584000	-2.475224000	0.650918000
H	-1.172903000	-3.445434000	3.577251000
H	2.166586000	-4.486922000	2.865158000
H	4.571502000	-1.068770000	-4.199284000
H	-5.804094000	-0.142802000	-2.924865000
H	-1.673415000	0.601879000	4.907770000
H	1.986998000	-0.660767000	4.794883000
H	6.316663000	-2.673328000	-0.626253000
H	-7.172450000	-1.611346000	-1.466575000
H	-1.338031000	-1.797822000	5.424127000
H	2.196946000	-3.124998000	4.937174000
H	6.454612000	-2.207725000	-3.055618000
Ir	-0.146777000	-1.367119000	-1.284397000
Cl	-1.835450000	-2.489253000	-2.653118000
H	-0.022231000	-0.196183000	-2.260190000
H	1.025009000	-2.835776000	-1.933298000
H	0.882856000	-1.998274000	-2.414790000

C	2.598326000	-4.352075000	-3.712642000
C	2.609067000	-4.426750000	-2.160175000
O	1.549978000	-4.006583000	-1.589964000
O	3.577176000	-4.946756000	-1.635918000
F	1.993038000	-3.253686000	-4.187988000
F	1.925901000	-5.411156000	-4.199314000
F	3.829279000	-4.388094000	-4.225769000

F1

Coordinates (Angstroms)			
	X	Y	Z
P	1.968858000	-0.410124000	-0.070422000
P	-1.668968000	-1.017801000	-0.159832000
O	-0.071657000	0.570115000	1.678831000
C	-0.493091000	2.908288000	3.125517000
C	0.820933000	2.665511000	2.385609000
C	-1.605891000	2.292556000	2.278362000
C	0.954277000	1.477650000	1.678332000
C	-1.328513000	1.107067000	1.607009000
C	-0.439946000	2.158426000	4.475175000
C	-0.733546000	4.395714000	3.383511000
C	2.080328000	1.126422000	0.944320000
C	-2.254329000	0.413886000	0.837387000
C	1.912892000	3.527323000	2.382325000
C	-2.894352000	2.801234000	2.154338000
C	3.166805000	1.998519000	0.992298000
C	-3.540426000	0.947762000	0.747912000
C	3.079515000	3.186811000	1.707133000
C	-3.852582000	2.131350000	1.401771000
C	2.174496000	-1.726796000	1.189871000
C	3.616021000	-0.396570000	-0.887133000
C	-3.273050000	-1.574230000	-0.896300000

C	-1.379198000	-2.386802000	1.029250000
C	2.547003000	-1.455332000	2.506344000
C	4.602256000	-1.348970000	-0.635329000
C	-4.157988000	-2.329134000	-0.119268000
C	-1.265969000	-3.671285000	0.489293000
C	2.009132000	-3.053228000	0.789548000
C	3.879429000	0.624385000	-1.805740000
C	-3.677267000	-1.172572000	-2.168663000
C	-1.306835000	-2.218940000	2.408419000
C	2.750224000	-2.494369000	3.407509000
C	5.829817000	-1.281967000	-1.289105000
C	-5.402663000	-2.694397000	-0.614965000
C	-1.112667000	-4.771534000	1.317898000
C	2.236023000	-4.090597000	1.684102000
C	5.109000000	0.699722000	-2.444090000
C	-4.925182000	-1.535656000	-2.663812000
C	-1.125013000	-3.323245000	3.237639000
C	2.602717000	-3.813575000	2.996411000
C	6.086924000	-0.257942000	-2.191279000
C	-5.788578000	-2.302452000	-1.892016000
C	-1.038912000	-4.598874000	2.696928000
H	-1.388047000	2.278539000	5.007471000
H	-0.258439000	1.089893000	4.331420000
H	0.363920000	2.562804000	5.097174000
H	0.064790000	4.812098000	4.001263000
H	-0.783469000	4.960358000	2.448557000
H	-1.667018000	4.544362000	3.930494000
H	1.863794000	4.470249000	2.913220000
H	-3.161871000	3.728765000	2.645502000
H	4.081515000	1.765280000	0.462787000
H	-4.294939000	0.459119000	0.144809000
H	3.928299000	3.860923000	1.729314000

H	-4.850403000	2.544892000	1.312262000
H	2.684872000	-0.432369000	2.837783000
H	4.427162000	-2.147112000	0.076331000
H	-3.884487000	-2.635911000	0.883385000
H	-1.315251000	-3.814249000	-0.585510000
H	1.705616000	-3.274842000	-0.228175000
H	3.120962000	1.368972000	-2.015705000
H	-3.021397000	-0.564988000	-2.778295000
H	-1.405262000	-1.237042000	2.854725000
H	3.028751000	-2.270307000	4.431489000
H	6.586755000	-2.031089000	-1.083522000
H	-6.070554000	-3.287302000	0.000221000
H	-1.037601000	-5.763575000	0.886355000
H	2.108423000	-5.117103000	1.359239000
H	5.300522000	1.502345000	-3.148002000
H	-5.218242000	-1.216092000	-3.657902000
H	-1.060891000	-3.180069000	4.310708000
H	2.765471000	-4.623809000	3.698919000
H	7.045981000	-0.202808000	-2.694988000
H	-6.758733000	-2.590815000	-2.282046000
H	-0.907576000	-5.457058000	3.347014000
Ir	0.027601000	-0.582438000	-1.599710000
Cl	1.414967000	-0.275650000	-3.672420000
H	-1.111019000	-0.711094000	-2.695953000
H	0.194526000	-2.132838000	-1.738962000
O	-0.076766000	1.722168000	-1.427308000
C	-1.102154000	2.410819000	-1.633340000
C	-0.931868000	3.913583000	-1.279143000
F	-0.743420000	4.634457000	-2.402394000
F	-2.025485000	4.406303000	-0.676672000
F	0.108173000	4.162664000	-0.474221000
O	-2.198364000	2.099262000	-2.096940000

F2

Coordinates (Angstroms)			
	X	Y	Z
P	1.968858000	-0.410124000	-0.070422000
P	-1.668968000	-1.017801000	-0.159832000
O	-0.071657000	0.570115000	1.678831000
C	-0.493091000	2.908288000	3.125517000
C	0.820933000	2.665511000	2.385609000
C	-1.605891000	2.292556000	2.278362000
C	0.954277000	1.477650000	1.678332000
C	-1.328513000	1.107067000	1.607009000
C	-0.439946000	2.158426000	4.475175000
C	-0.733546000	4.395714000	3.383511000
C	2.080328000	1.126422000	0.944320000
C	-2.254329000	0.413886000	0.837387000
C	1.912892000	3.527323000	2.382325000
C	-2.894352000	2.801234000	2.154338000
C	3.166805000	1.998519000	0.992298000
C	-3.540426000	0.947762000	0.747912000
C	3.079515000	3.186811000	1.707133000
C	-3.852582000	2.131350000	1.401771000
C	2.174496000	-1.726796000	1.189871000
C	3.616021000	-0.396570000	-0.887133000
C	-3.273050000	-1.574230000	-0.896300000
C	-1.379198000	-2.386802000	1.029250000
C	2.547003000	-1.455332000	2.506344000
C	4.602256000	-1.348970000	-0.635329000
C	-4.157988000	-2.329134000	-0.119268000
C	-1.265969000	-3.671285000	0.489293000
C	2.009132000	-3.053228000	0.789548000
C	3.879429000	0.624385000	-1.805740000

C	-3.677267000	-1.172572000	-2.168663000
C	-1.306835000	-2.218940000	2.408419000
C	2.750224000	-2.494369000	3.407509000
C	5.829817000	-1.281967000	-1.289105000
C	-5.402663000	-2.694397000	-0.614965000
C	-1.112667000	-4.771534000	1.317898000
C	2.236023000	-4.090597000	1.684102000
C	5.109000000	0.699722000	-2.444090000
C	-4.925182000	-1.535656000	-2.663812000
C	-1.125013000	-3.323245000	3.237639000
C	2.602717000	-3.813575000	2.996411000
C	6.086924000	-0.257942000	-2.191279000
C	-5.788578000	-2.302452000	-1.892016000
C	-1.038912000	-4.598874000	2.696928000
H	-1.388047000	2.278539000	5.007471000
H	-0.258439000	1.089893000	4.331420000
H	0.363920000	2.562804000	5.097174000
H	0.064790000	4.812098000	4.001263000
H	-0.783469000	4.960358000	2.448557000
H	-1.667018000	4.544362000	3.930494000
H	1.863794000	4.470249000	2.913220000
H	-3.161871000	3.728765000	2.645502000
H	4.081515000	1.765280000	0.462787000
H	-4.294939000	0.459119000	0.144809000
H	3.928299000	3.860923000	1.729314000
H	-4.850403000	2.544892000	1.312262000
H	2.684872000	-0.432369000	2.837783000
H	4.427162000	-2.147112000	0.076331000
H	-3.884487000	-2.635911000	0.883385000
H	-1.315251000	-3.814249000	-0.585510000
H	1.705616000	-3.274842000	-0.228175000
H	3.120962000	1.368972000	-2.015705000

H	-3.021397000	-0.564988000	-2.778295000
H	-1.405262000	-1.237042000	2.854725000
H	3.028751000	-2.270307000	4.431489000
H	6.586755000	-2.031089000	-1.083522000
H	-6.070554000	-3.287302000	0.000221000
H	-1.037601000	-5.763575000	0.886355000
H	2.108423000	-5.117103000	1.359239000
H	5.300522000	1.502345000	-3.148002000
H	-5.218242000	-1.216092000	-3.657902000
H	-1.060891000	-3.180069000	4.310708000
H	2.765471000	-4.623809000	3.698919000
H	7.045981000	-0.202808000	-2.694988000
H	-6.758733000	-2.590815000	-2.282046000
H	-0.907576000	-5.457058000	3.347014000
Ir	0.027601000	-0.582438000	-1.599710000
Cl	1.414967000	-0.275650000	-3.672420000
H	-1.111019000	-0.711094000	-2.695953000
H	0.194526000	-2.132838000	-1.738962000
O	-0.076766000	1.722168000	-1.427308000
C	-1.102154000	2.410819000	-1.633340000
C	-0.931868000	3.913583000	-1.279143000
F	-0.743420000	4.634457000	-2.402394000
F	-2.025485000	4.406303000	-0.676672000
F	0.108173000	4.162664000	-0.474221000
O	-2.198364000	2.099262000	-2.096940000

F3

Coordinates (Angstroms)			
	X	Y	Z
P	1.871860000	-0.570596000	0.059943000
P	-1.770523000	-0.883848000	-0.112753000

O	-0.259635000	0.614310000	1.665347000
C	-0.546969000	3.042942000	3.033305000
C	0.804468000	2.583489000	2.483162000
C	-1.632145000	2.523014000	2.091393000
C	0.861509000	1.379023000	1.791734000
C	-1.426338000	1.297768000	1.477374000
C	-0.757541000	2.384196000	4.414169000
C	-0.610477000	4.564281000	3.177214000
C	2.006118000	0.877172000	1.189590000
C	-2.348469000	0.667071000	0.656813000
C	2.004835000	3.265267000	2.648798000
C	-2.856063000	3.138700000	1.844151000
C	3.199331000	1.566832000	1.414133000
C	-3.574561000	1.294025000	0.451606000
C	3.193259000	2.743988000	2.148483000
C	-3.815699000	2.528232000	1.042024000
C	1.960883000	-2.050730000	1.118473000
C	3.513874000	-0.470734000	-0.750757000
C	-3.247360000	-1.449085000	-1.049187000
C	-1.635175000	-2.088924000	1.246619000
C	1.932201000	-1.964551000	2.508009000
C	4.521400000	-1.408088000	-0.545469000
C	-3.967587000	-2.582441000	-0.673954000
C	-1.138912000	-3.360895000	0.962048000
C	2.099098000	-3.298365000	0.504637000
C	3.773233000	0.651463000	-1.544419000
C	-3.677846000	-0.701094000	-2.150345000
C	-2.090852000	-1.797925000	2.531872000
C	2.055522000	-3.117306000	3.277417000
C	5.769378000	-1.235845000	-1.139842000
C	-5.087581000	-2.972837000	-1.402344000
C	-1.107971000	-4.333729000	1.950847000

C	2.250666000	-4.440608000	1.275928000
C	5.020049000	0.827781000	-2.121852000
C	-4.798869000	-1.089390000	-2.868459000
C	-2.039379000	-2.769295000	3.524126000
C	2.229084000	-4.351096000	2.664510000
C	6.020751000	-0.121037000	-1.926437000
C	-5.503119000	-2.231759000	-2.500021000
C	-1.552480000	-4.038079000	3.234598000
H	-1.735373000	2.661825000	4.818103000
H	-0.709460000	1.293868000	4.343289000
H	0.016439000	2.718731000	5.110881000
H	0.155389000	4.919416000	3.869213000
H	-0.471797000	5.061987000	2.213917000
H	-1.573178000	4.869407000	3.592674000
H	2.026931000	4.207360000	3.182939000
H	-3.077857000	4.102022000	2.286963000
H	4.132042000	1.203811000	1.004131000
H	-4.332944000	0.837910000	-0.171703000
H	4.124441000	3.273287000	2.313484000
H	-4.765005000	3.023108000	0.873986000
H	1.819402000	-1.004660000	2.998934000
H	4.355485000	-2.273448000	0.083269000
H	-3.666101000	-3.170207000	0.184225000
H	-0.783342000	-3.595347000	-0.034845000
H	2.098764000	-3.375856000	-0.577946000
H	3.001133000	1.396145000	-1.700422000
H	-3.147864000	0.200322000	-2.439138000
H	-2.493957000	-0.819902000	2.767750000
H	2.022599000	-3.043646000	4.358651000
H	6.545049000	-1.975508000	-0.975443000
H	-5.633508000	-3.861132000	-1.104627000
H	-0.722018000	-5.319940000	1.721265000

H	2.373675000	-5.403240000	0.792680000
H	5.210736000	1.705429000	-2.729357000
H	-5.122046000	-0.497636000	-3.717492000
H	-2.387626000	-2.533169000	4.523421000
H	2.335864000	-5.246520000	3.266852000
H	6.994600000	0.014623000	-2.384190000
H	-6.376093000	-2.538982000	-3.065334000
H	-1.516752000	-4.796333000	4.009032000
Ir	0.063788000	-0.621741000	-1.537943000
Cl	1.626424000	-0.602955000	-3.458296000
H	0.188051000	-2.181997000	-1.537722000
O	0.206251000	1.614657000	-1.342936000
C	-0.687927000	2.402965000	-1.742564000
C	-0.414240000	3.887475000	-1.388104000
F	-1.527004000	4.496825000	-0.954385000
F	0.521797000	4.048009000	-0.446680000
F	0.002652000	4.551312000	-2.481919000
O	-1.709762000	2.183064000	-2.385444000
H	-1.051016000	-0.360595000	-2.830286000
H	-0.976063000	-1.222996000	-2.746918000

TS_{F1-F2}

Coordinates (Angstroms)			
	X	Y	Z
P	-1.077531000	1.312848000	-1.602982000
P	0.089661000	-0.172255000	1.708565000
O	-0.405170000	2.510014000	1.105294000
C	-1.431059000	4.700982000	2.413789000
C	-1.569722000	4.570446000	0.896975000
C	-1.639195000	3.295001000	2.979911000
C	-1.072193000	3.402963000	0.316990000
C	-1.048070000	2.249673000	2.284119000

C	0.007766000	5.152412000	2.753117000
C	-2.422093000	5.706667000	2.995298000
C	-1.283935000	3.048351000	-0.998767000
C	-1.031256000	0.929325000	2.693604000
C	-2.185139000	5.483115000	0.053518000
C	-2.311286000	2.961125000	4.150403000
C	-1.877843000	4.005467000	-1.830693000
C	-1.691859000	0.631284000	3.884575000
C	-2.299719000	5.217073000	-1.311147000
C	-2.340756000	1.639614000	4.588663000
C	-0.156128000	1.720046000	-3.139558000
C	-2.832577000	0.979510000	-2.049591000
C	0.102942000	-1.629173000	2.828621000
C	1.663504000	0.714517000	2.123071000
C	-0.769861000	1.959676000	-4.366413000
C	-3.183007000	0.121929000	-3.094443000
C	1.227716000	-2.031811000	3.548849000
C	2.584878000	1.122958000	1.163033000
C	1.223884000	1.890087000	-3.018337000
C	-3.838116000	1.484934000	-1.222036000
C	-1.089951000	-2.338046000	2.983597000
C	1.888309000	1.064997000	3.460598000
C	-0.008630000	2.344041000	-5.465824000
C	-4.514139000	-0.207150000	-3.315909000
C	1.160550000	-3.126089000	4.403053000
C	3.707848000	1.860677000	1.529963000
C	1.979067000	2.283292000	-4.114616000
C	-5.166740000	1.143652000	-1.439247000
C	-1.160370000	-3.419113000	3.851379000
C	3.014014000	1.786271000	3.827484000
C	1.365225000	2.505409000	-5.343405000
C	-5.509235000	0.299271000	-2.487895000

C	-0.034044000	-3.819166000	4.560497000
C	3.928613000	2.189579000	2.859323000
H	0.134164000	5.215320000	3.837657000
H	0.753767000	4.456555000	2.360785000
H	0.197578000	6.139553000	2.322132000
H	-2.239585000	6.703471000	2.587649000
H	-3.457280000	5.427584000	2.780178000
H	-2.298926000	5.777441000	4.078377000
H	-2.587859000	6.407942000	0.448850000
H	-2.804897000	3.726970000	4.737037000
H	-2.050973000	3.788687000	-2.878131000
H	-1.701562000	-0.375880000	4.278508000
H	-2.763185000	5.947599000	-1.964136000
H	-2.862294000	1.393228000	5.506562000
H	-1.841169000	1.849204000	-4.480414000
H	-2.414616000	-0.312713000	-3.720033000
H	2.169781000	-1.509991000	3.438360000
H	2.435731000	0.880638000	0.119894000
H	1.713373000	1.706988000	-2.067510000
H	-3.592538000	2.135290000	-0.390227000
H	-1.974436000	-2.039124000	2.433587000
H	1.177793000	0.777263000	4.227234000
H	-0.496439000	2.518999000	-6.418553000
H	-4.770506000	-0.875064000	-4.130860000
H	2.046566000	-3.433590000	4.947425000
H	4.408757000	2.181684000	0.768124000
H	3.049773000	2.410921000	-4.009562000
H	-5.932488000	1.532339000	-0.777380000
H	-2.097375000	-3.952756000	3.964289000
H	3.171939000	2.038945000	4.870080000
H	1.957328000	2.805959000	-6.201001000
H	-6.546687000	0.030965000	-2.654417000

H	-0.086224000	-4.667661000	5.233948000
H	4.805709000	2.762125000	3.140767000
Ir	-0.224326000	-0.705646000	-0.560545000
H	1.211658000	-0.167982000	-0.755903000
Cl	-0.127441000	-1.394074000	-2.923874000
H	0.412758000	-2.357910000	-0.329578000
C	6.548597000	-0.241315000	0.206988000
C	7.532548000	0.739851000	0.150199000
C	7.424837000	1.809266000	-0.727618000
C	6.299064000	1.897943000	-1.541386000
C	5.323638000	0.930815000	-1.454272000
C	5.402128000	-0.181201000	-0.601661000
H	6.675365000	-1.071472000	0.889889000
H	8.398459000	0.652658000	0.797316000
H	8.194690000	2.569715000	-0.779075000
H	6.152257000	2.725781000	-2.225902000
C	2.987090000	-2.638897000	0.758231000
C	4.373568000	-2.057564000	0.569248000
N	4.378645000	-1.106883000	-0.527588000
C	3.666892000	-1.522016000	-1.742574000
C	3.260916000	-2.984417000	-1.649595000
N	2.472891000	-3.266879000	-0.451380000
H	3.009649000	-3.348051000	1.587633000
H	4.620047000	-1.533740000	1.495612000
H	2.778919000	-0.908403000	-1.910040000
H	2.706404000	-3.244944000	-2.544304000
C	-0.842088000	-4.646049000	0.743642000
C	0.643443000	-4.303150000	0.791224000
C	1.165443000	-3.627656000	-0.471043000
C	0.664270000	-4.287549000	-1.741910000
C	-0.818043000	-4.646986000	-1.739701000
C	-1.214815000	-5.438454000	-0.501619000

H	-1.096009000	-5.200138000	1.650667000
H	0.862836000	-3.709394000	1.672472000
H	0.871813000	-3.668722000	-2.609425000
H	-1.406284000	-3.727809000	-1.786912000
H	-0.701835000	-6.408775000	-0.494625000
H	1.229873000	-5.228982000	0.870899000
H	1.262690000	-5.203914000	-1.833887000
H	-1.030911000	-5.212007000	-2.652184000
H	-2.290274000	-5.639706000	-0.509611000
H	-1.422277000	-3.720413000	0.763636000
F	4.197835000	1.103182000	-2.193223000
O	-2.308266000	-1.737301000	-0.544320000
C	-3.284264000	-1.514123000	0.202776000
C	-4.461625000	-2.502801000	-0.011343000
F	-4.482354000	-3.053779000	-1.231181000
F	-5.653946000	-1.925414000	0.187268000
F	-4.362056000	-3.516626000	0.876925000
O	-3.434081000	-0.688311000	1.104418000
H	4.152687000	-3.618187000	-1.626255000
H	4.317580000	-1.418990000	-2.615546000
H	5.115241000	-2.859380000	0.438752000
H	2.299214000	-1.825125000	1.019983000

TSF3-E1

Coordinates (Angstroms)			
	X	Y	Z
P	-2.001250000	0.175216000	-0.074673000
P	1.515335000	1.223360000	-0.126776000
O	0.218138000	-0.278966000	1.802489000
C	0.881126000	-2.383883000	3.527505000
C	-0.502195000	-2.275046000	2.883218000
C	1.899015000	-1.806550000	2.544948000

C	-0.746305000	-1.218545000	2.012041000
C	1.504354000	-0.735253000	1.759862000
C	0.894925000	-1.506982000	4.799107000
C	1.217511000	-3.827907000	3.902754000
C	-1.933182000	-1.041573000	1.312976000
C	2.339967000	-0.048978000	0.890554000
C	-1.565134000	-3.134143000	3.138544000
C	3.223154000	-2.216311000	2.409431000
C	-2.989967000	-1.898584000	1.630553000
C	3.665337000	-0.463915000	0.797773000
C	-2.806473000	-2.924137000	2.546645000
C	4.093960000	-1.550462000	1.551706000
C	-2.536312000	1.751322000	0.664760000
C	-3.504642000	-0.455800000	-0.923032000
C	2.919523000	2.028291000	-1.004114000
C	0.972162000	2.525626000	1.027639000
C	-2.681916000	1.916576000	2.039372000
C	-4.708883000	0.239045000	-0.980017000
C	3.365545000	3.297111000	-0.630100000
C	0.243571000	3.594854000	0.507008000
C	-2.844640000	2.807359000	-0.196866000
C	-3.429302000	-1.738271000	-1.476240000
C	3.599559000	1.347433000	-2.018683000
C	1.333878000	2.527479000	2.373439000
C	-3.150845000	3.124567000	2.546796000
C	-5.821421000	-0.336070000	-1.591082000
C	4.451855000	3.881414000	-1.272856000
C	-0.110020000	4.660405000	1.322505000
C	-3.335185000	4.000450000	0.311455000
C	-4.539972000	-2.313692000	-2.071284000
C	4.688139000	1.929838000	-2.652832000
C	0.957788000	3.585434000	3.192558000

C	-3.489904000	4.159987000	1.685260000
C	-5.739943000	-1.609869000	-2.135411000
C	5.113184000	3.202699000	-2.286976000
C	0.240429000	4.653902000	2.668125000
H	1.882571000	-1.541002000	5.267933000
H	0.659170000	-0.464773000	4.566236000
H	0.155037000	-1.875366000	5.515622000
H	0.499299000	-4.215654000	4.627876000
H	1.216214000	-4.480734000	3.025707000
H	2.200541000	-3.881274000	4.375377000
H	-1.439312000	-3.967368000	3.819406000
H	3.591985000	-3.057130000	2.984327000
H	-3.952073000	-1.783431000	1.149108000
H	4.357977000	0.041160000	0.136027000
H	-3.632976000	-3.583957000	2.783641000
H	5.121320000	-1.885091000	1.468309000
H	-2.438393000	1.107399000	2.718993000
H	-4.802552000	1.224823000	-0.541710000
H	2.873648000	3.843275000	0.164552000
H	-0.037745000	3.600766000	-0.540257000
H	-2.710424000	2.690465000	-1.267664000
H	-2.500189000	-2.294549000	-1.429315000
H	3.303012000	0.347458000	-2.307760000
H	1.914278000	1.712291000	2.790272000
H	-3.258255000	3.250734000	3.618316000
H	-6.754338000	0.215417000	-1.629703000
H	4.778741000	4.871083000	-0.973629000
H	-0.670101000	5.490453000	0.908332000
H	-3.587437000	4.809806000	-0.364513000
H	-4.467581000	-3.310322000	-2.492457000
H	5.204368000	1.385143000	-3.435373000
H	1.232917000	3.575168000	4.241307000

H	-3.866719000	5.095466000	2.083989000
H	-6.608784000	-2.057927000	-2.605278000
H	5.960213000	3.659277000	-2.786982000
H	-0.047281000	5.481081000	3.307819000
Ir	-0.080260000	0.282026000	-1.537461000
Cl	-1.367286000	-0.489976000	-3.504688000
H	-0.405675000	1.743699000	-1.966649000
O	0.354335000	-1.899006000	-0.948706000
C	1.330313000	-2.334036000	-1.573405000
C	1.843332000	-3.739106000	-1.213025000
F	3.164456000	-3.721058000	-1.010992000
F	1.263523000	-4.211495000	-0.111565000
F	1.591725000	-4.592433000	-2.213109000
O	1.958512000	-1.740313000	-2.485999000
H	1.365053000	-0.533788000	-2.562648000
H	1.096566000	0.445434000	-2.708235000

E2c

Coordinates (Angstroms)			
	X	Y	Z
P	-1.915193000	-0.516674000	-0.116251000
P	1.791759000	-0.275232000	0.062312000
O	-0.134696000	1.756615000	-0.825541000
C	-0.460130000	4.436474000	-0.412439000
C	-1.684065000	3.531058000	-0.565014000
C	0.542652000	3.642474000	0.434499000
C	-1.435306000	2.169420000	-0.702817000
C	0.691719000	2.293131000	0.126573000
C	0.165763000	4.697601000	-1.800191000
C	-0.820020000	5.773265000	0.231994000
C	-2.415103000	1.191958000	-0.588520000
C	1.603632000	1.439889000	0.731648000

C	-3.013979000	3.927974000	-0.487906000
C	1.331936000	4.143289000	1.461782000
C	-3.742860000	1.624344000	-0.534329000
C	2.382441000	1.981666000	1.756719000
C	-4.034789000	2.981229000	-0.522346000
C	2.234457000	3.312618000	2.122738000
C	-3.493302000	-1.415623000	-0.382350000
C	-1.759452000	-0.372295000	1.709930000
C	2.606651000	-1.141588000	1.457874000
C	3.144865000	0.012483000	-1.156830000
C	-4.420491000	-1.621647000	0.638114000
C	-1.674328000	-1.552124000	2.456046000
C	3.946159000	-0.924046000	1.797318000
C	4.134494000	-0.947792000	-1.374078000
C	-3.809700000	-1.815867000	-1.683063000
C	-1.635537000	0.852278000	2.362577000
C	1.838227000	-1.990332000	2.253314000
C	3.130165000	1.158191000	-1.955382000
C	-5.636389000	-2.241435000	0.365358000
C	-1.465293000	-1.505309000	3.826199000
C	4.499997000	-1.547895000	2.907210000
C	5.101465000	-0.754146000	-2.353271000
C	-5.027545000	-2.422669000	-1.954507000
C	-1.402794000	0.896123000	3.734347000
C	2.390185000	-2.605013000	3.371514000
C	4.093267000	1.346206000	-2.939685000
C	-5.941834000	-2.642641000	-0.928546000
C	-1.316499000	-0.279058000	4.467789000
C	3.722462000	-2.387486000	3.698504000
C	5.084320000	0.392037000	-3.139137000
H	1.077509000	5.291690000	-1.691990000
H	0.420375000	3.766990000	-2.312518000

H	-0.538515000	5.252383000	-2.426490000
H	-1.524600000	6.322183000	-0.396695000
H	-1.267548000	5.640063000	1.220798000
H	0.071000000	6.396981000	0.333815000
H	-3.265170000	4.976995000	-0.385640000
H	1.252173000	5.182572000	1.757570000
H	-4.549113000	0.904252000	-0.463341000
H	3.098203000	1.365985000	2.286227000
H	-5.068378000	3.305219000	-0.482454000
H	2.837795000	3.712698000	2.929570000
H	-4.209078000	-1.296368000	1.649637000
H	-1.765031000	-2.514246000	1.962963000
H	4.564695000	-0.265523000	1.198886000
H	4.158220000	-1.852484000	-0.780427000
H	-3.102533000	-1.651379000	-2.488322000
H	-1.717078000	1.785170000	1.818751000
H	0.802010000	-2.172588000	2.001000000
H	2.369294000	1.918584000	-1.820347000
H	-6.346932000	-2.403088000	1.168353000
H	-1.404825000	-2.429133000	4.390693000
H	5.541327000	-1.374098000	3.154572000
H	5.867986000	-1.506785000	-2.502574000
H	-5.261234000	-2.726077000	-2.969004000
H	-1.292896000	1.856567000	4.225407000
H	1.775572000	-3.257179000	3.982252000
H	4.068818000	2.244586000	-3.546811000
H	-6.890592000	-3.123961000	-1.139087000
H	-1.136512000	-0.242201000	5.536536000
H	4.156766000	-2.870972000	4.566740000
H	5.839466000	0.540884000	-3.903286000
Ir	-0.085417000	-1.517821000	-1.030758000
H	0.277218000	-0.267585000	-2.340881000

H	-0.194969000	-2.516432000	0.184681000
H	-1.132362000	-2.522368000	-1.684469000
H	-0.294777000	-0.751841000	-2.675664000
Cl	1.621015000	-3.049535000	-2.009792000

E3c

Coordinates (Angstroms)			
	X	Y	Z
P	-1.123569000	-1.393767000	0.278586000
P	2.216908000	0.250208000	-0.251751000
O	-0.344290000	1.467953000	0.608068000
C	-1.074187000	3.354628000	2.448831000
C	-1.953543000	2.125761000	2.219737000
C	0.372435000	2.853434000	2.389363000
C	-1.496138000	1.194777000	1.291183000
C	0.672912000	1.916381000	1.402145000
C	-1.302853000	4.360429000	1.298282000
C	-1.383590000	4.040107000	3.778214000
C	-2.082778000	-0.046905000	1.091501000
C	1.937220000	1.389129000	1.181269000
C	-3.138823000	1.835247000	2.881313000
C	1.413071000	3.260805000	3.213053000
C	-3.288158000	-0.295471000	1.754171000
C	2.959871000	1.831888000	2.024309000
C	-3.819236000	0.648624000	2.619471000
C	2.696192000	2.748661000	3.030911000
C	-2.487421000	-2.541678000	-0.166385000
C	-0.283826000	-2.174615000	1.713302000
C	3.613734000	-0.771329000	0.358622000
C	2.960960000	1.447574000	-1.436093000
C	-2.922963000	-3.560046000	0.681456000
C	0.175406000	-3.489699000	1.590066000

C	4.930775000	-0.306956000	0.438469000
C	4.017043000	1.097199000	-2.277382000
C	-3.178924000	-2.302678000	-1.356258000
C	0.031957000	-1.448898000	2.859677000
C	3.318738000	-2.045652000	0.841703000
C	2.365783000	2.702688000	-1.583736000
C	-4.016430000	-4.345733000	0.330229000
C	0.922687000	-4.071055000	2.603888000
C	5.925546000	-1.107198000	0.985543000
C	4.488722000	1.996980000	-3.226266000
C	-4.277351000	-3.079543000	-1.697587000
C	0.804548000	-2.026105000	3.863592000
C	4.312367000	-2.841456000	1.399434000
C	2.830873000	3.596068000	-2.540638000
C	-4.693625000	-4.108859000	-0.859051000
C	1.247866000	-3.335962000	3.740549000
C	5.619020000	-2.374796000	1.469585000
C	3.898128000	3.247470000	-3.361255000
H	-0.618171000	5.207089000	1.401671000
H	-1.145682000	3.901553000	0.320524000
H	-2.329283000	4.736059000	1.335180000
H	-2.415969000	4.396498000	3.793374000
H	-1.235401000	3.366383000	4.626869000
H	-0.742387000	4.914330000	3.912303000
H	-3.542796000	2.530112000	3.607849000
H	1.238028000	3.982994000	4.001484000
H	-3.803078000	-1.238138000	1.616801000
H	3.967420000	1.454015000	1.907284000
H	-4.756949000	0.444754000	3.123450000
H	3.499831000	3.073109000	3.682094000
H	-2.424267000	-3.743391000	1.625330000
H	-0.039393000	-4.059015000	0.691875000

H	5.189576000	0.681244000	0.077382000
H	4.475635000	0.119414000	-2.203529000
H	-2.872364000	-1.496138000	-2.012320000
H	-0.313501000	-0.429202000	2.984122000
H	2.306038000	-2.421800000	0.780808000
H	1.528647000	2.993440000	-0.957599000
H	-4.340243000	-5.138815000	0.995154000
H	1.266917000	-5.093825000	2.497531000
H	6.942716000	-0.734840000	1.037732000
H	5.315210000	1.712018000	-3.868302000
H	-4.807262000	-2.879632000	-2.622342000
H	1.054199000	-1.446018000	4.745136000
H	4.061442000	-3.827951000	1.773970000
H	2.356591000	4.565885000	-2.642973000
H	-5.547418000	-4.720299000	-1.130436000
H	1.846506000	-3.784506000	4.525653000
H	6.397872000	-2.996324000	1.897872000
H	4.264323000	3.946648000	-4.105185000
Ir	0.367697000	-1.008339000	-1.408646000
H	-0.068957000	0.711612000	-1.863817000
H	0.980897000	-2.409418000	-0.991510000
H	-0.608654000	-1.908924000	-2.275389000
H	-0.667737000	0.245434000	-2.193406000
Cl	1.806017000	-1.094705000	-3.444059000
C	-4.223937000	1.866099000	-1.362411000
F	-5.136110000	2.502961000	-2.130454000
F	-4.126513000	2.563382000	-0.222153000
F	-4.754026000	0.671787000	-1.050297000
C	-2.876792000	1.746515000	-2.135952000
O	-2.843622000	0.814350000	-2.957644000
O	-2.033233000	2.616819000	-1.880101000

E4c

Coordinates (Angstroms)			
	X	Y	Z
P	-1.073479000	-1.398786000	0.226100000
P	2.191684000	0.258188000	-0.271381000
O	-0.383237000	1.473351000	0.535810000
C	-1.178692000	3.345961000	2.367098000
C	-2.061749000	2.132453000	2.069254000
C	0.269032000	2.839666000	2.354197000
C	-1.558734000	1.194378000	1.173443000
C	0.606193000	1.918084000	1.364230000
C	-1.345534000	4.389752000	1.241222000
C	-1.544037000	3.992594000	3.702490000
C	-2.123985000	-0.056586000	0.958140000
C	1.876807000	1.394833000	1.169229000
C	-3.290805000	1.854478000	2.654011000
C	1.282088000	3.235754000	3.217459000
C	-3.373611000	-0.288748000	1.538746000
C	2.869314000	1.828780000	2.051822000
C	-3.960157000	0.671606000	2.351511000
C	2.570918000	2.728464000	3.065419000
C	-2.373968000	-2.662564000	-0.116189000
C	-0.245944000	-2.050686000	1.743012000
C	3.643226000	-0.676840000	0.368921000
C	2.914876000	1.488681000	-1.440080000
C	-2.832820000	-3.525926000	0.881924000
C	0.247508000	-3.359495000	1.717261000
C	4.939678000	-0.155768000	0.427523000
C	3.972851000	1.160660000	-2.288728000
C	-2.993033000	-2.696133000	-1.366945000
C	0.030475000	-1.251086000	2.849376000
C	3.405064000	-1.941849000	0.905119000

C	2.311600000	2.741645000	-1.571772000
C	-3.868231000	-4.417902000	0.626998000
C	0.995337000	-3.854981000	2.774564000
C	5.969826000	-0.889134000	1.002893000
C	4.436558000	2.076107000	-3.226558000
C	-4.035130000	-3.580001000	-1.617663000
C	0.806062000	-1.739707000	3.898103000
C	4.432126000	-2.669955000	1.494648000
C	2.768516000	3.652327000	-2.516805000
C	-4.471835000	-4.448551000	-0.623912000
C	1.289636000	-3.040040000	3.864668000
C	5.718525000	-2.146841000	1.541404000
C	3.836690000	3.324048000	-3.344405000
H	-0.714480000	5.259823000	1.444580000
H	-1.069085000	3.982115000	0.267621000
H	-2.387632000	4.718197000	1.189245000
H	-2.569457000	4.368258000	3.676545000
H	-1.452769000	3.286569000	4.532751000
H	-0.895990000	4.849031000	3.901657000
H	-3.735552000	2.554215000	3.351505000
H	1.081456000	3.944405000	4.012126000
H	-3.883576000	-1.230650000	1.381024000
H	3.881538000	1.455691000	1.963778000
H	-4.932415000	0.478862000	2.790312000
H	3.353429000	3.043252000	3.746539000
H	-2.391486000	-3.505571000	1.870867000
H	0.057139000	-3.993329000	0.858207000
H	5.153534000	0.828750000	0.028732000
H	4.440377000	0.186628000	-2.227289000
H	-2.663618000	-2.028553000	-2.152280000
H	-0.349365000	-0.238703000	2.913908000
H	2.408949000	-2.362735000	0.858780000

H	1.472672000	3.017842000	-0.942040000
H	-4.203629000	-5.086659000	1.412095000
H	1.366216000	-4.873476000	2.738330000
H	6.970150000	-0.471382000	1.035819000
H	5.264283000	1.805555000	-3.873411000
H	-4.503871000	-3.590404000	-2.595525000
H	1.026050000	-1.095955000	4.742711000
H	4.223554000	-3.648950000	1.912793000
H	2.286714000	4.620057000	-2.604552000
H	-5.279065000	-5.144935000	-0.823295000
H	1.892358000	-3.419731000	4.682401000
H	6.523729000	-2.715253000	1.994177000
H	4.196284000	4.036041000	-4.079460000
Ir	0.435983000	-1.049999000	-1.420722000
H	-0.144957000	0.428075000	-2.038188000
H	1.058564000	-2.501777000	-0.960636000
H	-0.563612000	-1.875651000	-2.347496000
H	-1.539936000	0.405926000	-2.176518000
Cl	1.968393000	-1.202402000	-3.436629000
C	-4.413954000	1.832210000	-1.526081000
F	-5.028370000	2.357194000	-2.595658000
F	-4.636536000	2.642570000	-0.489877000
F	-4.983315000	0.655340000	-1.265146000
C	-2.896355000	1.721843000	-1.797245000
O	-2.556049000	0.532626000	-2.186365000
O	-2.197582000	2.692650000	-1.657197000

E5c

Coordinates (Angstroms)			
	X	Y	Z
P	-1.945019000	-0.169160000	-0.064122000
P	1.900388000	-0.578500000	0.009974000

O	0.341013000	1.733087000	-0.635305000
C	0.538316000	4.435184000	-0.150390000
C	-0.829594000	3.778355000	-0.341543000
C	1.391724000	3.439795000	0.640563000
C	-0.851164000	2.394236000	-0.511241000
C	1.274091000	2.099216000	0.294023000
C	1.198926000	4.642850000	-1.531984000
C	0.426867000	5.783980000	0.558654000
C	-2.009194000	1.633951000	-0.481362000
C	2.068473000	1.081363000	0.797610000
C	-2.053718000	4.433162000	-0.315502000
C	2.331761000	3.752113000	1.616982000
C	-3.222943000	2.329627000	-0.492188000
C	3.013360000	1.432108000	1.762049000
C	-3.241417000	3.714382000	-0.441052000
C	3.123965000	2.753791000	2.179289000
C	-3.377773000	-0.722071000	-1.084748000
C	-2.610878000	-0.085049000	1.657954000
C	3.201933000	-1.494309000	0.949629000
C	2.759450000	-0.272283000	-1.600579000
C	-4.671206000	-0.878478000	-0.591892000
C	-3.074762000	-1.264868000	2.250662000
C	4.520972000	-1.559655000	0.499309000
C	2.823460000	-1.319191000	-2.524290000
C	-3.140667000	-0.931064000	-2.445349000
C	-2.544161000	1.073701000	2.431059000
C	2.878092000	-2.086675000	2.172607000
C	3.388036000	0.933689000	-1.910100000
C	-5.707836000	-1.254509000	-1.442092000
C	-3.492921000	-1.273578000	3.573548000
C	5.491805000	-2.217902000	1.248080000
C	3.490714000	-1.160319000	-3.730672000

C	-4.176534000	-1.295053000	-3.294347000
C	-2.947935000	1.058277000	3.763959000
C	3.850058000	-2.733599000	2.924363000
C	4.044198000	1.097777000	-3.126920000
C	-5.464242000	-1.463926000	-2.792845000
C	-3.431625000	-0.110101000	4.336298000
C	5.160151000	-2.806354000	2.461372000
C	4.098095000	0.053260000	-4.039545000
H	2.191835000	5.084927000	-1.408601000
H	1.307258000	3.699935000	-2.073585000
H	0.589135000	5.318751000	-2.138318000
H	-0.161668000	6.483282000	-0.039313000
H	-0.041837000	5.685869000	1.541821000
H	1.415834000	6.229552000	0.687962000
H	-2.096126000	5.508912000	-0.193516000
H	2.465148000	4.778420000	1.938276000
H	-4.160065000	1.784701000	-0.490587000
H	3.667178000	0.680905000	2.188167000
H	-4.189490000	4.239994000	-0.445620000
H	3.852212000	3.014105000	2.938840000
H	-4.884284000	-0.707755000	0.456526000
H	-3.094817000	-2.183430000	1.673366000
H	4.806559000	-1.098859000	-0.438469000
H	2.344274000	-2.264983000	-2.300160000
H	-2.137184000	-0.816880000	-2.841759000
H	-2.167277000	1.998513000	2.010206000
H	1.858087000	-2.045010000	2.535927000
H	3.380458000	1.759067000	-1.208575000
H	-6.708305000	-1.379493000	-1.041894000
H	-3.861720000	-2.194116000	4.013158000
H	6.509672000	-2.268402000	0.876853000
H	3.530772000	-1.984629000	-4.434407000

H	-3.977339000	-1.454666000	-4.348551000
H	-2.884497000	1.968538000	4.350496000
H	3.580957000	-3.188190000	3.871638000
H	4.517771000	2.046878000	-3.353422000
H	-6.272326000	-1.756697000	-3.454535000
H	-3.752594000	-0.119130000	5.372336000
H	5.917025000	-3.320423000	3.043914000
H	4.609767000	0.181786000	-4.987175000
Ir	-0.051987000	-1.702898000	-0.146835000
H	-0.045000000	-1.674596000	-1.826381000
H	-0.076652000	-1.843942000	1.516764000
Cl	-1.790843000	-3.572276000	-0.247831000
H	1.000647000	-2.911910000	-0.193507000

TS_{E3c-E4c}

Coordinates (Angstroms)			
	X	Y	Z
P	-1.101800000	-1.442291000	0.192891000
P	2.164574000	0.275141000	-0.236415000
O	-0.434894000	1.427026000	0.589187000
C	-1.262235000	3.241586000	2.472662000
C	-2.121268000	2.019382000	2.145500000
C	0.194461000	2.764355000	2.439504000
C	-1.606909000	1.116894000	1.219788000
C	0.546268000	1.871513000	1.428316000
C	-1.457229000	4.311595000	1.376753000
C	-1.632802000	3.844104000	3.827203000
C	-2.156541000	-0.133423000	0.967787000
C	1.826997000	1.377930000	1.222272000
C	-3.342185000	1.702561000	2.727414000
C	1.202257000	3.163509000	3.307449000
C	-3.396563000	-0.407099000	1.549952000

C	2.814197000	1.815120000	2.109297000
C	-3.993354000	0.517621000	2.395553000
C	2.501201000	2.688127000	3.141202000
C	-2.404413000	-2.670305000	-0.243066000
C	-0.285894000	-2.161834000	1.681422000
C	3.614727000	-0.663897000	0.394086000
C	2.870225000	1.534564000	-1.382468000
C	-2.845838000	-3.642353000	0.656410000
C	0.220197000	-3.463271000	1.597964000
C	4.908838000	-0.139474000	0.468928000
C	3.948557000	1.246662000	-2.219704000
C	-3.048737000	-2.550618000	-1.476447000
C	-0.024862000	-1.409257000	2.824163000
C	3.375165000	-1.936171000	0.912794000
C	2.230740000	2.770280000	-1.508789000
C	-3.892293000	-4.494174000	0.317610000
C	0.963636000	-4.000399000	2.638140000
C	5.936479000	-0.877624000	1.042585000
C	4.399058000	2.186647000	-3.139412000
C	-4.100817000	-3.393511000	-1.808273000
C	0.745148000	-1.939955000	3.856162000
C	4.400066000	-2.669159000	1.499690000
C	2.675066000	3.704902000	-2.436029000
C	-4.521425000	-4.372828000	-0.914705000
C	1.239594000	-3.233917000	3.767344000
C	5.684590000	-2.142909000	1.562491000
C	3.765393000	3.418273000	-3.250287000
H	-0.815841000	5.173888000	1.581094000
H	-1.214850000	3.924799000	0.385775000
H	-2.498163000	4.647104000	1.366447000
H	-2.667629000	4.193526000	3.819028000
H	-1.516236000	3.120056000	4.638572000

H	-1.006480000	4.712551000	4.043267000
H	-3.795612000	2.374192000	3.446559000
H	0.988755000	3.850876000	4.117287000
H	-3.889316000	-1.353914000	1.367648000
H	3.833834000	1.465805000	2.009587000
H	-4.957882000	0.294297000	2.836906000
H	3.279337000	3.006607000	3.825551000
H	-2.384783000	-3.740166000	1.631622000
H	0.046006000	-4.055806000	0.706448000
H	5.122521000	0.851336000	0.085927000
H	4.440880000	0.284474000	-2.165456000
H	-2.733912000	-1.790862000	-2.180141000
H	-0.410869000	-0.402229000	2.927366000
H	2.379764000	-2.358124000	0.857567000
H	1.372263000	3.012667000	-0.891499000
H	-4.216927000	-5.249168000	1.025133000
H	1.345814000	-5.012117000	2.557790000
H	6.935098000	-0.457234000	1.089611000
H	5.243394000	1.947955000	-3.777206000
H	-4.590826000	-3.284601000	-2.769539000
H	0.953203000	-1.334887000	4.731772000
H	4.191047000	-3.653754000	1.904151000
H	2.166375000	4.659041000	-2.520423000
H	-5.337613000	-5.036913000	-1.177778000
H	1.838028000	-3.645666000	4.572582000
H	6.487927000	-2.714746000	2.014202000
H	4.115071000	4.149502000	-3.971055000
Ir	0.431088000	-1.036917000	-1.429277000
H	-0.082388000	0.500690000	-2.059971000
H	1.055345000	-2.455836000	-0.976520000
H	-0.534087000	-1.886058000	-2.368948000
H	-1.134091000	0.469743000	-2.126198000

Cl	1.993011000	-1.153856000	-3.407406000
C	-4.142320000	2.006218000	-1.499872000
F	-4.787218000	2.611537000	-2.511498000
F	-4.307827000	2.765836000	-0.410260000
F	-4.750259000	0.837908000	-1.278150000
C	-2.639343000	1.857864000	-1.846794000
O	-2.314452000	0.679913000	-2.208657000
O	-1.943523000	2.852522000	-1.764589000

TS_{E5c-E1}

Coordinates (Angstroms)			
	X	Y	Z
P	1.817492000	-0.408243000	1.426477000
P	0.019726000	-0.478458000	-1.600182000
O	1.281449000	1.749192000	-0.443892000
C	3.007920000	3.674900000	-1.257257000
C	2.986405000	3.242190000	0.214308000
C	2.884921000	2.371943000	-2.063657000
C	2.151494000	2.175652000	0.524874000
C	1.936604000	1.468558000	-1.614193000
C	1.784716000	4.564167000	-1.571433000
C	4.285180000	4.436671000	-1.601679000
C	2.292677000	1.374216000	1.649893000
C	1.601857000	0.273537000	-2.227405000
C	3.833943000	3.687853000	1.221983000
C	3.605002000	1.996178000	-3.193443000
C	3.151739000	1.851090000	2.644850000
C	2.333819000	-0.071138000	-3.360696000
C	3.862705000	3.030032000	2.449619000
C	3.339243000	0.778477000	-3.818031000
C	2.258184000	-1.095252000	3.072670000
C	3.243866000	-0.947822000	0.366079000

C	-0.222752000	-1.830317000	-2.819811000
C	-0.998369000	0.929895000	-2.263713000
C	3.083637000	-2.209830000	3.198839000
C	3.198537000	-2.219880000	-0.207334000
C	-1.292741000	-1.877077000	-3.710756000
C	-1.679436000	1.802348000	-1.421573000
C	1.720616000	-0.514418000	4.224274000
C	4.349424000	-0.137609000	0.096902000
C	0.710503000	-2.870068000	-2.830627000
C	-0.918936000	1.239532000	-3.628124000
C	3.368190000	-2.736221000	4.455978000
C	4.210954000	-2.662051000	-1.048488000
C	-1.418947000	-2.934851000	-4.605154000
C	-2.283975000	2.950379000	-1.929107000
C	2.017192000	-1.030055000	5.477192000
C	5.353059000	-0.571989000	-0.761880000
C	0.589327000	-3.921143000	-3.728359000
C	-1.534557000	2.372862000	-4.136268000
C	2.839595000	-2.146990000	5.596324000
C	5.285057000	-1.831474000	-1.343680000
C	-0.476979000	-3.954801000	-4.621390000
C	-2.219586000	3.235914000	-3.284994000
H	1.777618000	4.824367000	-2.633746000
H	0.843434000	4.061709000	-1.336017000
H	1.836776000	5.487961000	-0.988154000
H	4.341576000	5.367324000	-1.032071000
H	5.180274000	3.845029000	-1.389898000
H	4.290642000	4.703986000	-2.661182000
H	4.501969000	4.523359000	1.049576000
H	4.374871000	2.643696000	-3.596949000
H	3.320715000	1.282734000	3.549913000
H	2.123839000	-0.988201000	-3.897476000

H	4.518480000	3.390357000	3.234036000
H	3.912766000	0.494151000	-4.693129000
H	3.514427000	-2.679812000	2.322987000
H	2.351132000	-2.862979000	-0.005573000
H	-2.043382000	-1.096602000	-3.714177000
H	-1.737222000	1.593283000	-0.361445000
H	1.065384000	0.345343000	4.143672000
H	4.443922000	0.846194000	0.536635000
H	1.539721000	-2.859229000	-2.133749000
H	-0.356363000	0.605259000	-4.303676000
H	4.011413000	-3.605604000	4.537675000
H	4.147319000	-3.652194000	-1.486652000
H	-2.260013000	-2.957999000	-5.289397000
H	-2.800370000	3.623068000	-1.253292000
H	1.597044000	-0.564807000	6.362153000
H	6.189122000	0.084616000	-0.976467000
H	1.328081000	-4.714944000	-3.727394000
H	-1.464760000	2.589683000	-5.196574000
H	3.065072000	-2.555327000	6.575553000
H	6.064611000	-2.164048000	-2.020320000
H	-0.574201000	-4.775276000	-5.323974000
H	-2.689357000	4.130723000	-3.678841000
Ir	-0.276366000	-1.111913000	0.608445000
H	-0.989663000	0.341787000	0.918284000
H	0.342696000	-2.652036000	0.346973000
Cl	-0.914734000	-1.733487000	2.934316000
H	-1.862665000	-1.798498000	0.219666000
C	-4.912333000	3.762270000	0.630606000
C	-4.789862000	5.136533000	0.803268000
C	-3.719700000	5.669403000	1.508759000
C	-2.760922000	4.808413000	2.034281000
C	-2.888967000	3.450902000	1.837401000

C	-3.955921000	2.869951000	1.136738000
H	-5.766425000	3.371261000	0.091449000
H	-5.549177000	5.791307000	0.390008000
H	-3.621447000	6.739185000	1.649567000
H	-1.898119000	5.178305000	2.576519000
C	-4.279404000	-0.327262000	-0.658469000
C	-4.838803000	0.995458000	-0.161308000
N	-4.005608000	1.500667000	0.913972000
C	-3.807539000	0.585998000	2.046640000
C	-4.450880000	-0.762352000	1.752049000
N	-4.069306000	-1.270716000	0.438499000
H	-4.957893000	-0.749823000	-1.405823000
H	-4.796509000	1.691531000	-1.000557000
H	-2.745075000	0.439414000	2.239516000
H	-4.164197000	-1.460715000	2.530764000
C	-2.351530000	-4.107079000	-1.366317000
C	-3.277097000	-2.913563000	-1.163961000
C	-3.257385000	-2.334114000	0.242278000
C	-3.241934000	-3.385898000	1.335805000
C	-2.326011000	-4.575730000	1.074008000
C	-2.552027000	-5.180960000	-0.305207000
H	-2.521847000	-4.509063000	-2.368200000
H	-3.060563000	-2.144444000	-1.901555000
H	-2.975571000	-2.941701000	2.290310000
H	-1.285795000	-4.248614000	1.161715000
H	-3.567783000	-5.591828000	-0.372596000
H	-4.318313000	-3.225657000	-1.325176000
H	-4.281501000	-3.733612000	1.402762000
H	-2.498148000	-5.317288000	1.859880000
H	-1.857246000	-6.009200000	-0.474468000
H	-1.314969000	-3.764771000	-1.328805000
F	-1.903863000	2.648365000	2.308536000

H	-5.895909000	0.893236000	0.123657000
H	-3.313410000	-0.140064000	-1.138018000
H	-5.541099000	-0.678486000	1.778765000
H	-4.272629000	0.990299000	2.954423000

G1

Coordinates (Angstroms)			
	X	Y	Z
C	2.319114000	-3.461131000	-0.888288000
C	2.959666000	-4.054625000	0.234758000
H	2.593033000	-4.897354000	0.802801000
C	4.140517000	-3.311207000	0.511770000
H	4.828731000	-3.493390000	1.324483000
C	3.107010000	-2.354416000	-1.305891000
H	2.882297000	-1.693318000	-2.126863000
C	4.231197000	-2.257188000	-0.439980000
H	5.006746000	-1.506376000	-0.485474000
H	1.383229000	-3.776948000	-1.327603000
C	0.576229000	-1.577437000	1.208877000
C	1.263552000	-2.225568000	2.280162000
C	2.433109000	-1.489734000	2.599376000
H	3.170995000	-1.762871000	3.339464000
C	1.335903000	-0.398372000	0.878495000
C	2.490859000	-0.376801000	1.732971000
H	3.269762000	0.370027000	1.722049000
Fe	2.487843000	-2.101275000	0.640826000
P	0.744104000	1.086612000	0.009980000
C	1.214502000	2.374557000	1.258459000
C	1.099446000	3.824628000	0.746071000
C	0.462634000	2.206090000	2.583271000
C	0.947642000	4.821453000	1.909944000
H	1.999028000	4.066123000	0.170657000

C	1.144675000	3.033745000	3.685086000
H	-0.571508000	2.537985000	2.447644000
C	1.724876000	4.354717000	3.140073000
H	1.285677000	5.811088000	1.589508000
H	1.944571000	2.443115000	4.143845000
H	2.775176000	4.212730000	2.859216000
C	1.834144000	1.460882000	-1.425582000
C	1.419391000	0.639977000	-2.663757000
C	3.342664000	1.379924000	-1.189995000
C	2.519180000	0.647578000	-3.741552000
H	1.183651000	-0.390916000	-2.379295000
C	4.090340000	2.057846000	-2.356191000
H	3.625690000	1.853924000	-0.246609000
C	3.324633000	1.944415000	-3.688237000
H	3.205341000	-0.193663000	-3.591793000
H	5.079244000	1.599129000	-2.458161000
H	4.023480000	1.999447000	-4.527525000
H	0.249516000	3.929106000	0.067105000
H	-0.111075000	4.924370000	2.174047000
H	1.713556000	5.122066000	3.919047000
H	0.414689000	3.241970000	4.473825000
H	0.415006000	1.156031000	2.883255000
H	2.271604000	2.182491000	1.458841000
H	1.583603000	2.510138000	-1.621625000
H	0.498280000	1.068457000	-3.072777000
H	2.068589000	0.507893000	-4.728045000
H	2.637933000	2.791789000	-3.798853000
H	4.255815000	3.114442000	-2.122746000
H	3.633320000	0.330619000	-1.110828000
H	0.986905000	-3.158170000	2.744870000
C	-0.623232000	-2.182037000	0.495351000
H	-0.297619000	-2.359302000	-0.533640000

C	-0.930027000	-3.552557000	1.115027000
H	-0.080327000	-4.221344000	0.948496000
H	-1.090900000	-3.480620000	2.191218000
H	-1.804853000	-4.024386000	0.685388000
P	-2.089591000	-1.049915000	0.148405000
C	-2.891256000	-1.920663000	-1.353686000
C	-3.196011000	-1.076624000	1.678637000
C	-2.905950000	-3.453765000	-1.372711000
H	-3.415786000	-3.770692000	-2.289857000
H	-1.902618000	-3.883649000	-1.399581000
H	-3.456785000	-3.880341000	-0.532361000
C	-2.057243000	-1.454364000	-2.562539000
H	-2.103426000	-0.369454000	-2.698300000
H	-1.006224000	-1.747459000	-2.476643000
H	-2.454090000	-1.916763000	-3.473218000
C	-4.338405000	-1.443147000	-1.529780000
H	-4.699392000	-1.782809000	-2.507857000
H	-4.999876000	-1.871327000	-0.773246000
H	-4.422569000	-0.357569000	-1.500059000
C	-4.250279000	0.033307000	1.560309000
H	-4.961267000	-0.153687000	0.754720000
H	-4.812635000	0.078937000	2.500024000
H	-3.792970000	1.008620000	1.387178000
C	-3.917101000	-2.403270000	1.947010000
H	-4.545911000	-2.282234000	2.836756000
H	-4.571635000	-2.688750000	1.121357000
H	-3.232283000	-3.226413000	2.142424000
C	-2.280816000	-0.731370000	2.864950000
H	-1.532976000	-1.503496000	3.058225000
H	-1.761462000	0.217690000	2.705165000
H	-2.892494000	-0.629202000	3.768128000
Ir	-1.404123000	1.167417000	-0.628103000

Cl	-3.634731000	1.962206000	-1.537067000
H	-0.934460000	2.612550000	-1.183606000
H	-1.669858000	1.836767000	0.729218000

G2

Coordinates (Angstroms)			
	X	Y	Z
C	-3.440940000	-2.634840000	0.825466000
C	-3.970492000	-3.196366000	-0.369862000
H	-3.710870000	-4.157331000	-0.789748000
C	-4.856326000	-2.245367000	-0.948571000
H	-5.385885000	-2.360779000	-1.883124000
C	-4.009313000	-1.342307000	0.986046000
H	-3.810833000	-0.662309000	1.797119000
C	-4.878882000	-1.095665000	-0.109910000
H	-5.440598000	-0.189483000	-0.284683000
H	-2.717366000	-3.097193000	1.481724000
C	-0.929278000	-1.496292000	-1.051461000
C	-1.591792000	-2.050266000	-2.184077000
C	-2.452449000	-1.065593000	-2.737397000
H	-3.114294000	-1.207534000	-3.579050000
C	-1.388467000	-0.146037000	-0.914199000
C	-2.341295000	0.106327000	-1.954651000
H	-2.868833000	1.034734000	-2.115748000
Fe	-2.972605000	-1.461875000	-0.793179000
P	-0.527137000	1.114183000	0.024013000
C	-0.667027000	2.628568000	-1.018235000
C	-0.019701000	3.825167000	-0.281007000
C	-0.071494000	2.490768000	-2.424133000
C	0.425429000	4.921666000	-1.262514000
H	-0.738901000	4.236544000	0.433118000
C	-0.488107000	3.699479000	-3.278105000

H	1.018818000	2.451510000	-2.346255000
C	-0.531957000	5.000644000	-2.450819000
H	0.477690000	5.879962000	-0.738864000
H	-1.470579000	3.513452000	-3.723798000
H	-1.546879000	5.168105000	-2.071629000
C	-1.409984000	1.585310000	1.566505000
C	-1.325742000	0.510915000	2.651958000
C	-2.852186000	2.061998000	1.301975000
C	-1.892006000	1.025093000	3.995768000
H	-1.860285000	-0.383355000	2.324297000
C	-3.697073000	2.077698000	2.591663000
H	-2.812778000	3.070709000	0.881717000
C	-2.820440000	2.236722000	3.830102000
H	-2.443910000	0.213864000	4.480958000
H	-4.264575000	1.145478000	2.684504000
H	-3.437421000	2.354545000	4.725326000
H	0.846291000	3.486228000	0.304460000
H	1.436112000	4.708676000	-1.627955000
H	-0.291209000	5.859324000	-3.083325000
H	0.220061000	3.804624000	-4.105924000
H	-0.384826000	1.563179000	-2.907868000
H	-1.741134000	2.812537000	-1.125456000
H	-0.821567000	2.441313000	1.917787000
H	-0.285444000	0.216320000	2.786768000
H	-1.069282000	1.288351000	4.667131000
H	-2.227955000	3.154774000	3.737331000
H	-4.434901000	2.882241000	2.531631000
H	-3.334150000	1.424850000	0.554510000
H	-1.502164000	-3.062699000	-2.544792000
C	0.023070000	-2.224537000	-0.129287000
H	-0.336864000	-2.072361000	0.893978000
C	-0.036778000	-3.726117000	-0.440849000

H	-1.061102000	-4.066476000	-0.268286000
H	0.208728000	-3.931617000	-1.482263000
H	0.620062000	-4.323205000	0.179870000
P	1.738013000	-1.443871000	0.000130000
C	2.495157000	-2.159761000	1.601220000
C	2.710275000	-1.921061000	-1.546190000
C	2.230204000	-3.649276000	1.852430000
H	2.776221000	-3.926725000	2.760354000
H	1.175348000	-3.854495000	2.039455000
H	2.589396000	-4.290853000	1.046793000
C	1.859606000	-1.381557000	2.766331000
H	2.024837000	-0.299180000	2.695144000
H	0.786803000	-1.570785000	2.837404000
H	2.318776000	-1.719396000	3.700881000
C	4.014264000	-1.941843000	1.628263000
H	4.374135000	-2.228658000	2.621864000
H	4.533327000	-2.568420000	0.901383000
H	4.294258000	-0.902576000	1.460704000
C	3.977970000	-1.069093000	-1.698754000
H	4.638356000	-1.126173000	-0.834322000
H	4.526762000	-1.446200000	-2.568278000
H	3.741759000	-0.020192000	-1.878969000
C	3.123796000	-3.401294000	-1.534358000
H	3.566781000	-3.631951000	-2.508801000
H	3.878626000	-3.607529000	-0.774304000
H	2.288918000	-4.082639000	-1.383804000
C	1.812493000	-1.647820000	-2.764332000
H	0.989605000	-2.358018000	-2.844722000
H	1.399800000	-0.634843000	-2.751997000
H	2.424547000	-1.746557000	-3.666472000
Ir	1.712070000	0.792134000	0.366094000
Cl	4.082853000	1.480958000	0.686536000

H 1.842103000 0.950091000 -1.149679000

G3

Coordinates (Angstroms)			
	X	Y	Z
C	-2.953815000	-3.226670000	0.745998000
C	-3.498918000	-3.720862000	-0.472198000
H	-3.176421000	-4.606472000	-1.000362000
C	-4.506037000	-2.813273000	-0.903504000
H	-5.080215000	-2.891028000	-1.815357000
C	-3.628417000	-2.018972000	1.065228000
H	-3.437319000	-1.403122000	1.928061000
C	-4.585266000	-1.757221000	0.046865000
H	-5.240177000	-0.899497000	-0.006651000
H	-2.151180000	-3.674198000	1.314495000
C	-0.675484000	-1.583596000	-1.044106000
C	-1.260086000	-2.213083000	-2.181207000
C	-2.264439000	-1.364785000	-2.712343000
H	-2.908238000	-1.592626000	-3.549029000
C	-1.328338000	-0.313652000	-0.883532000
C	-2.321536000	-0.202001000	-1.913602000
H	-2.998249000	0.625499000	-2.059356000
Fe	-2.696124000	-1.864029000	-0.769704000
P	-0.693372000	1.083230000	0.063976000
C	-1.226562000	2.527264000	-0.967899000
C	-1.157684000	3.896771000	-0.249470000
C	-0.502221000	2.588104000	-2.318487000
C	-1.018095000	5.050697000	-1.256944000
H	-2.073463000	4.035010000	0.331071000
C	-1.245098000	3.538973000	-3.268978000
H	0.517443000	2.948340000	-2.152927000
C	-1.817920000	4.763334000	-2.525822000

H	-1.352849000	5.979743000	-0.787634000
H	-2.054762000	2.998870000	-3.769838000
H	-2.861139000	4.576960000	-2.244979000
C	-1.597084000	1.346328000	1.642140000
C	-1.222524000	0.330903000	2.721470000
C	-3.122343000	1.473166000	1.452458000
C	-1.799990000	0.744017000	4.093702000
H	-1.582513000	-0.659666000	2.430861000
C	-3.879809000	1.279415000	2.780362000
H	-3.345011000	2.464487000	1.050290000
C	-3.014538000	1.677533000	3.972522000
H	-2.089680000	-0.158474000	4.641115000
H	-4.175590000	0.232157000	2.901248000
H	-3.596546000	1.650932000	4.897823000
H	-0.331390000	3.947241000	0.462801000
H	0.036287000	5.194374000	-1.518541000
H	-1.824161000	5.635747000	-3.184660000
H	-0.551757000	3.864453000	-4.050716000
H	-0.413916000	1.597850000	-2.772900000
H	-2.283256000	2.322035000	-1.164333000
H	-1.201863000	2.317986000	1.964554000
H	-0.137526000	0.256132000	2.792742000
H	-1.022464000	1.234530000	4.687097000
H	-2.681495000	2.714192000	3.843515000
H	-4.805680000	1.860478000	2.758266000
H	-3.475650000	0.748585000	0.714972000
H	-1.025075000	-3.195653000	-2.558171000
C	0.376666000	-2.204898000	-0.150155000
H	0.022529000	-2.110953000	0.882129000
C	0.488726000	-3.699114000	-0.484285000
H	-0.487016000	-4.161638000	-0.318845000
H	0.753123000	-3.859862000	-1.528687000

H	1.213530000	-4.224972000	0.125158000
P	1.987344000	-1.228652000	-0.048952000
C	2.854162000	-1.863791000	1.527973000
C	2.974644000	-1.576709000	-1.622688000
C	2.741090000	-3.369613000	1.790065000
H	3.327767000	-3.590973000	2.688051000
H	1.713862000	-3.676561000	1.993710000
H	3.146869000	-3.973911000	0.977364000
C	2.174887000	-1.142002000	2.703570000
H	2.257611000	-0.050480000	2.636583000
H	1.120267000	-1.411695000	2.786871000
H	2.666982000	-1.446673000	3.633168000
C	4.343760000	-1.497164000	1.516712000
H	4.752190000	-1.732148000	2.505507000
H	4.905952000	-2.080737000	0.786102000
H	4.511622000	-0.437860000	1.328620000
C	4.125124000	-0.576259000	-1.786062000
H	4.824815000	-0.592576000	-0.951796000
H	4.674991000	-0.848456000	-2.693401000
H	3.759955000	0.443919000	-1.904670000
C	3.562666000	-2.995331000	-1.648997000
H	4.047848000	-3.140417000	-2.620115000
H	4.323429000	-3.135868000	-0.879848000
H	2.812953000	-3.775670000	-1.536035000
C	2.023413000	-1.388024000	-2.815142000
H	1.281728000	-2.182550000	-2.888702000
H	1.501987000	-0.426799000	-2.775932000
H	2.619472000	-1.405425000	-3.733268000
Ir	1.606578000	1.090398000	0.341615000
Cl	3.986830000	1.847882000	0.582376000
H	1.671793000	1.267817000	-1.180545000
H	1.352161000	2.746811000	0.933838000

H	1.520883000	2.817357000	0.111569000
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TS_{G3-G1}

Coordinates (Angstroms)			
	X	Y	Z
C	5.684460000	-0.971040000	-0.522769000
C	6.146248000	-1.826099000	0.516390000
H	6.361335000	-2.880764000	0.422569000
C	6.224515000	-1.060450000	1.712995000
H	6.511205000	-1.433584000	2.685632000
C	5.474780000	0.316457000	0.032729000
H	5.114131000	1.175069000	-0.508767000
C	5.804122000	0.265844000	1.416483000
H	5.730844000	1.080991000	2.121797000
H	5.501509000	-1.251753000	-1.549377000
C	2.506425000	-1.753416000	0.250890000
C	3.118109000	-2.744421000	1.067956000
C	3.279425000	-2.209947000	2.372901000
H	3.749858000	-2.705116000	3.209766000
C	2.272636000	-0.596191000	1.057004000
C	2.776721000	-0.888017000	2.368960000
H	2.778114000	-0.224333000	3.219285000
Fe	4.302980000	-1.078995000	1.004148000
P	1.130199000	0.757256000	0.631035000
C	0.701512000	1.336327000	2.331869000
C	0.011648000	2.705014000	2.332534000
C	-0.155220000	0.328657000	3.101856000
C	-0.781747000	2.957869000	3.628037000
H	0.753471000	3.495445000	2.193579000
C	-0.210184000	0.705150000	4.592651000
H	-1.158713000	0.337401000	2.668197000
C	-0.145528000	2.228308000	4.808815000

H	-0.842146000	4.033149000	3.816885000
H	0.617527000	0.223564000	5.123432000
H	0.898323000	2.549377000	4.904757000
C	2.015065000	2.179984000	-0.114769000
C	2.362033000	1.935250000	-1.587467000
C	3.179607000	2.787848000	0.679235000
C	2.657850000	3.276742000	-2.289374000
H	3.220680000	1.259726000	-1.652930000
C	4.019504000	3.727964000	-0.207591000
H	2.771232000	3.355799000	1.519450000
C	3.163668000	4.351431000	-1.309941000
H	3.402126000	3.114774000	-3.075290000
H	4.844212000	3.180109000	-0.676710000
H	3.730001000	5.112347000	-1.853963000
H	-0.657960000	2.745579000	1.479012000
H	-1.811789000	2.603206000	3.511928000
H	-0.641530000	2.498405000	5.745171000
H	-1.134414000	0.305688000	5.022428000
H	0.217789000	-0.690633000	2.993625000
H	1.670129000	1.438731000	2.830450000
H	1.208950000	2.915431000	-0.117168000
H	1.530047000	1.426825000	-2.095793000
H	1.750275000	3.638488000	-2.783373000
H	2.311336000	4.867159000	-0.850646000
H	4.479060000	4.502809000	0.412006000
H	3.806794000	2.006144000	1.109393000
H	3.437075000	-3.724148000	0.746421000
C	2.165785000	-1.896584000	-1.201944000
H	2.418890000	-0.948733000	-1.686074000
C	3.045195000	-2.985870000	-1.835252000
H	4.007174000	-2.997517000	-1.323599000
H	2.622704000	-3.986487000	-1.764403000

H	3.250203000	-2.765471000	-2.878560000
P	0.283721000	-1.910445000	-1.438539000
C	0.071341000	-2.386468000	-3.298871000
C	-0.499716000	-3.231707000	-0.315183000
C	0.918759000	-3.557299000	-3.842959000
H	0.464944000	-3.855666000	-4.793711000
H	1.943509000	-3.278144000	-4.064571000
H	0.922857000	-4.435540000	-3.199187000
C	0.498521000	-1.132593000	-4.082832000
H	-0.139971000	-0.274031000	-3.876239000
H	1.537785000	-0.863815000	-3.867219000
H	0.434632000	-1.351047000	-5.154591000
C	-1.375682000	-2.793025000	-3.639463000
H	-1.514541000	-2.652480000	-4.717522000
H	-1.526840000	-3.854352000	-3.430466000
H	-2.137161000	-2.216071000	-3.130962000
C	-2.010599000	-3.315313000	-0.591326000
H	-2.241265000	-3.857740000	-1.505409000
H	-2.476124000	-3.856050000	0.238032000
H	-2.472897000	-2.327402000	-0.643750000
C	0.131754000	-4.613600000	-0.509363000
H	-0.369798000	-5.320182000	0.161381000
H	0.005501000	-4.987090000	-1.526443000
H	1.194459000	-4.619021000	-0.256943000
C	-0.358923000	-2.835037000	1.164588000
H	0.672911000	-2.742221000	1.493472000
H	-0.881866000	-1.905160000	1.384431000
H	-0.827174000	-3.624184000	1.762461000
Ir	-0.567689000	0.290438000	-0.886178000
Cl	-2.364391000	0.050482000	-2.540195000
H	-1.455697000	1.899867000	-0.564875000
H	-1.396191000	-0.353295000	0.227100000

C	-2.651568000	2.909930000	-0.662372000
C	-2.716466000	3.205689000	-2.145558000
C	-1.406835000	3.761103000	-2.701342000
C	-0.965423000	5.020974000	-1.964498000
C	-0.854043000	4.748025000	-0.468931000
C	-2.116776000	4.118321000	0.103262000
H	-3.004741000	2.322630000	-2.705240000
H	-0.627140000	2.993435000	-2.620464000
H	-0.006308000	5.376680000	-2.353836000
H	-0.009169000	4.082648000	-0.292919000
H	-2.942157000	4.838769000	0.014156000
C	-3.662814000	2.058706000	1.369649000
C	-4.830517000	1.690396000	-0.767286000
C	-4.621823000	0.947869000	1.767946000
H	-2.646982000	1.744117000	1.630013000
C	-5.038051000	0.196496000	-0.475838000
H	-5.716123000	2.248337000	-0.444360000
H	-4.380065000	0.633043000	2.778784000
H	-4.549026000	-0.406999000	-1.239777000
H	-3.508272000	3.956937000	-2.265730000
H	-1.540895000	3.965134000	-3.767225000
H	-1.699215000	5.817329000	-2.139896000
H	-0.644591000	5.670478000	0.080047000
H	-2.008770000	3.927666000	1.166070000
H	-4.737932000	1.833825000	-1.838729000
H	-3.901761000	2.974448000	1.920060000
H	-5.662235000	1.302767000	1.778988000
H	-6.122043000	0.007739000	-0.516261000
C	-4.580498000	-1.473222000	1.239221000
C	-3.853288000	-1.952608000	2.339302000
C	-5.340380000	-2.430977000	0.552957000
C	-3.891711000	-3.260085000	2.767081000

C	-5.377070000	-3.761540000	0.958608000
H	-5.911100000	-2.134655000	-0.317302000
C	-4.666669000	-4.184236000	2.072024000
H	-3.298090000	-3.544452000	3.628395000
H	-5.978242000	-4.466103000	0.394672000
H	-4.698713000	-5.217883000	2.395129000
F	-3.036447000	-1.098123000	3.005926000
N	-3.690256000	2.277878000	-0.076068000
N	-4.474375000	-0.149410000	0.819732000

TS_{G3-G1}

Coordinates (Angstroms)			
	X	Y	Z
C	-3.582328000	-2.220671000	-2.227233000
C	-4.780907000	-2.426385000	-1.489057000
H	-5.673303000	-1.819655000	-1.542116000
C	-4.579965000	-3.537691000	-0.623465000
H	-5.293953000	-3.919726000	0.091713000
C	-2.648254000	-3.210358000	-1.821615000
H	-1.648625000	-3.323644000	-2.205429000
C	-3.256755000	-4.021119000	-0.825891000
H	-2.791406000	-4.846159000	-0.306178000
H	-3.405290000	-1.439438000	-2.952579000
C	-2.642678000	-0.113771000	0.196025000
C	-3.898031000	-0.413197000	0.803504000
C	-3.730749000	-1.498101000	1.700672000
H	-4.513192000	-1.972820000	2.274419000
C	-1.682698000	-1.031152000	0.742437000
C	-2.375853000	-1.894808000	1.653800000
H	-1.941169000	-2.705232000	2.218115000
Fe	-3.232093000	-2.051723000	-0.207155000
P	0.113341000	-0.826196000	0.693581000

C	0.652389000	-1.617358000	2.279508000
C	2.168424000	-1.938239000	2.333829000
C	0.213168000	-0.801613000	3.501907000
C	2.725342000	-1.821100000	3.758400000
H	2.321546000	-2.961493000	1.980363000
C	0.424792000	-1.603340000	4.793165000
H	0.797025000	0.122210000	3.536553000
C	1.741641000	-2.408427000	4.768632000
H	3.688461000	-2.336729000	3.810552000
H	-0.420097000	-2.283065000	4.944794000
H	1.538287000	-3.448334000	4.486607000
C	0.855719000	-1.895012000	-0.609125000
C	0.485891000	-1.408785000	-2.012039000
C	0.580223000	-3.397866000	-0.423537000
C	1.301095000	-2.146566000	-3.097876000
H	-0.585965000	-1.551272000	-2.167216000
C	0.944858000	-4.207221000	-1.689251000
H	1.166753000	-3.765257000	0.420614000
C	1.923996000	-3.451679000	-2.584835000
H	0.646955000	-2.369349000	-3.947162000
H	0.043656000	-4.428212000	-2.271159000
H	2.224911000	-4.075798000	-3.431411000
H	2.748994000	-1.297384000	1.670538000
H	2.919874000	-0.770030000	4.000310000
H	2.186012000	-2.440307000	5.767157000
H	0.423401000	-0.907346000	5.637654000
H	-0.835209000	-0.502745000	3.418132000
H	0.115661000	-2.570314000	2.301172000
H	1.929241000	-1.723195000	-0.469253000
H	0.664812000	-0.337587000	-2.085397000
H	2.091585000	-1.490707000	-3.472294000
H	2.838085000	-3.233987000	-2.021934000

H	1.362888000	-5.173929000	-1.395787000
H	-0.470700000	-3.559202000	-0.169809000
H	-4.839628000	0.068505000	0.594374000
C	-2.423891000	0.948672000	-0.862987000
H	-1.892666000	0.475696000	-1.696581000
C	-3.793504000	1.415836000	-1.373640000
H	-4.316698000	0.555231000	-1.798446000
H	-4.412236000	1.810348000	-0.568439000
H	-3.730398000	2.175520000	-2.142143000
P	-1.172935000	2.277266000	-0.371585000
C	-0.731265000	3.174629000	-2.000064000
C	-2.044781000	3.439244000	0.843720000
C	-1.871462000	3.410571000	-2.996713000
H	-1.464431000	3.995560000	-3.828799000
H	-2.251158000	2.478395000	-3.418096000
H	-2.699643000	3.979617000	-2.571717000
C	0.309271000	2.283101000	-2.695155000
H	1.176107000	2.082776000	-2.058408000
H	-0.126015000	1.330019000	-3.005315000
H	0.666757000	2.790661000	-3.597468000
C	-0.086051000	4.535482000	-1.701023000
H	0.326687000	4.925509000	-2.638065000
H	-0.812763000	5.264699000	-1.339340000
H	0.728332000	4.460369000	-0.982317000
C	-1.029911000	4.332324000	1.571630000
H	-0.431674000	4.942499000	0.896669000
H	-1.590445000	5.005892000	2.229537000
H	-0.348334000	3.746727000	2.189628000
C	-3.091548000	4.343662000	0.176638000
H	-3.626240000	4.883827000	0.966016000
H	-2.633753000	5.089517000	-0.474274000
H	-3.830808000	3.792966000	-0.402358000

C	-2.734960000	2.573075000	1.910490000
H	-3.629534000	2.080961000	1.530157000
H	-2.065222000	1.811604000	2.321280000
H	-3.042788000	3.224584000	2.735163000
Ir	0.837738000	1.334307000	0.513113000
Cl	2.211434000	3.468243000	0.669346000
H	0.222765000	1.546995000	1.902457000
H	2.801618000	0.683058000	0.802875000
H	2.115838000	0.767107000	1.463895000
C	3.931247000	0.054446000	-0.934719000
O	3.992737000	0.276636000	0.309551000
O	3.141297000	0.494988000	-1.757895000
C	5.014677000	-0.943997000	-1.414561000
F	4.879179000	-2.122436000	-0.779318000
F	6.247238000	-0.488972000	-1.150077000
F	4.941368000	-1.182981000	-2.724653000

H1

Coordinates (Angstroms)			
	X	Y	Z
C	-3.825196000	0.323527000	-2.733597000
C	-4.997180000	0.867472000	-2.137155000
H	-5.312911000	1.899795000	-2.181996000
C	-5.652849000	-0.174932000	-1.423979000
H	-6.553502000	-0.070227000	-0.836347000
C	-3.766141000	-1.054547000	-2.395258000
H	-2.999169000	-1.743871000	-2.703169000
C	-4.887578000	-1.364834000	-1.579247000
H	-5.108828000	-2.327577000	-1.141669000
H	-3.097018000	0.865258000	-3.320358000
C	-2.198116000	1.260083000	0.038260000
C	-3.458875000	1.733707000	0.506869000

C	-4.098333000	0.700571000	1.238873000
H	-5.080214000	0.752796000	1.686297000
C	-2.055096000	-0.094128000	0.499076000
C	-3.248316000	-0.429538000	1.220623000
H	-3.461802000	-1.379259000	1.686380000
Fe	-3.762225000	0.116273000	-0.689610000
P	-0.485677000	-1.016854000	0.620278000
C	-0.848103000	-2.223371000	1.986010000
C	0.219469000	-3.340304000	2.093818000
C	-1.033572000	-1.544410000	3.348615000
C	0.333515000	-3.890547000	3.524011000
H	-0.048020000	-4.158271000	1.419758000
C	-1.625641000	-2.535967000	4.361413000
H	-0.059018000	-1.189555000	3.694410000
C	-1.038399000	-3.953030000	4.192113000
H	0.797375000	-4.880728000	3.493709000
H	-2.714382000	-2.571547000	4.246700000
H	-1.702204000	-4.561426000	3.566191000
C	-0.286070000	-2.116198000	-0.845049000
C	-0.103235000	-1.339851000	-2.152293000
C	-1.354323000	-3.212778000	-1.003353000
C	0.453398000	-2.264367000	-3.255920000
H	-1.064952000	-0.917769000	-2.454542000
C	-1.261301000	-3.891870000	-2.388922000
H	-1.212633000	-3.969953000	-0.229956000
C	0.134043000	-3.743818000	-2.993336000
H	0.031869000	-1.964978000	-4.221331000
H	-1.984030000	-3.451084000	-3.084766000
H	0.211829000	-4.314396000	-3.923364000
H	1.196453000	-2.974185000	1.772286000
H	0.997738000	-3.253941000	4.119613000
H	-0.976928000	-4.456855000	5.160892000

H	-1.428390000	-2.164891000	5.372318000
H	-1.672697000	-0.661357000	3.276892000
H	-1.798554000	-2.690948000	1.707562000
H	0.669230000	-2.599333000	-0.616008000
H	0.571092000	-0.499344000	-2.002197000
H	1.536577000	-2.136230000	-3.335361000
H	0.875540000	-4.166223000	-2.305053000
H	-1.532123000	-4.947403000	-2.296699000
H	-2.354112000	-2.796080000	-0.852333000
H	-3.887499000	2.703530000	0.308494000
C	-1.245958000	2.062244000	-0.825590000
H	-0.952931000	1.413014000	-1.656424000
C	-1.981465000	3.271350000	-1.411490000
H	-2.864580000	2.926239000	-1.955922000
H	-2.322993000	3.958319000	-0.636487000
H	-1.366114000	3.834494000	-2.103928000
P	0.444015000	2.373617000	-0.028943000
C	1.514829000	3.041851000	-1.472479000
C	0.187519000	3.760805000	1.263506000
C	1.029117000	4.242255000	-2.305308000
H	1.886416000	4.608549000	-2.882392000
H	0.270926000	3.948407000	-3.032387000
H	0.649343000	5.077941000	-1.723874000
C	1.711473000	1.890724000	-2.470420000
H	2.170332000	1.019135000	-2.010099000
H	0.769453000	1.593189000	-2.940208000
H	2.373979000	2.240148000	-3.271352000
C	2.881075000	3.404432000	-0.869544000
H	3.604154000	3.534209000	-1.683068000
H	2.836566000	4.347168000	-0.317911000
H	3.257302000	2.630274000	-0.197203000
C	1.374255000	3.791462000	2.235994000

H	2.327054000	3.967026000	1.737250000
H	1.210888000	4.607190000	2.950546000
H	1.464746000	2.859703000	2.792427000
C	0.026195000	5.175739000	0.694004000
H	-0.246843000	5.846719000	1.517192000
H	0.961244000	5.549287000	0.271927000
H	-0.754052000	5.252650000	-0.062867000
C	-1.063973000	3.420800000	2.087718000
H	-1.985356000	3.608041000	1.536834000
H	-1.068149000	2.382091000	2.428491000
H	-1.077062000	4.061741000	2.976728000
Ir	1.304116000	0.281312000	1.045340000
Cl	3.535325000	1.189732000	1.947976000
H	0.517498000	0.749869000	2.308997000
O	2.696559000	-0.473560000	-0.670168000
C	3.182874000	-1.610490000	-0.842351000
C	4.200393000	-1.667387000	-2.016877000
O	3.019389000	-2.665797000	-0.226633000
F	5.440106000	-1.384584000	-1.569116000
F	3.929272000	-0.789889000	-2.994885000
F	4.253134000	-2.881793000	-2.582610000
H	1.783952000	-0.997065000	1.881974000

H2

Coordinates (Angstroms)			
	X	Y	Z
C	3.126318000	0.854971000	-2.682132000
C	3.679785000	-0.157242000	-3.515241000
H	3.368530000	-0.390332000	-4.523326000
C	4.674603000	-0.848051000	-2.768574000
H	5.252967000	-1.693276000	-3.112922000
C	3.784110000	0.791405000	-1.423648000

H	3.573219000	1.413500000	-0.568817000
C	4.739425000	-0.261046000	-1.474081000
H	5.383695000	-0.574946000	-0.665330000
H	2.322154000	1.527339000	-2.943717000
C	0.830522000	-1.307607000	-1.765082000
C	1.458129000	-2.285513000	-2.587744000
C	2.400446000	-3.006830000	-1.809707000
H	3.057536000	-3.784778000	-2.170264000
C	1.398272000	-1.436815000	-0.449551000
C	2.373253000	-2.485732000	-0.496408000
H	2.977029000	-2.820194000	0.334101000
Fe	2.851351000	-0.995045000	-1.840703000
P	0.705315000	-0.714628000	1.047310000
C	0.592390000	-2.117468000	2.273102000
C	-0.093743000	-1.612047000	3.582374000
C	-0.039026000	-3.422459000	1.787074000
C	-1.350326000	-2.407007000	3.933199000
H	0.622046000	-1.685391000	4.407456000
C	-0.124006000	-4.413453000	2.949729000
H	-1.042033000	-3.244246000	1.393467000
C	-1.062467000	-3.905622000	4.067692000
H	-1.775330000	-2.019146000	4.863689000
H	0.885543000	-4.565952000	3.348235000
H	-0.609856000	-4.102362000	5.045023000
C	1.976117000	0.276870000	2.011192000
C	1.973872000	1.795983000	1.858090000
C	3.402988000	-0.309262000	1.888584000
C	2.804481000	2.454542000	2.978110000
H	2.359156000	2.083617000	0.879447000
C	4.479383000	0.719249000	2.266106000
H	3.489237000	-1.178000000	2.548437000
C	4.007117000	1.599924000	3.417680000

H	3.152066000	3.429161000	2.620960000
H	4.710095000	1.353031000	1.402011000
H	4.816212000	2.242074000	3.776602000
H	-0.364199000	-0.552638000	3.510001000
H	-2.106125000	-2.241227000	3.158394000
H	-2.009242000	-4.453756000	4.046794000
H	-0.462025000	-5.385222000	2.579531000
H	0.556150000	-3.848570000	0.976314000
H	1.638870000	-2.346516000	2.498008000
H	1.634275000	0.092952000	3.034640000
H	0.955554000	2.169289000	1.920714000
H	2.159327000	2.650441000	3.840622000
H	3.723183000	0.955378000	4.258338000
H	5.404013000	0.194486000	2.523524000
H	3.592430000	-0.657978000	0.875857000
H	1.276914000	-2.438002000	-3.640300000
C	-0.205289000	-0.314633000	-2.244203000
H	0.110249000	0.675255000	-1.903601000
C	-0.242772000	-0.290541000	-3.772964000
H	0.784969000	-0.265549000	-4.142368000
H	-0.734919000	-1.164500000	-4.203067000
H	-0.731022000	0.604400000	-4.142477000
P	-1.835929000	-0.452173000	-1.314341000
C	-3.091397000	0.759816000	-2.137188000
C	-2.553095000	-2.214528000	-1.496637000
C	-3.190019000	0.683820000	-3.679355000
H	-4.186726000	1.040893000	-3.957405000
H	-2.474303000	1.354282000	-4.153354000
H	-3.066505000	-0.304908000	-4.109257000
C	-2.695220000	2.203504000	-1.804405000
H	-2.807252000	2.425745000	-0.745400000
H	-1.670944000	2.422549000	-2.113239000

H	-3.359708000	2.869443000	-2.365302000
C	-4.499084000	0.512374000	-1.567270000
H	-5.129279000	1.353197000	-1.876621000
H	-4.958154000	-0.394652000	-1.959874000
H	-4.511247000	0.477459000	-0.479924000
C	-3.567690000	-2.498135000	-0.376191000
H	-4.332812000	-1.729336000	-0.276272000
H	-4.070225000	-3.442907000	-0.608184000
H	-3.077998000	-2.614744000	0.591480000
C	-3.236208000	-2.448511000	-2.854539000
H	-3.514278000	-3.507006000	-2.896689000
H	-4.147974000	-1.870668000	-2.995300000
H	-2.560526000	-2.261197000	-3.690699000
C	-1.434868000	-3.260748000	-1.406921000
H	-0.875406000	-3.322400000	-2.340075000
H	-0.735056000	-3.071258000	-0.601038000
H	-1.897405000	-4.237253000	-1.228390000
Ir	-1.398599000	0.227973000	0.834595000
Cl	-3.590712000	1.021922000	1.714539000
H	-1.837583000	-1.203038000	1.208805000
O	-0.961107000	2.495048000	0.712778000
C	-0.165026000	3.073462000	-0.066647000
C	-0.149417000	4.608472000	0.151821000
O	0.573938000	2.618722000	-0.935736000
F	0.248493000	4.911547000	1.401475000
F	-1.376120000	5.133832000	-0.011830000
F	0.670852000	5.242072000	-0.690800000

H3

Coordinates (Angstroms)			
	X	Y	Z
C	-4.014414000	-0.070578000	-2.571539000

C	-5.204841000	0.343524000	-1.911148000
H	-5.644431000	1.329562000	-1.951422000
C	-5.686589000	-0.752544000	-1.142344000
H	-6.553332000	-0.741272000	-0.497322000
C	-3.767366000	-1.421908000	-2.212370000
H	-2.938736000	-2.018858000	-2.552177000
C	-4.793068000	-1.845209000	-1.324304000
H	-4.870811000	-2.816169000	-0.856925000
H	-3.392916000	0.540428000	-3.210306000
C	-2.322294000	1.080767000	0.074080000
C	-3.591918000	1.466789000	0.591427000
C	-4.100605000	0.411816000	1.391582000
H	-5.060538000	0.396535000	1.886321000
C	-2.042939000	-0.235671000	0.568749000
C	-3.161833000	-0.644709000	1.368161000
H	-3.272011000	-1.591728000	1.873270000
Fe	-3.805199000	-0.220280000	-0.532654000
P	-0.407238000	-1.001196000	0.609373000
C	-0.536804000	-2.141097000	2.066273000
C	0.611398000	-3.180264000	2.153090000
C	-0.689672000	-1.388339000	3.395542000
C	0.887391000	-3.599056000	3.604661000
H	0.327477000	-4.066310000	1.579818000
C	-1.119690000	-2.355839000	4.507365000
H	0.265955000	-0.926626000	3.656120000
C	-0.420471000	-3.725406000	4.383033000
H	1.433584000	-4.546470000	3.606270000
H	-2.205701000	-2.491255000	4.475316000
H	-1.071599000	-4.429382000	3.851453000
C	-0.136512000	-2.133852000	-0.810292000
C	-0.073381000	-1.404041000	-2.153236000
C	-1.116708000	-3.321379000	-0.866217000

C	0.499930000	-2.333001000	-3.243518000
H	-1.077170000	-1.066538000	-2.422484000
C	-1.055008000	-4.037339000	-2.233439000
H	-0.863215000	-4.034811000	-0.080383000
C	0.293336000	-3.820319000	-2.916351000
H	0.018774000	-2.099762000	-4.198835000
H	-1.841589000	-3.666777000	-2.899519000
H	0.360541000	-4.416419000	-3.830757000
H	1.533909000	-2.810235000	1.702598000
H	1.536016000	-2.863386000	4.093667000
H	-0.243998000	-4.153213000	5.373615000
H	-0.888108000	-1.899392000	5.474663000
H	-1.411721000	-0.573040000	3.312926000
H	-1.466529000	-2.690520000	1.885599000
H	0.867094000	-2.519653000	-0.594056000
H	0.543799000	-0.513086000	-2.068817000
H	1.566853000	-2.133826000	-3.373833000
H	1.093218000	-4.172961000	-2.255076000
H	-1.251125000	-5.103661000	-2.092577000
H	-2.136432000	-2.981165000	-0.665883000
H	-4.108272000	2.390820000	0.383661000
C	-1.468854000	1.900589000	-0.865662000
H	-1.161508000	1.235347000	-1.678646000
C	-2.317643000	3.027201000	-1.465355000
H	-3.198208000	2.585713000	-1.937804000
H	-2.668050000	3.724334000	-0.704265000
H	-1.790419000	3.594509000	-2.222454000
P	0.212946000	2.393216000	-0.161980000
C	1.185053000	3.071184000	-1.667241000
C	-0.090727000	3.772056000	1.125167000
C	0.540627000	4.194596000	-2.503015000
H	1.335356000	4.622428000	-3.123687000

H	-0.210771000	3.806059000	-3.190380000
H	0.106335000	5.007707000	-1.928963000
C	1.426345000	1.912398000	-2.644690000
H	1.995994000	1.100589000	-2.200335000
H	0.490005000	1.517223000	-3.047579000
H	1.999329000	2.304301000	-3.492411000
C	2.539324000	3.583680000	-1.158062000
H	3.171548000	3.800416000	-2.025916000
H	2.430511000	4.511888000	-0.591913000
H	3.056511000	2.855226000	-0.534108000
C	1.117562000	3.946418000	2.052918000
H	2.042238000	4.153598000	1.516302000
H	0.908216000	4.797095000	2.710868000
H	1.282869000	3.068396000	2.675321000
C	-0.383374000	5.142784000	0.499992000
H	-0.685694000	5.818864000	1.307146000
H	0.506231000	5.571597000	0.035577000
H	-1.190607000	5.125840000	-0.231008000
C	-1.286463000	3.368993000	2.001727000
H	-2.236165000	3.468790000	1.478192000
H	-1.202769000	2.348513000	2.384318000
H	-1.313732000	4.043784000	2.863854000
Ir	1.317919000	0.501773000	0.905046000
Cl	3.456181000	1.649197000	1.641164000
H	2.215891000	-0.871735000	1.540474000
H	0.503272000	1.025757000	2.118609000
O	2.683270000	-0.274690000	-0.829289000
C	3.346256000	-1.327655000	-0.697566000
C	4.213756000	-1.704752000	-1.926280000
O	3.428853000	-2.100591000	0.258777000
F	5.517668000	-1.543465000	-1.641955000
F	3.951454000	-0.971368000	-3.013809000

F	4.035755000	-2.992968000	-2.260749000
H	1.859659000	-0.479484000	2.209572000

TS_{H1-H2}

Coordinates (Angstroms)			
	X	Y	Z
C	5.120994000	-1.631521000	-0.583619000
C	5.407363000	-3.013744000	-0.405450000
H	5.459721000	-3.758319000	-1.186681000
C	5.555119000	-3.257286000	0.988623000
H	5.743023000	-4.216971000	1.448059000
C	5.099581000	-1.023663000	0.699572000
H	4.902114000	0.016165000	0.897619000
C	5.362568000	-2.024626000	1.673588000
H	5.391125000	-1.878778000	2.743863000
H	4.924282000	-1.133720000	-1.521986000
C	1.889293000	-2.425255000	-0.411423000
C	2.289678000	-3.777885000	-0.219981000
C	2.416901000	-4.022365000	1.171168000
H	2.744338000	-4.944480000	1.628915000
C	1.755597000	-1.818972000	0.883645000
C	2.104170000	-2.822813000	1.851505000
H	2.130861000	-2.694544000	2.922104000
Fe	3.685935000	-2.521908000	0.586542000
P	0.866948000	-0.266209000	1.273452000
C	0.031101000	-0.824557000	2.859772000
C	-0.601927000	0.349079000	3.627954000
C	-0.955560000	-1.980917000	2.743832000
C	-1.737091000	-0.092970000	4.560447000
H	0.165862000	0.853245000	4.222496000
C	-1.313715000	-2.531618000	4.136243000
H	-1.856433000	-1.634947000	2.231458000

C	-1.394292000	-1.430093000	5.209403000
H	-1.910442000	0.680703000	5.314123000
H	-0.571164000	-3.280057000	4.431785000
H	-0.430345000	-1.333551000	5.723160000
C	2.035973000	0.953351000	2.077277000
C	2.788727000	1.875298000	1.121652000
C	2.956815000	0.323639000	3.146261000
C	3.518352000	3.017306000	1.866392000
H	3.489766000	1.299113000	0.518791000
C	4.150135000	1.229114000	3.497315000
H	2.374926000	0.152015000	4.056239000
C	3.779562000	2.699666000	3.343666000
H	4.474260000	3.205673000	1.366669000
H	4.999612000	1.012630000	2.839832000
H	4.570687000	3.347539000	3.732231000
H	-0.970037000	1.076589000	2.911181000
H	-2.672839000	-0.201841000	4.001481000
H	-2.130341000	-1.695723000	5.973117000
H	-2.273186000	-3.053499000	4.064022000
H	-0.534798000	-2.791506000	2.151574000
H	0.872335000	-1.190947000	3.451493000
H	1.319897000	1.590309000	2.603492000
H	2.074724000	2.309538000	0.427356000
H	2.940239000	3.942876000	1.787181000
H	2.881994000	2.908350000	3.939335000
H	4.482625000	1.009208000	4.515977000
H	3.325478000	-0.647806000	2.816381000
H	2.498502000	-4.490765000	-1.003162000
C	1.699729000	-1.778937000	-1.755858000
H	2.142721000	-0.782357000	-1.689865000
C	2.489136000	-2.539870000	-2.824721000
H	3.445342000	-2.845154000	-2.398223000

H	1.986213000	-3.435479000	-3.189488000
H	2.714754000	-1.893535000	-3.667671000
P	-0.094902000	-1.271650000	-2.060094000
C	-0.177029000	-0.864599000	-3.960900000
C	-1.312565000	-2.711508000	-1.778714000
C	0.454627000	-1.908555000	-4.917424000
H	-0.032404000	-1.786656000	-5.890391000
H	1.514622000	-1.731810000	-5.079437000
H	0.322421000	-2.944757000	-4.618993000
C	0.571799000	0.450781000	-4.202299000
H	0.100186000	1.285989000	-3.689559000
H	1.615196000	0.376064000	-3.888202000
H	0.567407000	0.654028000	-5.279452000
C	-1.631366000	-0.716068000	-4.449236000
H	-1.597874000	-0.197929000	-5.414551000
H	-2.088593000	-1.690816000	-4.627338000
H	-2.258339000	-0.134295000	-3.782291000
C	-2.760600000	-2.198921000	-1.887095000
H	-3.072451000	-1.996434000	-2.907721000
H	-3.422360000	-2.975897000	-1.491751000
H	-2.914244000	-1.296336000	-1.293500000
C	-1.107372000	-3.886291000	-2.739912000
H	-1.768261000	-4.702713000	-2.426927000
H	-1.368545000	-3.637336000	-3.768304000
H	-0.081891000	-4.264914000	-2.714709000
C	-1.166301000	-3.227879000	-0.347828000
H	-0.197376000	-3.680619000	-0.146780000
H	-1.338629000	-2.421935000	0.356889000
H	-1.935259000	-3.988821000	-0.173973000
Ir	-0.460790000	0.573470000	-0.475315000
Cl	-1.995219000	1.558951000	-2.123044000
H	-1.067886000	1.994545000	0.508307000

H	-1.609211000	-0.234910000	0.183783000
C	-2.045628000	3.137208000	0.908081000
C	-1.826185000	4.181296000	-0.168973000
C	-0.395721000	4.708752000	-0.252105000
C	0.133635000	5.183937000	1.095540000
C	0.018261000	4.054036000	2.110551000
C	-1.410239000	3.547245000	2.231989000
H	-2.119945000	3.787720000	-1.138704000
H	0.250630000	3.915366000	-0.633078000
H	1.176712000	5.501067000	0.999543000
H	0.656193000	3.230587000	1.788572000
H	-2.056304000	4.364106000	2.584831000
C	-3.574176000	1.683504000	2.109697000
C	-4.357998000	2.756990000	0.034441000
C	-4.871424000	0.932407000	1.872706000
H	-2.769201000	0.945409000	2.155694000
C	-4.962312000	1.441852000	-0.480550000
H	-5.136922000	3.343554000	0.533972000
H	-4.950757000	0.141580000	2.611805000
H	-4.443406000	1.123901000	-1.384776000
H	-2.509195000	5.004527000	0.081688000
H	-0.373086000	5.519548000	-0.986306000
H	-0.439312000	6.053791000	1.441427000
H	0.368388000	4.368388000	3.098000000
H	-1.473799000	2.767725000	2.982827000
H	-4.019389000	3.335710000	-0.817631000
H	-3.618874000	2.223395000	3.060762000
H	-5.745545000	1.585223000	2.002230000
H	-6.014904000	1.648389000	-0.729966000
C	-5.297550000	-0.876780000	0.216313000
C	-4.972293000	-1.992809000	1.004784000
C	-6.032309000	-1.155457000	-0.946296000

C	-5.361251000	-3.277936000	0.705527000
C	-6.417672000	-2.451375000	-1.275028000
H	-6.302719000	-0.345499000	-1.611174000
C	-6.097983000	-3.519947000	-0.450695000
H	-5.060851000	-4.079516000	1.370686000
H	-6.979077000	-2.616430000	-2.188069000
H	-6.400075000	-4.529941000	-0.700638000
F	-4.192112000	-1.817049000	2.103205000
O	1.053085000	2.038845000	-1.563311000
C	2.224142000	2.048201000	-1.989430000
C	2.640918000	3.437266000	-2.548257000
O	3.092296000	1.172925000	-2.004175000
F	2.950411000	4.270246000	-1.530613000
F	1.660543000	4.026183000	-3.250060000
F	3.714917000	3.374013000	-3.343832000
N	-3.273681000	2.581124000	0.996308000
N	-4.837017000	0.395468000	0.520770000

TS_{H3-G1}

Coordinates (Angstroms)			
	X	Y	Z
C	-4.137072000	-0.356528000	-2.427447000
C	-5.322860000	-0.047168000	-1.703908000
H	-5.839217000	0.901794000	-1.704991000
C	-5.677877000	-1.187960000	-0.931749000
H	-6.509285000	-1.253195000	-0.244762000
C	-3.768435000	-1.689854000	-2.105499000
H	-2.915571000	-2.216493000	-2.497970000
C	-4.712091000	-2.204535000	-1.175949000
H	-4.689212000	-3.184600000	-0.721855000
H	-3.597066000	0.309763000	-3.084901000
C	-2.417947000	0.894528000	0.160332000

C	-3.688487000	1.160763000	0.747880000
C	-4.067831000	0.052853000	1.547878000
H	-4.998756000	-0.052777000	2.085365000
C	-2.007965000	-0.405313000	0.609504000
C	-3.047036000	-0.920017000	1.454176000
H	-3.053093000	-1.881528000	1.943683000
Fe	-3.817624000	-0.517133000	-0.403542000
P	-0.309578000	-1.027896000	0.569347000
C	-0.285596000	-2.205508000	2.002307000
C	0.938319000	-3.158298000	2.004453000
C	-0.411228000	-1.483753000	3.350731000
C	1.360232000	-3.543274000	3.429280000
H	0.676825000	-4.068713000	1.459269000
C	-0.685826000	-2.490068000	4.476088000
H	0.521203000	-0.949946000	3.549711000
C	0.132284000	-3.787325000	4.304452000
H	1.990648000	-4.436169000	3.387567000
H	-1.754661000	-2.726206000	4.504739000
H	-0.484343000	-4.557413000	3.826049000
C	-0.006452000	-2.104537000	-0.887867000
C	-0.054407000	-1.336919000	-2.209920000
C	-0.878364000	-3.372083000	-0.954630000
C	0.605703000	-2.168652000	-3.325976000
H	-1.096304000	-1.114705000	-2.454943000
C	-0.811461000	-4.019638000	-2.355008000
H	-0.529807000	-4.090454000	-0.210270000
C	0.498240000	-3.681995000	-3.065571000
H	0.132951000	-1.924130000	-4.282493000
H	-1.641733000	-3.671500000	-2.978985000
H	0.574309000	-4.230249000	-4.008674000
H	1.792764000	-2.724638000	1.484445000
H	1.973527000	-2.748544000	3.869142000

H	0.424211000	-4.185096000	5.280219000
H	-0.4444632000	-2.015523000	5.432436000
H	-1.199265000	-0.727669000	3.328133000
H	-1.182142000	-2.817941000	1.861459000
H	1.034400000	-2.410625000	-0.723712000
H	0.453379000	-0.380206000	-2.111155000
H	1.659883000	-1.888841000	-3.414189000
H	1.337781000	-4.015053000	-2.444868000
H	-0.933795000	-5.102028000	-2.260723000
H	-1.915032000	-3.133628000	-0.700342000
H	-4.290761000	2.040878000	0.586398000
C	-1.687889000	1.813442000	-0.794434000
H	-1.369935000	1.203356000	-1.645940000
C	-2.665269000	2.874561000	-1.311818000
H	-3.518411000	2.370611000	-1.772788000
H	-3.050588000	3.501783000	-0.508045000
H	-2.224668000	3.523718000	-2.058139000
P	-0.012006000	2.421156000	-0.155385000
C	0.814854000	3.233014000	-1.684454000
C	-0.375134000	3.747806000	1.169963000
C	0.015437000	4.283810000	-2.477673000
H	0.727920000	4.810409000	-3.122331000
H	-0.715775000	3.819100000	-3.140101000
H	-0.484858000	5.032311000	-1.869476000
C	1.158060000	2.125948000	-2.691249000
H	1.854545000	1.393266000	-2.292807000
H	0.264287000	1.610688000	-3.052491000
H	1.628931000	2.596458000	-3.561832000
C	2.119333000	3.891034000	-1.212975000
H	2.711071000	4.155654000	-2.096350000
H	1.927933000	4.813848000	-0.660064000
H	2.718643000	3.229882000	-0.586250000

C	0.866706000	4.015375000	2.030368000
H	1.733812000	4.320537000	1.446415000
H	0.622332000	4.826392000	2.725645000
H	1.151257000	3.141063000	2.614231000
C	-0.839287000	5.097755000	0.606306000
H	-1.148747000	5.725166000	1.449707000
H	-0.030050000	5.621562000	0.094322000
H	-1.689413000	5.018041000	-0.070030000
C	-1.469262000	3.209863000	2.106098000
H	-2.456280000	3.237964000	1.645936000
H	-1.270060000	2.188357000	2.440122000
H	-1.501896000	3.849513000	2.994666000
Ir	1.278974000	0.604702000	0.799567000
Cl	3.375468000	1.891541000	1.450800000
H	2.680664000	-0.848347000	1.137076000
H	0.533100000	0.968723000	2.103856000
O	2.698038000	-0.056831000	-1.043818000
C	3.481982000	-0.944709000	-0.707998000
C	4.411909000	-1.539577000	-1.783273000
O	3.605637000	-1.456848000	0.436509000
F	5.689956000	-1.485878000	-1.396166000
F	4.305423000	-0.898563000	-2.946024000
F	4.101751000	-2.827772000	-1.993277000
H	2.011767000	-0.525217000	1.806492000

G2c

Coordinates (Angstroms)			
	X	Y	Z
C	-2.800428000	-3.355343000	0.748159000
C	-3.183374000	-3.950369000	-0.486523000
H	-2.724621000	-4.814178000	-0.945367000
C	-4.240587000	-3.175213000	-1.040329000

H	-4.721831000	-3.348590000	-1.991959000
C	-3.625957000	-2.218647000	0.955298000
H	-3.585374000	-1.560069000	1.805591000
C	-4.512373000	-2.099518000	-0.148812000
H	-5.247397000	-1.320920000	-0.293427000
H	-2.007956000	-3.691547000	1.401429000
C	-0.544604000	-1.604711000	-1.001638000
C	-1.052257000	-2.275658000	-2.152778000
C	-2.091867000	-1.497764000	-2.723097000
H	-2.689537000	-1.767709000	-3.581483000
C	-1.287687000	-0.380925000	-0.866087000
C	-2.253773000	-0.342070000	-1.925146000
H	-2.977311000	0.440695000	-2.094294000
Fe	-2.559877000	-2.029903000	-0.803312000
P	-0.762174000	1.072415000	0.086303000
C	-1.578391000	2.471564000	-0.815144000
C	-1.534587000	3.801720000	-0.024499000
C	-1.015198000	2.682187000	-2.225779000
C	-1.618131000	5.021183000	-0.958510000
H	-2.370877000	3.831005000	0.678193000
C	-1.937900000	3.611966000	-3.028271000
H	-0.019612000	3.124484000	-2.137576000
C	-2.531125000	4.731195000	-2.148387000
H	-1.977202000	5.886159000	-0.393749000
H	-2.747879000	3.028699000	-3.478614000
H	-3.513574000	4.427444000	-1.767919000
C	-1.583283000	1.106252000	1.737253000
C	-1.150555000	-0.042784000	2.649739000
C	-3.120008000	1.210918000	1.690776000
C	-1.545796000	0.256361000	4.109786000
H	-1.620811000	-0.966922000	2.304344000
C	-3.751871000	0.889003000	3.062496000

H	-3.404855000	2.222910000	1.397003000
C	-2.778650000	1.172111000	4.204974000
H	-1.746410000	-0.688278000	4.625444000
H	-4.045577000	-0.164856000	3.113894000
H	-3.271785000	1.037538000	5.171775000
H	-0.618806000	3.868909000	0.568695000
H	-0.618784000	5.280864000	-1.325818000
H	-2.693855000	5.635431000	-2.741353000
H	-1.366571000	4.046954000	-3.854465000
H	-0.884916000	1.735785000	-2.755398000
H	-2.626367000	2.168093000	-0.909019000
H	-1.179235000	2.033585000	2.162650000
H	-0.076111000	-0.202325000	2.583317000
H	-0.703479000	0.725790000	4.628140000
H	-2.469077000	2.222631000	4.157842000
H	-4.672067000	1.466653000	3.185007000
H	-3.520390000	0.537806000	0.927148000
H	-0.735691000	-3.239793000	-2.517787000
C	0.538509000	-2.153339000	-0.091632000
H	0.177209000	-2.038675000	0.935468000
C	0.710344000	-3.651544000	-0.369198000
H	-0.253854000	-4.148376000	-0.236001000
H	1.036568000	-3.843232000	-1.391419000
H	1.418418000	-4.125268000	0.299436000
P	2.104790000	-1.087967000	-0.024915000
C	3.108575000	-1.785763000	1.455091000
C	3.059232000	-1.412876000	-1.646632000
C	3.304076000	-3.310352000	1.539887000
H	4.093400000	-3.498887000	2.276249000
H	2.407046000	-3.809588000	1.909568000
H	3.609866000	-3.778400000	0.607512000
C	2.411090000	-1.386742000	2.764446000

H	2.438292000	-0.312479000	2.947165000
H	1.374443000	-1.729616000	2.806109000
H	2.943916000	-1.865278000	3.593291000
C	4.494382000	-1.123438000	1.433009000
H	4.984099000	-1.311534000	2.395203000
H	5.135283000	-1.542525000	0.654523000
H	4.431274000	-0.043575000	1.287839000
C	4.107008000	-0.314519000	-1.875764000
H	4.842041000	-0.254277000	-1.074111000
H	4.639867000	-0.544790000	-2.805704000
H	3.647297000	0.667714000	-1.979061000
C	3.778896000	-2.766723000	-1.714060000
H	4.183789000	-2.886864000	-2.725452000
H	4.620928000	-2.816379000	-1.021753000
H	3.119947000	-3.613036000	-1.522162000
C	2.059755000	-1.339244000	-2.811656000
H	1.421923000	-2.220904000	-2.862526000
H	1.422797000	-0.452492000	-2.761162000
H	2.626562000	-1.288101000	-3.747740000
Ir	1.490836000	1.302961000	0.211951000
Cl	3.853190000	2.264992000	0.340500000
H	1.489706000	1.303707000	-1.377858000
H	1.126764000	2.857747000	0.071327000
H	1.369733000	1.853781000	1.895236000
H	1.648841000	1.061466000	1.978523000

G3c

Coordinates (Angstroms)			
	X	Y	Z
C	2.717868000	3.522923000	-1.734392000
C	3.566743000	4.179011000	-0.799741000
H	4.632079000	4.032212000	-0.695538000

C	2.757168000	5.017766000	0.016408000
H	3.103176000	5.622375000	0.842387000
C	1.388719000	3.961621000	-1.497568000
H	0.518237000	3.646781000	-2.047841000
C	1.407040000	4.881036000	-0.412962000
H	0.547459000	5.372279000	0.019837000
H	3.023315000	2.796951000	-2.474206000
C	2.378535000	1.026649000	0.464126000
C	3.309852000	1.757701000	1.260465000
C	2.598269000	2.608701000	2.143651000
H	3.033595000	3.309093000	2.841393000
C	1.062202000	1.435255000	0.875003000
C	1.218295000	2.427168000	1.898092000
H	0.418517000	2.944485000	2.405568000
Fe	2.167351000	3.065487000	0.194944000
P	-0.490154000	0.544733000	0.555250000
C	-1.553361000	1.040486000	1.988754000
C	-3.037021000	0.652219000	1.777733000
C	-1.046822000	0.498788000	3.329810000
C	-3.764121000	0.430906000	3.113093000
H	-3.540794000	1.449340000	1.227031000
C	-1.783577000	1.188896000	4.487339000
H	-1.226085000	-0.578549000	3.359249000
C	-3.273447000	1.426140000	4.163073000
H	-4.841996000	0.529136000	2.957123000
H	-1.298847000	2.144485000	4.713883000
H	-3.413818000	2.440289000	3.770118000
C	-1.352616000	1.308347000	-0.890138000
C	-0.564049000	1.076334000	-2.186294000
C	-1.741134000	2.778839000	-0.658202000
C	-1.198833000	1.765495000	-3.418598000
H	0.461617000	1.428965000	-2.053468000

C	-2.299815000	3.460379000	-1.932912000
H	-2.497326000	2.824620000	0.126182000
C	-2.506406000	2.481510000	-3.087426000
H	-0.495771000	2.501501000	-3.825914000
H	-1.608905000	4.242811000	-2.267035000
H	-2.869349000	3.018629000	-3.969328000
H	-3.120894000	-0.251561000	1.169395000
H	-3.591281000	-0.590775000	3.469919000
H	-3.874698000	1.360155000	5.074213000
H	-1.688786000	0.568242000	5.384101000
H	0.031794000	0.636630000	3.439003000
H	-1.490203000	2.132721000	2.022670000
H	-2.272649000	0.720157000	-0.955838000
H	-0.502864000	0.003514000	-2.361203000
H	-1.368193000	1.027402000	-4.207519000
H	-3.273522000	1.746669000	-2.827295000
H	-3.241845000	3.963102000	-1.696913000
H	-0.878877000	3.333393000	-0.283361000
H	4.384491000	1.709305000	1.183524000
C	2.767956000	0.055713000	-0.634177000
H	2.195853000	0.333750000	-1.524159000
C	4.254172000	0.240727000	-0.962724000
H	4.428519000	1.284854000	-1.235598000
H	4.895775000	0.014587000	-0.111363000
H	4.578026000	-0.374785000	-1.792853000
P	2.140531000	-1.710226000	-0.364896000
C	2.382597000	-2.565098000	-2.063837000
C	3.307933000	-2.499322000	0.925104000
C	3.746167000	-2.412058000	-2.761276000
H	3.785196000	-3.147329000	-3.572910000
H	3.854449000	-1.429546000	-3.223575000
H	4.602449000	-2.594579000	-2.116272000

C	1.345505000	-2.006878000	-3.050737000
H	0.323307000	-2.274476000	-2.785325000
H	1.408836000	-0.920910000	-3.155289000
H	1.544678000	-2.442031000	-4.036079000
C	2.104974000	-4.063996000	-1.875203000
H	2.003575000	-4.526247000	-2.863716000
H	2.926538000	-4.568782000	-1.362065000
H	1.183385000	-4.245350000	-1.318965000
C	2.671345000	-3.762540000	1.521167000
H	2.447515000	-4.519757000	0.770678000
H	3.381888000	-4.193464000	2.236194000
H	1.745532000	-3.540001000	2.050637000
C	4.696305000	-2.888528000	0.398703000
H	5.303629000	-3.211845000	1.252156000
H	4.648408000	-3.727272000	-0.298399000
H	5.222562000	-2.065384000	-0.083085000
C	3.485568000	-1.495439000	2.075904000
H	4.145461000	-0.670692000	1.808520000
H	2.533434000	-1.081785000	2.417679000
H	3.942275000	-2.019963000	2.922380000
Ir	-0.218951000	-1.701177000	0.418183000
Cl	-0.555087000	-4.231131000	0.582994000
H	0.422107000	-1.611914000	1.868838000
H	-1.620486000	-1.717219000	1.191626000
H	-1.448099000	-1.807671000	-0.872638000
H	-0.737177000	-1.934358000	-1.294584000
C	-4.157742000	-1.239053000	-1.419241000
O	-4.044477000	-2.238823000	-0.697136000
O	-3.535579000	-0.914479000	-2.444582000
C	-5.281773000	-0.234584000	-1.014268000
F	-5.807926000	-0.481822000	0.193391000
F	-6.295296000	-0.282685000	-1.902370000

F	-4.850648000	1.042634000	-0.996067000
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G4c

Coordinates (Angstroms)			
	X	Y	Z
C	2.796813000	3.007285000	-2.290377000
C	3.901441000	3.561095000	-1.584421000
H	4.930820000	3.242189000	-1.663405000
C	3.405326000	4.569396000	-0.711826000
H	3.994275000	5.151967000	-0.018161000
C	1.623998000	3.681286000	-1.859732000
H	0.626582000	3.492801000	-2.219105000
C	1.993489000	4.641519000	-0.878768000
H	1.321681000	5.297679000	-0.344330000
H	2.836147000	2.200784000	-3.008579000
C	2.523532000	0.731427000	0.142594000
C	3.675325000	1.352829000	0.711853000
C	3.257417000	2.355926000	1.623388000
H	3.904108000	3.017754000	2.181045000
C	1.370492000	1.360400000	0.729999000
C	1.843341000	2.374250000	1.625301000
H	1.226932000	3.034268000	2.216442000
Fe	2.560580000	2.759965000	-0.259802000
P	-0.321005000	0.675366000	0.752841000
C	-1.045187000	1.442594000	2.283477000
C	-2.584029000	1.288000000	2.350490000
C	-0.413953000	0.938267000	3.584105000
C	-3.101147000	1.357899000	3.797282000
H	-3.054601000	2.082888000	1.765405000
C	-0.818698000	1.850840000	4.752932000
H	-0.757212000	-0.082818000	3.766189000
C	-2.274455000	2.343582000	4.620880000

H	-4.157580000	1.641816000	3.792402000
H	-0.141468000	2.710492000	4.800550000
H	-2.296143000	3.319564000	4.121289000
C	-1.302398000	1.517440000	-0.577433000
C	-0.801588000	1.110918000	-1.968086000
C	-1.427177000	3.039808000	-0.400762000
C	-1.555686000	1.819420000	-3.119307000
H	0.268267000	1.321261000	-2.040482000
C	-2.133977000	3.723241000	-1.599331000
H	-1.994596000	3.250816000	0.505740000
C	-2.680599000	2.720700000	-2.614601000
H	-0.855433000	2.437902000	-3.692779000
H	-1.429722000	4.382828000	-2.119069000
H	-3.139937000	3.251396000	-3.454376000
H	-2.896218000	0.341606000	1.902924000
H	-3.046759000	0.367098000	4.262556000
H	-2.717432000	2.491598000	5.609898000
H	-0.693430000	1.300781000	5.691222000
H	0.675062000	0.885635000	3.508785000
H	-0.817660000	2.509691000	2.196108000
H	-2.298307000	1.084273000	-0.439294000
H	-0.912980000	0.032866000	-2.061069000
H	-1.953842000	1.076593000	-3.815804000
H	-3.471666000	2.114447000	-2.159953000
H	-2.940999000	4.364752000	-1.234253000
H	-0.438790000	3.476629000	-0.248207000
H	4.703143000	1.139591000	0.464041000
C	2.568170000	-0.343006000	-0.928477000
H	1.893127000	-0.021350000	-1.726939000
C	3.982225000	-0.406795000	-1.518643000
H	4.246271000	0.576015000	-1.918600000
H	4.729796000	-0.665490000	-0.769154000

H	4.066909000	-1.124376000	-2.325778000
P	1.741316000	-1.975362000	-0.429993000
C	1.525476000	-2.900812000	-2.103016000
C	3.039028000	-2.904246000	0.629928000
C	2.726588000	-2.977490000	-3.061791000
H	2.481095000	-3.708767000	-3.840778000
H	2.898056000	-2.026273000	-3.568592000
H	3.654375000	-3.301092000	-2.595617000
C	0.403766000	-2.218841000	-2.901776000
H	-0.555491000	-2.260934000	-2.387916000
H	0.632435000	-1.172926000	-3.122648000
H	0.301160000	-2.738944000	-3.861064000
C	1.078734000	-4.334866000	-1.780745000
H	0.707608000	-4.802283000	-2.700329000
H	1.908317000	-4.945735000	-1.417188000
H	0.279244000	-4.359594000	-1.037485000
C	2.361339000	-4.043930000	1.403795000
H	1.914379000	-4.790983000	0.748146000
H	3.123119000	-4.543473000	2.014549000
H	1.576513000	-3.675347000	2.062668000
C	4.221502000	-3.513829000	-0.135875000
H	4.936264000	-3.905465000	0.597888000
H	3.912094000	-4.353405000	-0.761370000
H	4.754874000	-2.795644000	-0.757488000
C	3.590732000	-1.914284000	1.669822000
H	4.285525000	-1.195521000	1.235283000
H	2.794479000	-1.363525000	2.176664000
H	4.139595000	-2.481140000	2.430353000
Ir	-0.362095000	-1.569188000	0.770492000
Cl	-1.032255000	-4.053144000	1.161385000
H	0.519946000	-1.549599000	2.175482000
H	-1.675421000	-1.328136000	1.669475000

H	-2.604069000	-1.391990000	-0.307717000
H	-1.289992000	-1.662608000	-0.623676000
C	-4.017026000	-0.765466000	-1.483285000
O	-3.602449000	-1.131049000	-0.309950000
O	-3.460883000	-0.871154000	-2.546334000
C	-5.417740000	-0.121124000	-1.377761000
F	-6.323289000	-1.016300000	-0.966179000
F	-5.812761000	0.359186000	-2.553142000
F	-5.412437000	0.888031000	-0.496449000

G5c

Coordinates (Angstroms)			
	X	Y	Z
C	-2.644809000	-3.476133000	0.736263000
C	-3.028278000	-4.063050000	-0.502374000
H	-2.551565000	-4.906238000	-0.981021000
C	-4.116474000	-3.310975000	-1.028165000
H	-4.607012000	-3.484259000	-1.975116000
C	-3.500180000	-2.368529000	0.973749000
H	-3.464797000	-1.722213000	1.833450000
C	-4.406520000	-2.258125000	-0.115396000
H	-5.165810000	-1.498962000	-0.236599000
H	-1.833433000	-3.798302000	1.373239000
C	-0.468562000	-1.609563000	-0.996362000
C	-0.951577000	-2.298200000	-2.148450000
C	-2.024773000	-1.561357000	-2.712045000
H	-2.614316000	-1.851496000	-3.569679000
C	-1.256837000	-0.416282000	-0.853520000
C	-2.228265000	-0.415277000	-1.907814000
H	-2.982847000	0.338441000	-2.073226000
Fe	-2.465834000	-2.119647000	-0.797705000
P	-0.759097000	1.061337000	0.096787000

C	-1.695335000	2.410336000	-0.778760000
C	-1.707127000	3.742641000	0.007124000
C	-1.219967000	2.665534000	-2.213921000
C	-1.969726000	4.946151000	-0.915718000
H	-2.484259000	3.705461000	0.774598000
C	-2.263949000	3.505936000	-2.966633000
H	-0.265415000	3.196297000	-2.175315000
C	-2.915728000	4.563984000	-2.052595000
H	-2.380627000	5.772524000	-0.328552000
H	-3.037214000	2.848747000	-3.379146000
H	-3.840356000	4.164879000	-1.618543000
C	-1.609741000	1.043903000	1.741367000
C	-1.129850000	-0.077998000	2.662081000
C	-3.149671000	1.068776000	1.687419000
C	-1.548826000	0.204048000	4.119082000
H	-1.549924000	-1.026388000	2.316604000
C	-3.774444000	0.726823000	3.058340000
H	-3.488739000	2.061094000	1.383874000
C	-2.822491000	1.062850000	4.204495000
H	-1.710803000	-0.747589000	4.636313000
H	-4.017640000	-0.339545000	3.117512000
H	-3.314209000	0.912181000	5.169988000
H	-0.755780000	3.887736000	0.524808000
H	-1.025963000	5.305768000	-1.341267000
H	-3.200892000	5.445458000	-2.634097000
H	-1.778802000	3.993677000	-3.818482000
H	-1.028608000	1.734367000	-2.751296000
H	-2.725706000	2.041707000	-0.828534000
H	-1.257063000	1.989693000	2.171700000
H	-0.048377000	-0.175498000	2.601084000
H	-0.731885000	0.711861000	4.642398000
H	-2.561662000	2.126278000	4.151654000

H	-4.722161000	1.260637000	3.172561000
H	-3.510815000	0.369947000	0.927342000
H	-0.596851000	-3.247756000	-2.517157000
C	0.637755000	-2.112567000	-0.089093000
H	0.272216000	-2.006587000	0.937627000
C	0.865561000	-3.604716000	-0.357754000
H	-0.077915000	-4.139562000	-0.220622000
H	1.198436000	-3.791564000	-1.378685000
H	1.593865000	-4.045409000	0.312263000
P	2.158405000	-0.975848000	-0.021484000
C	3.154634000	-1.638567000	1.488570000
C	3.163407000	-1.345203000	-1.612103000
C	3.420163000	-3.151027000	1.601277000
H	4.188398000	-3.293936000	2.370493000
H	2.535448000	-3.691069000	1.942728000
H	3.785942000	-3.615890000	0.689274000
C	2.407495000	-1.260028000	2.776238000
H	2.286730000	-0.183434000	2.887615000
H	1.421306000	-1.729525000	2.827574000
H	2.986504000	-1.630653000	3.630049000
C	4.510543000	-0.916154000	1.493194000
H	4.988392000	-1.072020000	2.467598000
H	5.186667000	-1.315534000	0.733525000
H	4.403480000	0.158310000	1.331816000
C	4.189262000	-0.227554000	-1.851741000
H	4.918943000	-0.144010000	-1.046776000
H	4.732552000	-0.454782000	-2.777013000
H	3.710052000	0.744058000	-1.963374000
C	3.925947000	-2.676921000	-1.633649000
H	4.353605000	-2.809901000	-2.634637000
H	4.757164000	-2.681411000	-0.926502000
H	3.293025000	-3.540629000	-1.431857000

C	2.187667000	-1.330401000	-2.800162000
H	1.580973000	-2.234660000	-2.846701000
H	1.521012000	-0.464583000	-2.775401000
H	2.768658000	-1.277956000	-3.727985000
Ir	1.459838000	1.373770000	0.158342000
Cl	3.846962000	2.436385000	0.344216000
H	1.517677000	1.499867000	-1.513195000
H	1.434419000	1.421633000	1.824711000
H	1.036382000	2.926281000	0.207503000

TS_{G3c-G4c}

Coordinates (Angstroms)			
	X	Y	Z
C	-2.932067000	-2.800545000	-2.340757000
C	-4.092546000	-3.271543000	-1.664471000
H	-5.089368000	-2.864785000	-1.755495000
C	-3.698687000	-4.333240000	-0.802852000
H	-4.346237000	-4.876668000	-0.129962000
C	-1.827809000	-3.577106000	-1.901075000
H	-0.810902000	-3.468165000	-2.238384000
C	-2.295330000	-4.520465000	-0.946568000
H	-1.689949000	-5.238900000	-0.412683000
H	-2.891404000	-1.981986000	-3.045071000
C	-2.554295000	-0.591209000	0.137969000
C	-3.747238000	-1.148716000	0.688108000
C	-3.402437000	-2.192057000	1.584487000
H	-4.094745000	-2.821238000	2.124844000
C	-1.449292000	-1.302178000	0.723779000
C	-1.992675000	-2.301440000	1.595778000
H	-1.424091000	-3.010229000	2.178311000
Fe	-2.717439000	-2.605928000	-0.301631000
P	0.280399000	-0.731135000	0.768270000

C	0.937188000	-1.534114000	2.308807000
C	2.481913000	-1.468603000	2.392470000
C	0.317005000	-0.980660000	3.595889000
C	2.976566000	-1.535410000	3.846685000
H	2.910349000	-2.304176000	1.832306000
C	0.660072000	-1.894104000	4.783303000
H	0.711823000	0.023579000	3.767659000
C	2.090676000	-2.461421000	4.678074000
H	4.016415000	-1.874752000	3.861079000
H	-0.060492000	-2.717360000	4.835320000
H	2.067958000	-3.446421000	4.196580000
C	1.225107000	-1.614173000	-0.558534000
C	0.752864000	-1.178028000	-1.951213000
C	1.259500000	-3.141937000	-0.386488000
C	1.476362000	-1.923254000	-3.098893000
H	-0.325770000	-1.332864000	-2.029846000
C	1.942774000	-3.858754000	-1.579303000
H	1.799732000	-3.389189000	0.527529000
C	2.547881000	-2.883046000	-2.587279000
H	0.748230000	-2.502870000	-3.678113000
H	1.210120000	-4.481049000	-2.105926000
H	2.986968000	-3.434493000	-3.424437000
H	2.856300000	-0.553792000	1.926789000
H	2.969313000	-0.534113000	4.292189000
H	2.514324000	-2.612807000	5.674980000
H	0.550749000	-1.323134000	5.711015000
H	-0.766938000	-0.873446000	3.504679000
H	0.649034000	-2.586557000	2.224916000
H	2.242136000	-1.234641000	-0.413141000
H	0.921050000	-0.107477000	-2.044506000
H	1.918875000	-1.201428000	-3.790230000
H	3.364891000	-2.319920000	-2.123365000

H	2.713313000	-4.540294000	-1.208091000
H	0.244354000	-3.520629000	-0.251525000
H	-4.756800000	-0.865582000	0.435318000
C	-2.527539000	0.495553000	-0.922735000
H	-1.873634000	0.139542000	-1.724228000
C	-3.934580000	0.653477000	-1.512785000
H	-4.260620000	-0.307865000	-1.918760000
H	-4.664463000	0.954227000	-0.761332000
H	-3.973200000	1.379385000	-2.315811000
P	-1.599083000	2.066847000	-0.412387000
C	-1.321656000	2.994623000	-2.073660000
C	-2.825561000	3.063920000	0.663909000
C	-2.512419000	3.141993000	-3.036542000
H	-2.221533000	3.860143000	-3.811826000
H	-2.735820000	2.203277000	-3.546501000
H	-3.421883000	3.517325000	-2.572508000
C	-0.233488000	2.259056000	-2.871670000
H	0.729825000	2.262657000	-2.364104000
H	-0.507915000	1.223164000	-3.087528000
H	-0.110321000	2.769828000	-3.833341000
C	-0.797494000	4.400074000	-1.741738000
H	-0.402805000	4.851405000	-2.659551000
H	-1.590567000	5.054624000	-1.372969000
H	0.005018000	4.376108000	-1.001765000
C	-2.078482000	4.152738000	1.447182000
H	-1.570071000	4.864995000	0.797950000
H	-2.811251000	4.705755000	2.046950000
H	-1.332447000	3.731121000	2.119852000
C	-3.969249000	3.751304000	-0.095285000
H	-4.658721000	4.178993000	0.642286000
H	-3.610257000	4.575671000	-0.714086000
H	-4.544943000	3.071824000	-0.722202000

C	-3.436266000	2.098888000	1.693835000
H	-4.166518000	1.422992000	1.249017000
H	-2.675666000	1.500826000	2.201743000
H	-3.957431000	2.690164000	2.455168000
Ir	0.479871000	1.510756000	0.783950000
Cl	1.322135000	3.925148000	1.154905000
H	-0.405764000	1.544798000	2.153189000
H	1.756634000	1.194598000	1.706555000
H	2.371690000	1.311575000	-0.369336000
H	1.370349000	1.545718000	-0.667941000
C	3.957881000	0.630076000	-1.526239000
O	3.536816000	1.023350000	-0.386854000
O	3.445097000	0.753198000	-2.621347000
C	5.324137000	-0.089909000	-1.404076000
F	6.279222000	0.767837000	-1.014735000
F	5.707511000	-0.628174000	-2.562079000
F	5.274401000	-1.074757000	-0.492976000

II

Coordinates (Angstroms)			
	X	Y	Z
C	-3.531676000	3.183761000	-0.551757000
C	-2.576279000	2.342761000	0.003326000
C	-2.696800000	0.958001000	-0.039172000
C	-3.796790000	0.378101000	-0.676606000
C	-4.766885000	1.202342000	-1.247859000
C	-4.620567000	2.586751000	-1.170520000
H	-3.414276000	4.259006000	-0.503025000
H	-5.630010000	0.784439000	-1.748107000
H	-5.382424000	3.215481000	-1.618367000
O	-3.833611000	-0.969491000	-0.683340000
C	-4.926962000	-1.620139000	-1.320243000

H	-5.873514000	-1.358859000	-0.838534000
H	-4.966558000	-1.371961000	-2.384810000
H	-4.741582000	-2.686343000	-1.202214000
O	-1.481164000	2.851747000	0.633250000
P	-1.307696000	0.178002000	0.812749000
C	-0.466773000	1.854920000	0.832247000
C	-1.861441000	-0.081504000	2.581218000
C	-2.464909000	1.180167000	3.202210000
H	-3.335472000	1.529099000	2.639715000
H	-2.798918000	0.947762000	4.219160000
H	-1.743076000	1.997560000	3.271989000
C	-2.908032000	-1.202088000	2.577087000
H	-2.527701000	-2.109066000	2.101053000
H	-3.175435000	-1.440999000	3.612167000
H	-3.819564000	-0.893797000	2.057504000
C	-0.614808000	-0.519282000	3.359473000
H	-0.191686000	-1.442846000	2.952749000
H	0.164818000	0.249529000	3.344696000
H	-0.882979000	-0.702418000	4.405068000
C	3.711709000	2.563314000	1.578008000
C	4.740022000	1.713656000	1.960100000
C	4.810102000	0.387564000	1.534090000
C	3.821977000	-0.111956000	0.686302000
C	2.782310000	0.730197000	0.281492000
C	2.736224000	2.042526000	0.738691000
H	3.653956000	3.588353000	1.921829000
O	3.782641000	-1.374190000	0.212512000
C	4.825354000	-2.272042000	0.578447000
H	4.591270000	-3.211564000	0.081091000
H	5.795577000	-1.906076000	0.230706000
H	4.848223000	-2.427049000	1.660870000
C	2.904790000	-0.418962000	-2.956296000

H	2.427048000	-1.398188000	-2.882403000
H	3.209393000	-0.264945000	-3.996544000
H	3.806943000	-0.424540000	-2.338358000
C	0.716179000	0.715470000	-3.459755000
H	-0.022688000	1.458701000	-3.143501000
H	1.026164000	0.964573000	-4.479611000
H	0.231926000	-0.263229000	-3.482405000
C	2.683840000	2.054632000	-2.652585000
H	2.032649000	2.903028000	-2.428167000
H	3.552762000	2.094770000	-1.990077000
H	3.043663000	2.178375000	-3.678810000
C	1.951532000	0.711052000	-2.552107000
P	1.377550000	0.402064000	-0.801991000
O	1.696318000	2.813166000	0.312897000
C	0.625335000	2.023054000	-0.228226000
H	5.513166000	2.086702000	2.622872000
H	5.626150000	-0.237902000	1.869539000
Ir	0.112909000	-1.374805000	-0.316910000
H	-0.698476000	-1.091943000	-1.591167000
H	1.085794000	-2.306375000	-1.217061000
Cl	-1.124514000	-3.479279000	0.228783000
H	0.213438000	2.570327000	-1.076231000
H	-0.021803000	2.033500000	1.811855000

I2

Coordinates (Angstroms)			
	X	Y	Z
C	-4.424771000	2.639551000	1.796986000
C	-3.348284000	1.763897000	1.779754000
C	-3.232185000	0.763039000	0.823839000
C	-4.192456000	0.648873000	-0.188821000
C	-5.276403000	1.523630000	-0.195830000

C	-5.376758000	2.495596000	0.799195000
H	-4.496740000	3.408017000	2.555877000
H	-6.038801000	1.459937000	-0.960135000
H	-6.226217000	3.169466000	0.782130000
O	-3.975964000	-0.314264000	-1.098894000
C	-4.909075000	-0.479455000	-2.161925000
H	-5.898917000	-0.737499000	-1.775563000
H	-4.967232000	0.424515000	-2.774492000
H	-4.524605000	-1.302562000	-2.761615000
O	-2.357260000	1.871337000	2.704919000
P	-1.722823000	-0.164691000	1.079837000
C	-1.222669000	1.044140000	2.440095000
C	-2.116335000	-1.774721000	1.943104000
C	-2.833788000	-1.487615000	3.269292000
H	-3.727443000	-0.873369000	3.127246000
H	-3.156831000	-2.446055000	3.686675000
H	-2.189536000	-1.013182000	4.011469000
C	-3.045446000	-2.620064000	1.065460000
H	-2.621632000	-2.813612000	0.080774000
H	-3.205322000	-3.580371000	1.565880000
H	-4.018331000	-2.137497000	0.942157000
C	-0.783036000	-2.487474000	2.194744000
H	-0.297505000	-2.772307000	1.257850000
H	-0.093442000	-1.862011000	2.771464000
H	-0.970587000	-3.399649000	2.769223000
C	3.469421000	1.337125000	2.961831000
C	4.642813000	1.323319000	2.222479000
C	4.654281000	1.453915000	0.833639000
C	3.447978000	1.600302000	0.153185000
C	2.255566000	1.639487000	0.881691000
C	2.279752000	1.494682000	2.264612000
H	3.466182000	1.232023000	4.039297000

O	3.322066000	1.712526000	-1.182941000
C	4.505201000	1.769338000	-1.976138000
H	4.164909000	1.896236000	-3.002125000
H	5.124845000	2.622672000	-1.687090000
H	5.077139000	0.841567000	-1.890972000
C	0.470978000	3.182966000	-2.040646000
H	-0.135131000	2.389876000	-2.486088000
H	0.223507000	4.122009000	-2.545341000
H	1.524641000	2.963879000	-2.221752000
C	-1.320451000	3.622433000	-0.339734000
H	-1.566949000	3.794707000	0.710970000
H	-1.581861000	4.529079000	-0.893584000
H	-1.943352000	2.806441000	-0.715986000
C	1.025415000	4.466416000	0.052363000
H	0.863375000	4.582199000	1.127483000
H	2.091076000	4.298338000	-0.121920000
H	0.746782000	5.408825000	-0.429265000
C	0.174986000	3.343276000	-0.545532000
P	0.558722000	1.741448000	0.316847000
O	1.087348000	1.489726000	2.915682000
C	-0.012423000	1.902218000	2.095579000
H	5.588956000	1.207183000	2.739241000
H	5.596307000	1.437924000	0.302891000
Ir	-0.245507000	-0.191207000	-0.585878000
H	-1.290162000	0.651580000	-1.320521000
Cl	-0.985920000	-2.293499000	-1.761646000
H	-0.239922000	2.944310000	2.329500000
H	-0.986650000	0.498787000	3.352542000

I3

Coordinates (Angstroms)

X	Y	Z
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C	-4.391522000	2.621669000	1.762515000
C	-3.330372000	1.727536000	1.773969000
C	-3.205743000	0.721269000	0.825302000
C	-4.144729000	0.617796000	-0.207699000
C	-5.212502000	1.512119000	-0.245593000
C	-5.320584000	2.491101000	0.741531000
H	-4.466475000	3.396674000	2.514467000
H	-5.956966000	1.458027000	-1.028131000
H	-6.155768000	3.181481000	0.698883000
O	-3.926151000	-0.356043000	-1.107018000
C	-4.831082000	-0.502309000	-2.196631000
H	-5.838313000	-0.734628000	-1.839897000
H	-4.849130000	0.400487000	-2.813604000
H	-4.449367000	-1.336961000	-2.781942000
O	-2.356713000	1.822089000	2.719385000
P	-1.698805000	-0.213110000	1.101812000
C	-1.210755000	1.011114000	2.450833000
C	-2.112027000	-1.803701000	1.985157000
C	-2.869812000	-1.502020000	3.284189000
H	-3.773868000	-0.914387000	3.100884000
H	-3.179972000	-2.455686000	3.722096000
H	-2.257739000	-0.988097000	4.027862000
C	-3.006039000	-2.665406000	1.086374000
H	-2.541345000	-2.875849000	0.123327000
H	-3.188720000	-3.616421000	1.596857000
H	-3.972134000	-2.184244000	0.913474000
C	-0.780999000	-2.503287000	2.280805000
H	-0.259866000	-2.777117000	1.359323000
H	-0.118700000	-1.872474000	2.883220000
H	-0.977239000	-3.419928000	2.845301000
C	3.471093000	1.287660000	2.925341000
C	4.634673000	1.246170000	2.172111000

C	4.633717000	1.389933000	0.784496000
C	3.425676000	1.586804000	0.120074000
C	2.242910000	1.658436000	0.863917000
C	2.278932000	1.488431000	2.243516000
H	3.476306000	1.165623000	4.000989000
O	3.289446000	1.716708000	-1.212343000
C	4.458417000	1.658255000	-2.025909000
H	4.109726000	1.783494000	-3.049235000
H	5.149630000	2.466108000	-1.771586000
H	4.956042000	0.690278000	-1.922370000
C	0.457433000	3.271123000	-2.015083000
H	-0.156784000	2.507175000	-2.497713000
H	0.233523000	4.232066000	-2.488052000
H	1.509911000	3.040930000	-2.190910000
C	-1.360906000	3.631228000	-0.326910000
H	-1.621928000	3.786323000	0.722831000
H	-1.634989000	4.538127000	-0.874122000
H	-1.960704000	2.805566000	-0.719843000
C	0.969008000	4.506920000	0.113645000
H	0.789302000	4.602432000	1.187765000
H	2.039069000	4.352761000	-0.047272000
H	0.687443000	5.454293000	-0.356016000
C	0.141934000	3.385257000	-0.519814000
P	0.542863000	1.774444000	0.315056000
O	1.094487000	1.492198000	2.907436000
C	-0.018074000	1.893492000	2.100728000
H	5.582461000	1.093841000	2.676370000
H	5.568415000	1.346143000	0.242463000
Ir	-0.187465000	-0.164382000	-0.635887000
H	-1.322797000	0.614044000	-1.321672000
H	0.903075000	0.424200000	-2.022492000
Cl	-0.891272000	-2.300219000	-1.745357000

H	-0.262832000	2.928088000	2.349694000
H	-0.960458000	0.474842000	3.365334000
H	0.921295000	-0.377379000	-2.099781000

TS11-12

Coordinates (Angstroms)			
	X	Y	Z
C	-4.225148000	2.766916000	1.663497000
C	-3.202368000	1.828647000	1.634062000
C	-3.192803000	0.777089000	0.727875000
C	-4.212369000	0.674245000	-0.223473000
C	-5.255808000	1.597809000	-0.207609000
C	-5.244982000	2.625165000	0.734318000
H	-4.209210000	3.576179000	2.382536000
H	-6.062780000	1.535964000	-0.924537000
H	-6.058064000	3.342781000	0.730776000
O	-4.094945000	-0.330350000	-1.112075000
C	-5.195013000	-0.617074000	-1.968258000
H	-6.075557000	-0.895021000	-1.380922000
H	-5.431992000	0.232186000	-2.611903000
H	-4.881289000	-1.462060000	-2.578717000
O	-2.153081000	1.928836000	2.493966000
P	-1.752869000	-0.271657000	0.991022000
C	-1.140631000	0.940865000	2.286805000
C	-2.337267000	-1.749360000	1.990933000
C	-3.041931000	-1.289797000	3.274390000
H	-3.867459000	-0.604536000	3.062338000
H	-3.464410000	-2.173454000	3.763133000
H	-2.367376000	-0.817909000	3.991051000
C	-3.337289000	-2.575639000	1.173517000
H	-2.923134000	-2.898378000	0.219494000
H	-3.602235000	-3.465413000	1.754712000

H	-4.256710000	-2.014039000	0.987368000
C	-1.086537000	-2.567234000	2.328527000
H	-0.614877000	-2.963619000	1.425536000
H	-0.348670000	-1.968155000	2.873177000
H	-1.367978000	-3.411346000	2.966120000
C	3.584943000	0.713411000	2.661654000
C	4.777796000	0.931474000	1.988664000
C	4.810385000	1.431492000	0.689251000
C	3.615413000	1.690897000	0.018527000
C	2.397043000	1.432900000	0.658126000
C	2.410919000	0.991490000	1.978224000
H	3.555348000	0.365227000	3.686374000
O	3.543276000	2.203986000	-1.221760000
C	4.732022000	2.669516000	-1.847568000
H	4.421782000	3.056266000	-2.817114000
H	5.187650000	3.472538000	-1.260998000
H	5.454448000	1.862434000	-1.993058000
C	0.768951000	3.229018000	-2.086812000
H	0.510665000	2.299839000	-2.588606000
H	0.269820000	4.051132000	-2.608674000
H	1.845408000	3.368259000	-2.164252000
C	-1.211088000	3.409261000	-0.561266000
H	-1.562698000	3.462929000	0.470883000
H	-1.458382000	4.357835000	-1.047213000
H	-1.753570000	2.611957000	-1.076176000
C	1.018819000	4.314717000	0.158672000
H	0.662531000	4.393451000	1.188467000
H	2.101955000	4.171548000	0.172153000
H	0.813338000	5.270293000	-0.334887000
C	0.307863000	3.208800000	-0.626058000
P	0.671640000	1.524542000	0.097880000
O	1.202919000	0.846011000	2.590543000

C	0.177273000	1.589374000	1.914653000
H	5.716204000	0.732467000	2.494197000
H	5.763181000	1.623129000	0.214911000
Ir	-0.228849000	-0.402995000	-0.778719000
H	-1.244497000	0.454158000	-1.531366000
H	0.744500000	-0.467407000	-2.231635000
Cl	-1.140572000	-2.566882000	-1.519909000
H	0.193768000	2.619708000	2.279381000
H	-0.980330000	0.429673000	3.235456000
C	-1.264457000	1.674659000	-4.386584000
C	0.032696000	1.079472000	-4.920002000
C	-0.969671000	-1.097637000	-4.920704000
C	-2.273327000	-0.498998000	-4.414427000
C	-3.667079000	1.461577000	-4.573845000
C	-3.877064000	2.489580000	-3.650506000
C	-5.144141000	3.028047000	-3.444091000
C	-6.239282000	2.539757000	-4.141299000
C	-6.060378000	1.511412000	-5.063390000
C	-4.795098000	1.004666000	-5.265101000
H	-1.349216000	2.700910000	-4.750889000
H	0.876686000	1.682233000	-4.600973000
H	-0.977796000	-1.108239000	-6.016213000
H	-2.305843000	-0.562100000	-3.318432000
H	-3.041233000	2.878638000	-3.082593000
H	-5.269173000	3.824339000	-2.719114000
H	-7.227879000	2.953120000	-3.979759000
H	-6.887207000	1.108779000	-5.636934000
N	-2.404943000	0.897209000	-4.852500000
N	0.188195000	-0.308460000	-4.496537000
H	-3.096396000	-1.089635000	-4.815424000
H	-0.896604000	-2.122077000	-4.575161000
H	0.010550000	1.094562000	-6.014964000

H	-1.229186000	1.703720000	-3.289838000
C	1.146321000	-0.748474000	-3.652765000
C	1.353242000	-2.254100000	-3.619640000
C	2.447235000	0.043195000	-3.581948000
C	2.372745000	-2.747090000	-2.602660000
H	0.414881000	-2.770942000	-3.449746000
C	3.450664000	-0.515396000	-2.574278000
H	2.874192000	-0.006716000	-4.592258000
C	3.694716000	-2.008069000	-2.737065000
H	1.970552000	-2.605538000	-1.592786000
H	3.078539000	-0.331353000	-1.562183000
H	4.408941000	-2.353773000	-1.983971000
H	2.263856000	1.092009000	-3.356986000
H	1.695306000	-2.506270000	-4.632160000
H	2.503951000	-3.823482000	-2.744472000
H	4.136439000	-2.212104000	-3.720488000
H	4.384470000	0.039777000	-2.679199000
F	-4.636078000	0.023474000	-6.182633000

TS_{13-II}

Coordinates (Angstroms)			
	X	Y	Z
C	-4.294354000	2.838214000	1.684784000
C	-3.296413000	1.872027000	1.680284000
C	-3.355065000	0.757470000	0.854423000
C	-4.423814000	0.611224000	-0.037110000
C	-5.433476000	1.571319000	-0.056023000
C	-5.353533000	2.663263000	0.807780000
H	-4.226209000	3.696329000	2.341337000
H	-6.273685000	1.483749000	-0.731381000
H	-6.144664000	3.404534000	0.782932000
O	-4.383935000	-0.475133000	-0.828817000

C	-5.427401000	-0.676476000	-1.774984000
H	-6.393634000	-0.786755000	-1.274821000
H	-5.467501000	0.145571000	-2.495053000
H	-5.178192000	-1.601482000	-2.292107000
O	-2.205628000	2.011588000	2.477463000
P	-1.880287000	-0.252056000	1.045259000
C	-1.206866000	1.007149000	2.281999000
C	-2.278507000	-1.756083000	2.075833000
C	-3.038976000	-1.370860000	3.347979000
H	-3.971354000	-0.847649000	3.117239000
H	-3.296040000	-2.288042000	3.887620000
H	-2.449091000	-0.749491000	4.025493000
C	-3.138067000	-2.714949000	1.245856000
H	-2.661831000	-2.974111000	0.298669000
H	-3.287271000	-3.635066000	1.820531000
H	-4.119802000	-2.284559000	1.035044000
C	-0.929669000	-2.403611000	2.415646000
H	-0.394492000	-2.710677000	1.511802000
H	-0.282675000	-1.729580000	2.986486000
H	-1.103906000	-3.296214000	3.024483000
C	3.524467000	0.665570000	2.536587000
C	4.673797000	0.639487000	1.759771000
C	4.655712000	0.918281000	0.394279000
C	3.446646000	1.223669000	-0.226665000
C	2.274331000	1.248789000	0.535652000
C	2.332645000	0.976356000	1.898146000
H	3.543409000	0.463227000	3.599961000
O	3.312429000	1.511701000	-1.534720000
C	4.488475000	1.709309000	-2.316174000
H	4.139055000	2.008678000	-3.302269000
H	5.106227000	2.503892000	-1.888794000
H	5.066991000	0.786303000	-2.398688000

C	0.439337000	2.925561000	-2.299055000
H	-0.290603000	2.229577000	-2.717590000
H	0.292546000	3.899504000	-2.776614000
H	1.440883000	2.569960000	-2.544949000
C	-1.200028000	3.500334000	-0.492540000
H	-1.366254000	3.692807000	0.570280000
H	-1.421974000	4.423014000	-1.037362000
H	-1.909349000	2.736435000	-0.823817000
C	1.224102000	4.149330000	-0.247676000
H	1.147886000	4.270911000	0.836170000
H	2.259663000	3.906239000	-0.497670000
H	0.983970000	5.113122000	-0.707604000
C	0.251485000	3.096737000	-0.786572000
P	0.553521000	1.463132000	0.055626000
O	1.160919000	1.008745000	2.591908000
C	0.105364000	1.654552000	1.867111000
H	5.622282000	0.404528000	2.229825000
H	5.578581000	0.896528000	-0.168944000
Ir	-0.438379000	-0.387128000	-0.806078000
H	-1.410231000	0.547639000	-1.535796000
H	0.478878000	-0.208325000	-2.218777000
Cl	-1.410903000	-2.370031000	-1.929520000
H	0.087638000	2.711188000	2.147101000
H	-1.033605000	0.522090000	3.242697000
H	1.179641000	-0.770301000	-1.853333000
C	3.265464000	-1.504974000	-2.368095000
O	2.284567000	-1.482601000	-1.561223000
O	4.426419000	-1.777263000	-2.115996000
C	2.898612000	-1.189244000	-3.847295000
F	2.290050000	0.003360000	-3.975531000
F	2.049003000	-2.114483000	-4.324017000
F	3.971252000	-1.174954000	-4.636794000

J1

Coordinates (Angstroms)			
	X	Y	Z
C	-4.274887000	1.679284000	2.226688000
C	-3.191317000	0.868716000	1.915637000
C	-3.106870000	0.172174000	0.716762000
C	-4.116965000	0.315941000	-0.236842000
C	-5.209909000	1.137155000	0.044180000
C	-5.274848000	1.795613000	1.271202000
H	-4.317309000	2.206986000	3.171231000
H	-6.005543000	1.270906000	-0.676177000
H	-6.131468000	2.427983000	1.477703000
O	-3.948100000	-0.365769000	-1.388322000
C	-4.951131000	-0.269271000	-2.391886000
H	-5.910168000	-0.646544000	-2.024671000
H	-5.062018000	0.761323000	-2.741091000
H	-4.604654000	-0.895127000	-3.212538000
O	-2.150689000	0.722687000	2.784842000
P	-1.571444000	-0.785827000	0.644462000
C	-0.976223000	0.231425000	2.113331000
C	-2.049947000	-2.472413000	1.313010000
C	-2.678904000	-2.398181000	2.706090000
H	-3.580123000	-1.778860000	2.714290000
H	-2.969094000	-3.408577000	3.015082000
H	-1.980380000	-2.011860000	3.452783000
C	-3.059453000	-3.067794000	0.321575000
H	-2.661170000	-3.083429000	-0.696303000
H	-3.277703000	-4.099456000	0.618699000
H	-4.002101000	-2.514062000	0.321704000
C	-0.789163000	-3.341140000	1.348919000
H	-0.318414000	-3.402260000	0.364021000

H	-0.052911000	-2.956413000	2.057762000
H	-1.062688000	-4.355228000	1.660158000
C	3.443274000	1.582953000	2.523615000
C	4.601778000	1.584735000	1.763874000
C	4.577175000	1.576718000	0.369386000
C	3.349831000	1.574989000	-0.289943000
C	2.167561000	1.592453000	0.456916000
C	2.231154000	1.571011000	1.843334000
H	3.465654000	1.562896000	3.605931000
O	3.203431000	1.552306000	-1.629553000
C	4.368964000	1.514220000	-2.444116000
H	4.007128000	1.485728000	-3.470510000
H	4.979679000	2.409543000	-2.295769000
H	4.959959000	0.617277000	-2.241588000
C	0.335431000	3.247102000	-2.208776000
H	-0.130424000	2.485850000	-2.837904000
H	0.027865000	4.231118000	-2.578143000
H	1.419270000	3.164842000	-2.316700000
C	-1.634081000	3.171470000	-0.664268000
H	-2.002966000	3.117153000	0.363908000
H	-1.969994000	4.123920000	-1.086630000
H	-2.099720000	2.365985000	-1.237074000
C	0.520725000	4.239542000	0.083296000
H	0.278636000	4.165287000	1.147354000
H	1.608769000	4.258131000	-0.019647000
H	0.131354000	5.197452000	-0.276399000
C	-0.102554000	3.111547000	-0.745778000
P	0.462870000	1.448666000	-0.098632000
O	1.065166000	1.502073000	2.533187000
C	-0.104364000	1.429270000	1.704661000
H	5.562702000	1.579899000	2.266507000
H	5.507209000	1.563502000	-0.182202000

Ir	-0.124130000	-0.395218000	-1.204228000
H	-1.271607000	0.422026000	-1.864430000
H	0.788217000	0.076980000	-2.460054000
Cl	-0.803860000	-2.374488000	-2.623225000
H	-0.686278000	2.329691000	1.905775000
H	-0.427498000	-0.387802000	2.820467000
O	1.751208000	-1.655019000	-0.561671000
C	2.281894000	-1.686753000	0.573489000
C	3.728889000	-2.249106000	0.535733000
O	1.836592000	-1.376103000	1.675733000
F	3.709544000	-3.589986000	0.400211000
F	4.417819000	-1.974742000	1.649932000
F	4.435175000	-1.762017000	-0.497573000

J2

Coordinates (Angstroms)			
	X	Y	Z
C	-4.314957000	1.604185000	2.173395000
C	-3.198158000	0.840839000	1.871395000
C	-3.071736000	0.156624000	0.666813000
C	-4.085213000	0.247503000	-0.292404000
C	-5.209262000	1.026387000	-0.017663000
C	-5.308540000	1.682267000	1.207639000
H	-4.388436000	2.123593000	3.120283000
H	-6.005629000	1.126072000	-0.742426000
H	-6.191699000	2.279141000	1.406958000
O	-3.888011000	-0.432970000	-1.435363000
C	-4.889684000	-0.378810000	-2.445982000
H	-5.836727000	-0.783593000	-2.078386000
H	-5.030172000	0.644760000	-2.804133000
H	-4.517890000	-1.001249000	-3.257753000
O	-2.168942000	0.726537000	2.761683000

P	-1.510970000	-0.741151000	0.645933000
C	-0.963399000	0.301990000	2.118808000
C	-1.896459000	-2.465661000	1.266353000
C	-2.497127000	-2.382552000	2.676555000
H	-3.416117000	-1.791762000	2.702215000
H	-2.752533000	-3.400385000	2.987670000
H	-1.792929000	-1.981463000	3.408584000
C	-2.931156000	-3.089805000	0.320863000
H	-2.582700000	-3.110079000	-0.712672000
H	-3.105508000	-4.121748000	0.642096000
H	-3.886822000	-2.561761000	0.366204000
C	-0.615774000	-3.303344000	1.299855000
H	-0.172224000	-3.406562000	0.307898000
H	0.129141000	-2.874467000	1.972464000
H	-0.869750000	-4.303271000	1.665967000
C	3.405411000	1.817630000	2.409692000
C	4.538156000	1.791472000	1.611048000
C	4.474094000	1.685695000	0.220819000
C	3.228402000	1.620655000	-0.396617000
C	2.074535000	1.688450000	0.388612000
C	2.173991000	1.744216000	1.771770000
H	3.465466000	1.864611000	3.489463000
O	3.026085000	1.471996000	-1.720946000
C	4.159201000	1.370260000	-2.577883000
H	3.755776000	1.240869000	-3.580600000
H	4.760407000	2.282867000	-2.539636000
H	4.770944000	0.503756000	-2.315197000
C	0.203146000	3.062490000	-2.354797000
H	-0.144896000	2.178114000	-2.896681000
H	-0.212448000	3.946374000	-2.848873000
H	1.291420000	3.109547000	-2.428683000
C	-1.803154000	3.036942000	-0.853253000

H	-2.196066000	3.004780000	0.166735000
H	-2.167145000	3.956836000	-1.321143000
H	-2.215200000	2.191518000	-1.408381000
C	0.280343000	4.268396000	-0.149139000
H	-0.024516000	4.286450000	0.901143000
H	1.371649000	4.309682000	-0.193151000
H	-0.111741000	5.174423000	-0.621610000
C	-0.269384000	3.049651000	-0.895516000
P	0.366154000	1.490629000	-0.099624000
O	1.023360000	1.684619000	2.491950000
C	-0.156397000	1.535767000	1.695654000
H	5.513789000	1.835002000	2.082110000
H	5.387915000	1.641470000	-0.355596000
Ir	-0.135609000	-0.485704000	-1.079933000
H	-1.370410000	0.182979000	-1.740057000
Cl	-0.599015000	-2.557492000	-2.353624000
H	-0.778285000	2.414309000	1.873585000
H	-0.388382000	-0.289547000	2.828642000
O	1.864737000	-1.438608000	-0.560928000
C	2.391477000	-1.510561000	0.579157000
C	3.838097000	-2.067527000	0.537023000
O	1.927800000	-1.254588000	1.684775000
F	3.809711000	-3.414131000	0.503721000
F	4.549827000	-1.712023000	1.611994000
F	4.517142000	-1.661817000	-0.545471000

J3

Coordinates (Angstroms)			
	X	Y	Z
C	-4.333770000	1.335523000	2.324305000
C	-3.217546000	0.604332000	1.947394000
C	-3.094012000	0.048595000	0.679697000

C	-4.097701000	0.247997000	-0.271240000
C	-5.222984000	0.992757000	0.080306000
C	-5.324064000	1.515074000	1.368651000
H	-4.408488000	1.758862000	3.317764000
H	-6.016797000	1.171924000	-0.631901000
H	-6.206295000	2.090489000	1.626848000
O	-3.884280000	-0.300527000	-1.480997000
C	-4.871092000	-0.128488000	-2.493239000
H	-5.820171000	-0.581317000	-2.193306000
H	-5.015374000	0.930877000	-2.722803000
H	-4.481772000	-0.641989000	-3.370293000
O	-2.185947000	0.398980000	2.815322000
P	-1.541092000	-0.844643000	0.553454000
C	-0.988001000	0.000952000	2.139546000
C	-1.931944000	-2.624831000	0.980830000
C	-2.602457000	-2.700929000	2.358171000
H	-3.530468000	-2.124996000	2.399132000
H	-2.855556000	-3.748492000	2.549791000
H	-1.941101000	-2.369886000	3.162157000
C	-2.901100000	-3.159241000	-0.082541000
H	-2.493519000	-3.060647000	-1.090075000
H	-3.073855000	-4.222156000	0.114978000
H	-3.867362000	-2.650725000	-0.037520000
C	-0.638760000	-3.444500000	0.990687000
H	-0.154724000	-3.447845000	0.013228000
H	0.074131000	-3.069757000	1.729225000
H	-0.889331000	-4.476896000	1.255304000
C	3.491018000	1.207936000	2.527664000
C	4.600196000	1.373381000	1.712936000
C	4.492114000	1.654244000	0.351202000
C	3.228785000	1.787615000	-0.217788000
C	2.095983000	1.650912000	0.592042000

C	2.240984000	1.332822000	1.935834000
H	3.581133000	0.960693000	3.577549000
O	2.992992000	2.026518000	-1.521126000
C	4.086353000	1.985712000	-2.432318000
H	3.647562000	2.115744000	-3.420116000
H	4.791816000	2.797683000	-2.235672000
H	4.597387000	1.021009000	-2.380225000
C	0.061168000	3.478325000	-1.829395000
H	-0.352514000	2.717594000	-2.496117000
H	-0.359383000	4.446525000	-2.118409000
H	1.142307000	3.516986000	-1.972346000
C	-1.838509000	3.160702000	-0.230987000
H	-2.161524000	3.005394000	0.801592000
H	-2.244021000	4.120565000	-0.565125000
H	-2.271293000	2.376358000	-0.856066000
C	0.282521000	4.291402000	0.538640000
H	0.067747000	4.116362000	1.596545000
H	1.365526000	4.369171000	0.413874000
H	-0.160071000	5.254632000	0.266784000
C	-0.311488000	3.208493000	-0.366717000
P	0.370933000	1.548417000	0.121236000
O	1.114200000	1.093516000	2.655267000
C	-0.100890000	1.232691000	1.911520000
H	5.589338000	1.264714000	2.143594000
H	5.387175000	1.751909000	-0.247614000
Ir	-0.080763000	-0.272782000	-1.156711000
H	-1.257955000	0.453650000	-1.872841000
H	0.642340000	0.454798000	-2.587579000
Cl	-0.467219000	-2.248599000	-2.608610000
H	-0.631410000	2.101925000	2.304400000
H	-0.455264000	-0.697351000	2.783736000
O	1.468519000	-1.379484000	0.107070000

C	2.644965000	-1.540079000	-0.307940000
C	3.540067000	-2.302913000	0.700198000
O	3.153644000	-1.229358000	-1.380394000
F	3.183893000	-2.100906000	1.975393000
F	4.829060000	-1.964583000	0.584562000
F	3.449572000	-3.627085000	0.469637000
H	1.300855000	0.073060000	-2.237888000

TS_{J1-J2}

Coordinates (Angstroms)			
	X	Y	Z
C	-4.161443000	2.574163000	1.983410000
C	-3.145320000	1.633935000	1.886670000
C	-3.071245000	0.724751000	0.838682000
C	-4.043477000	0.753760000	-0.164420000
C	-5.073878000	1.690933000	-0.092106000
C	-5.115962000	2.583718000	0.976773000
H	-4.189739000	3.272142000	2.810699000
H	-5.836097000	1.735444000	-0.858173000
H	-5.919132000	3.311385000	1.016601000
O	-3.910370000	-0.148088000	-1.158005000
C	-5.045192000	-0.430294000	-1.969503000
H	-5.883347000	-0.763154000	-1.349536000
H	-5.344726000	0.437151000	-2.560477000
H	-4.739460000	-1.234760000	-2.636063000
O	-2.178603000	1.558166000	2.843033000
P	-1.645590000	-0.369791000	1.064430000
C	-1.049284000	0.788020000	2.410916000
C	-2.376837000	-1.871197000	1.942783000
C	-2.988338000	-1.461746000	3.289429000
H	-3.771717000	-0.707948000	3.175782000
H	-3.451178000	-2.349796000	3.732463000

H	-2.242507000	-1.095416000	3.998318000
C	-3.494549000	-2.454297000	1.066662000
H	-3.140808000	-2.716059000	0.069603000
H	-3.868122000	-3.363073000	1.550506000
H	-4.332819000	-1.758971000	0.975494000
C	-1.275676000	-2.909038000	2.173373000
H	-0.814952000	-3.222479000	1.234586000
H	-0.494697000	-2.524940000	2.831537000
H	-1.720271000	-3.789807000	2.648970000
C	3.549988000	1.589643000	2.912940000
C	4.742295000	1.660996000	2.214618000
C	4.775772000	1.772706000	0.825632000
C	3.582086000	1.768970000	0.107667000
C	2.362776000	1.641125000	0.785381000
C	2.372024000	1.603909000	2.175223000
H	3.514817000	1.530053000	3.993273000
O	3.509180000	1.916101000	-1.227430000
C	4.672865000	2.327099000	-1.931077000
H	4.364744000	2.452943000	-2.968063000
H	5.042356000	3.279922000	-1.539986000
H	5.463811000	1.574742000	-1.877582000
C	0.813458000	3.147259000	-2.068742000
H	0.674248000	2.179096000	-2.545207000
H	0.305664000	3.905606000	-2.672555000
H	1.880538000	3.365817000	-2.059022000
C	-1.297083000	3.262987000	-0.710405000
H	-1.744804000	3.317447000	0.285356000
H	-1.559088000	4.183331000	-1.241770000
H	-1.747331000	2.422297000	-1.241175000
C	0.812874000	4.335942000	0.128335000
H	0.373684000	4.445256000	1.122942000
H	1.897798000	4.258024000	0.234743000

H	0.594514000	5.254427000	-0.426459000
C	0.231815000	3.152714000	-0.651071000
P	0.664069000	1.521664000	0.167694000
O	1.182044000	1.584898000	2.817071000
C	0.056116000	1.732825000	1.947624000
H	5.679208000	1.649168000	2.760448000
H	5.726742000	1.863155000	0.319280000
Ir	-0.116238000	-0.464623000	-0.692106000
H	-1.206994000	0.301603000	-1.485282000
H	0.758300000	-0.530703000	-2.225295000
Cl	-1.042408000	-2.637931000	-1.444774000
H	-0.318262000	2.750965000	2.067803000
H	-0.684412000	0.224860000	3.267606000
O	1.716602000	-1.589478000	0.188180000
C	2.105398000	-1.629276000	1.379083000
C	3.537338000	-2.215473000	1.504721000
O	1.536863000	-1.309347000	2.418891000
F	3.524344000	-3.542086000	1.268497000
F	4.064916000	-2.032434000	2.719486000
F	4.385815000	-1.669611000	0.617035000
C	-1.212011000	1.673505000	-4.377562000
C	0.065699000	1.039612000	-4.910557000
C	-1.002395000	-1.108992000	-4.895611000
C	-2.283078000	-0.466480000	-4.388176000
C	-3.620058000	1.534176000	-4.581860000
C	-3.798899000	2.599400000	-3.694470000
C	-5.051464000	3.172093000	-3.493170000
C	-6.164548000	2.685601000	-4.163117000
C	-6.015845000	1.626816000	-5.055491000
C	-4.764096000	1.085829000	-5.252457000
H	-1.265957000	2.700977000	-4.743876000
H	0.926283000	1.617169000	-4.589074000

H	-1.017618000	-1.135554000	-5.991202000
H	-2.305174000	-0.514194000	-3.291110000
H	-2.948910000	2.989516000	-3.150361000
H	-5.150693000	3.994990000	-2.794222000
H	-7.142589000	3.124565000	-4.005067000
H	-6.856118000	1.225352000	-5.610005000
N	-2.374969000	0.928152000	-4.843250000
N	0.179784000	-0.350751000	-4.485537000
H	-3.126212000	-1.037980000	-4.774152000
H	-0.959936000	-2.129242000	-4.533257000
H	0.045842000	1.055299000	-6.006028000
H	-1.174404000	1.697702000	-3.281744000
C	1.149231000	-0.829183000	-3.676453000
C	1.307049000	-2.342288000	-3.691821000
C	2.472786000	-0.075724000	-3.643109000
C	2.393549000	-2.912797000	-2.791741000
H	0.368824000	-2.829363000	-3.447604000
C	3.520975000	-0.704172000	-2.726288000
H	2.838753000	-0.086006000	-4.678806000
C	3.718731000	-2.191642000	-2.979659000
H	2.080691000	-2.829314000	-1.749266000
H	3.223413000	-0.555291000	-1.686091000
H	4.470445000	-2.589154000	-2.291302000
H	2.328634000	0.965040000	-3.359661000
H	1.540769000	-2.573966000	-4.740068000
H	2.490923000	-3.979502000	-3.015922000
H	4.094322000	-2.352792000	-3.998656000
H	4.460951000	-0.168698000	-2.871980000
F	-4.637302000	0.075054000	-6.143198000

TSJ3-11

Coordinates (Angstroms)

	X	Y	Z
C	4.942392000	-1.922931000	-0.361307000
C	3.714010000	-1.499942000	0.125974000
C	3.416441000	-0.155709000	0.320368000
C	4.385171000	0.812414000	0.040262000
C	5.628192000	0.410697000	-0.449426000
C	5.883300000	-0.944732000	-0.647620000
H	5.144537000	-2.977064000	-0.502908000
H	6.398578000	1.137153000	-0.669451000
H	6.854470000	-1.241181000	-1.028341000
O	4.040874000	2.087422000	0.292893000
C	4.944438000	3.126297000	-0.063904000
H	5.875616000	3.051602000	0.504958000
H	5.156815000	3.107279000	-1.136647000
H	4.437928000	4.056128000	0.189323000
O	2.734681000	-2.403428000	0.407169000
P	1.680254000	0.001716000	0.784637000
C	1.674768000	-1.835845000	1.187030000
C	1.468771000	0.904174000	2.405411000
C	2.672222000	0.658530000	3.318034000
H	3.585030000	1.091074000	2.901049000
H	2.482736000	1.137232000	4.284429000
H	2.845763000	-0.404991000	3.502550000
C	1.310499000	2.404579000	2.129613000
H	0.433538000	2.610127000	1.513590000
H	1.179533000	2.915876000	3.089190000
H	2.189955000	2.821905000	1.637459000
C	0.181806000	0.366152000	3.047414000
H	-0.673238000	0.444680000	2.370927000
H	0.286995000	-0.674816000	3.361207000
H	-0.040839000	0.962065000	3.938090000
C	-2.537184000	-2.377159000	2.984886000

C	-3.810103000	-1.854437000	2.815731000
C	-4.223107000	-1.264053000	1.620896000
C	-3.331828000	-1.194083000	0.553307000
C	-2.049045000	-1.732791000	0.696350000
C	-1.667128000	-2.298561000	1.904687000
H	-2.217927000	-2.825319000	3.917208000
O	-3.603150000	-0.634979000	-0.640628000
C	-4.917407000	-0.147181000	-0.887858000
H	-4.891804000	0.269655000	-1.892721000
H	-5.646547000	-0.961253000	-0.843795000
H	-5.190854000	0.634029000	-0.175418000
C	-1.900974000	-2.383993000	-2.851273000
H	-1.509182000	-1.475192000	-3.312804000
H	-2.035939000	-3.131203000	-3.639969000
H	-2.878806000	-2.162275000	-2.419321000
C	0.425490000	-3.233487000	-2.461548000
H	1.162482000	-3.614844000	-1.749268000
H	0.290069000	-3.992403000	-3.238408000
H	0.835555000	-2.337263000	-2.932771000
C	-1.522361000	-4.236917000	-1.210413000
H	-0.866648000	-4.697030000	-0.466491000
H	-2.495723000	-4.055587000	-0.747152000
H	-1.662599000	-4.963687000	-2.016545000
C	-0.933590000	-2.953386000	-1.807597000
P	-0.665693000	-1.702211000	-0.447298000
O	-0.395000000	-2.761752000	2.012907000
C	0.398002000	-2.581006000	0.835850000
H	-4.512451000	-1.899418000	3.640812000
H	-5.224464000	-0.863973000	1.538051000
Ir	0.153308000	0.349648000	-0.955251000
H	1.174366000	-0.377492000	-1.866269000
H	-0.803304000	0.389531000	-2.366718000

Cl	1.117703000	2.514676000	-1.713010000
H	0.683937000	-3.570422000	0.477145000
H	1.897639000	-1.995962000	2.245631000
O	-1.461000000	1.693989000	0.289665000
C	-2.306548000	2.142434000	-0.492074000
C	-3.357593000	3.082873000	0.130575000
O	-2.394983000	1.939225000	-1.728148000
F	-4.354449000	3.365990000	-0.705807000
F	-2.778230000	4.236696000	0.489316000
F	-3.885803000	2.535383000	1.232513000
H	-1.426118000	1.069986000	-2.006452000

I2c

Coordinates (Angstroms)			
	X	Y	Z
C	-3.353506000	3.227336000	-0.447320000
C	-2.516617000	2.312154000	0.176333000
C	-2.619957000	0.944490000	-0.047343000
C	-3.575640000	0.458778000	-0.943252000
C	-4.422406000	1.359519000	-1.590050000
C	-4.300608000	2.723286000	-1.327737000
H	-3.251261000	4.288198000	-0.256583000
H	-5.169717000	1.015673000	-2.292164000
H	-4.965025000	3.411513000	-1.838638000
O	-3.604269000	-0.877798000	-1.111867000
C	-4.546955000	-1.431383000	-2.022727000
H	-5.571583000	-1.216039000	-1.706112000
H	-4.380912000	-1.055000000	-3.036028000
H	-4.377211000	-2.506407000	-2.001159000
O	-1.556684000	2.723928000	1.052323000
P	-1.386811000	0.054309000	0.923859000
C	-0.566649000	1.707903000	1.278197000

C	-2.232489000	-0.417998000	2.524249000
C	-2.919954000	0.778960000	3.187931000
H	-3.664774000	1.235589000	2.530603000
H	-3.441182000	0.426872000	4.084318000
H	-2.208726000	1.547073000	3.500963000
C	-3.277831000	-1.489872000	2.191794000
H	-2.833660000	-2.337069000	1.663759000
H	-3.716871000	-1.857102000	3.125702000
H	-4.086364000	-1.082245000	1.578975000
C	-1.159868000	-0.992480000	3.455237000
H	-0.721289000	-1.906842000	3.047346000
H	-0.354416000	-0.274415000	3.641591000
H	-1.617765000	-1.237849000	4.418792000
C	3.941523000	2.092119000	1.992338000
C	5.062997000	1.281904000	1.910030000
C	5.126621000	0.181215000	1.055110000
C	4.033659000	-0.117508000	0.244331000
C	2.897806000	0.698317000	0.298433000
C	2.861335000	1.772318000	1.178014000
H	3.891398000	2.938081000	2.666195000
O	3.976379000	-1.154824000	-0.613378000
C	5.095565000	-2.030020000	-0.704316000
H	4.819230000	-2.780954000	-1.442165000
H	5.986481000	-1.493881000	-1.043127000
H	5.291124000	-2.515383000	0.255950000
C	2.172536000	0.115049000	-3.182895000
H	1.538532000	-0.771939000	-3.242214000
H	2.302614000	0.511797000	-4.194894000
H	3.152754000	-0.185514000	-2.805427000
C	0.148184000	1.558729000	-2.856249000
H	-0.346842000	2.339134000	-2.270764000
H	0.263004000	1.936053000	-3.877213000

H	-0.508694000	0.686677000	-2.890435000
C	2.440073000	2.441848000	-2.292143000
H	2.045704000	3.243962000	-1.662021000
H	3.448860000	2.199234000	-1.948310000
H	2.517712000	2.833897000	-3.310954000
C	1.537528000	1.202748000	-2.309669000
P	1.333347000	0.545203000	-0.572506000
O	1.724991000	2.513666000	1.225539000
C	0.659639000	2.006433000	0.409221000
H	5.921549000	1.505240000	2.533868000
H	6.021496000	-0.425526000	1.030404000
Ir	0.162780000	-1.340993000	-0.238982000
H	-0.661278000	-1.029109000	-1.550233000
H	1.140059000	-2.109122000	-1.265297000
Cl	-1.049026000	-3.523035000	-0.008032000
H	0.381025000	2.804476000	-0.279208000
H	-0.272104000	1.761956000	2.326410000
H	1.412712000	-2.024000000	0.878065000
H	0.883510000	-1.664494000	1.411830000

I3c

Coordinates (Angstroms)			
	X	Y	Z
C	-4.765766000	1.580464000	1.928526000
C	-3.608099000	0.833378000	1.750660000
C	-3.459719000	-0.058446000	0.697773000
C	-4.482769000	-0.189765000	-0.246070000
C	-5.652065000	0.555036000	-0.095067000
C	-5.775032000	1.421316000	0.990675000
H	-4.855095000	2.269634000	2.758883000
H	-6.460693000	0.473631000	-0.808790000
H	-6.689524000	1.994621000	1.096666000

O	-4.248070000	-1.048661000	-1.257144000
C	-5.241658000	-1.209559000	-2.262305000
H	-6.168244000	-1.605995000	-1.837174000
H	-5.437653000	-0.263271000	-2.774522000
H	-4.829943000	-1.927357000	-2.969700000
O	-2.563777000	0.958962000	2.613397000
P	-1.825450000	-0.819900000	0.730614000
C	-1.355198000	0.351863000	2.132025000
C	-2.015943000	-2.486533000	1.557962000
C	-2.778999000	-2.376128000	2.881157000
H	-3.772940000	-1.942621000	2.738732000
H	-2.910860000	-3.380623000	3.296744000
H	-2.243112000	-1.782069000	3.625576000
C	-2.787237000	-3.401292000	0.599193000
H	-2.303068000	-3.463573000	-0.378238000
H	-2.829136000	-4.407648000	1.029582000
H	-3.814099000	-3.054438000	0.456763000
C	-0.604302000	-3.035575000	1.794932000
H	-0.075370000	-3.203399000	0.853240000
H	0.001382000	-2.363257000	2.411185000
H	-0.677183000	-3.995108000	2.316958000
C	3.215527000	1.458397000	2.468451000
C	4.346596000	1.614064000	1.683071000
C	4.276537000	1.758105000	0.298106000
C	3.031645000	1.750130000	-0.327122000
C	1.876037000	1.629334000	0.449219000
C	1.985651000	1.460677000	1.823305000
H	3.274489000	1.321940000	3.540695000
O	2.841827000	1.850574000	-1.656947000
C	3.983576000	1.821633000	-2.507828000
H	3.591303000	1.835890000	-3.523189000
H	4.615451000	2.699710000	-2.347032000

H	4.557860000	0.905770000	-2.348306000
C	-0.172750000	3.233174000	-2.199527000
H	-0.699409000	2.461931000	-2.764470000
H	-0.514653000	4.210720000	-2.554965000
H	0.895636000	3.145649000	-2.407950000
C	-1.982882000	3.173544000	-0.464984000
H	-2.238873000	3.168700000	0.598111000
H	-2.377156000	4.099346000	-0.895427000
H	-2.491094000	2.334536000	-0.947585000
C	0.226466000	4.276382000	0.043737000
H	0.079683000	4.227633000	1.126153000
H	1.300872000	4.293829000	-0.156267000
H	-0.197500000	5.223804000	-0.303966000
C	-0.466059000	3.128923000	-0.698928000
P	0.159203000	1.487600000	-0.061825000
O	0.841599000	1.260478000	2.526891000
C	-0.352762000	1.441456000	1.754751000
H	5.321682000	1.615405000	2.156642000
H	5.187519000	1.858480000	-0.274822000
Ir	-0.401306000	-0.401174000	-1.139213000
H	-1.621422000	0.359681000	-1.818065000
H	0.406792000	0.112780000	-2.437932000
Cl	-0.928583000	-2.443391000	-2.503529000
H	-0.783665000	2.403850000	2.037164000
H	-0.922653000	-0.215333000	2.956265000
H	1.228657000	-1.097199000	-0.888416000
H	0.790761000	-1.384992000	-0.228523000
C	3.820780000	-1.564836000	0.121954000
O	3.560159000	-1.422037000	-1.083931000
O	3.072694000	-1.693206000	1.101917000
C	5.345379000	-1.671826000	0.436389000
F	5.768059000	-2.937068000	0.219847000

F	6.101598000	-0.877985000	-0.340959000
F	5.648595000	-1.377221000	1.709972000

I4c

Coordinates (Angstroms)			
	X	Y	Z
C	-4.787683000	1.852950000	1.637020000
C	-3.656845000	1.050181000	1.556472000
C	-3.492024000	0.100282000	0.558214000
C	-4.474039000	-0.040903000	-0.425217000
C	-5.616000000	0.759579000	-0.374315000
C	-5.755643000	1.687114000	0.657168000
H	-4.888523000	2.587053000	2.426739000
H	-6.392410000	0.673398000	-1.122422000
H	-6.647478000	2.303843000	0.685028000
O	-4.232894000	-0.967956000	-1.375793000
C	-5.180143000	-1.131551000	-2.423539000
H	-6.145003000	-1.466451000	-2.031209000
H	-5.306914000	-0.202689000	-2.987001000
H	-4.767306000	-1.898638000	-3.076418000
O	-2.651695000	1.174023000	2.467662000
P	-1.893869000	-0.733626000	0.719324000
C	-1.438508000	0.530518000	2.043943000
C	-2.273814000	-2.297178000	1.683644000
C	-3.069525000	-2.013411000	2.961452000
H	-4.016860000	-1.509959000	2.749078000
H	-3.304174000	-2.966831000	3.447235000
H	-2.507169000	-1.411452000	3.679548000
C	-3.096363000	-3.211960000	0.767215000
H	-2.592119000	-3.381610000	-0.187407000
H	-3.235252000	-4.179776000	1.261814000
H	-4.086016000	-2.791428000	0.569809000

C	-0.938011000	-2.962150000	2.031236000
H	-0.392422000	-3.252049000	1.130438000
H	-0.296137000	-2.301517000	2.623201000
H	-1.129838000	-3.863558000	2.623310000
C	3.083285000	1.805893000	2.517481000
C	4.260879000	1.889382000	1.793501000
C	4.277713000	1.862439000	0.398366000
C	3.073696000	1.755365000	-0.296052000
C	1.871807000	1.683930000	0.413103000
C	1.896682000	1.691938000	1.800479000
H	3.071669000	1.811071000	3.600245000
O	2.967634000	1.701629000	-1.638275000
C	4.156433000	1.709848000	-2.419260000
H	3.828390000	1.622529000	-3.453656000
H	4.705166000	2.646830000	-2.286859000
H	4.794721000	0.860366000	-2.166256000
C	0.012338000	2.899559000	-2.524753000
H	-0.435734000	2.042591000	-3.030699000
H	-0.340213000	3.810886000	-3.019348000
H	1.096063000	2.842136000	-2.643473000
C	-1.927236000	3.001678000	-0.948622000
H	-2.274371000	3.115627000	0.082013000
H	-2.289501000	3.865701000	-1.515002000
H	-2.385941000	2.104050000	-1.370985000
C	0.220170000	4.194431000	-0.392218000
H	0.002092000	4.259638000	0.677447000
H	1.305347000	4.217541000	-0.521338000
H	-0.195136000	5.089199000	-0.867470000
C	-0.396263000	2.954794000	-1.048362000
P	0.191300000	1.400664000	-0.182657000
O	0.715582000	1.548393000	2.454070000
C	-0.432381000	1.589683000	1.590759000

H	5.203717000	1.971608000	2.322613000
H	5.220809000	1.926236000	-0.126784000
Ir	-0.284765000	-0.611536000	-0.995392000
H	-1.373794000	-0.035714000	-2.107754000
H	0.860622000	-0.385356000	-2.133281000
Cl	-0.627137000	-2.942973000	-1.988086000
H	-0.899071000	2.568166000	1.718407000
H	-1.016894000	0.020770000	2.910488000
H	2.146091000	-1.245850000	-0.559801000
H	0.814915000	-1.282514000	0.082203000
C	3.735284000	-1.424086000	0.486132000
O	3.147211000	-1.363449000	-0.672246000
O	3.237194000	-1.387818000	1.581318000
C	5.258828000	-1.637307000	0.340098000
F	5.514676000	-2.949289000	0.234346000
F	5.767655000	-1.037808000	-0.738528000
F	5.901600000	-1.179047000	1.412256000

I5c

Coordinates (Angstroms)			
	X	Y	Z
C	-3.227128000	3.298160000	0.040932000
C	-2.460667000	2.247986000	0.531803000
C	-2.629987000	0.942360000	0.097108000
C	-3.566027000	0.666958000	-0.903025000
C	-4.342157000	1.703467000	-1.422530000
C	-4.164965000	2.998619000	-0.935803000
H	-3.075831000	4.307543000	0.402969000
H	-5.078054000	1.518980000	-2.193524000
H	-4.775451000	3.796485000	-1.344667000
O	-3.643999000	-0.620948000	-1.297701000
C	-4.518022000	-0.955674000	-2.367699000

H	-5.561215000	-0.758950000	-2.103087000
H	-4.253413000	-0.407806000	-3.276883000
H	-4.380775000	-2.022639000	-2.534889000
O	-1.491685000	2.477413000	1.459282000
P	-1.429902000	-0.166058000	0.876406000
C	-0.625727000	1.350985000	1.669921000
C	-2.357588000	-0.962171000	2.302576000
C	-3.122990000	0.071576000	3.133970000
H	-3.850089000	0.619216000	2.528097000
H	-3.674136000	-0.448465000	3.925092000
H	-2.461128000	0.794057000	3.618349000
C	-3.349961000	-1.975015000	1.718413000
H	-2.852281000	-2.694307000	1.063647000
H	-3.823993000	-2.522175000	2.541021000
H	-4.139477000	-1.477040000	1.149482000
C	-1.326179000	-1.684228000	3.175057000
H	-0.823021000	-2.481227000	2.623180000
H	-0.561378000	-1.000503000	3.557509000
H	-1.833652000	-2.132912000	4.035727000
C	3.985225000	0.859851000	2.642016000
C	5.152706000	0.296152000	2.151271000
C	5.256533000	-0.171684000	0.841445000
C	4.154850000	-0.074650000	-0.007690000
C	2.973885000	0.506909000	0.459403000
C	2.903965000	0.949350000	1.772923000
H	3.901880000	1.217401000	3.660805000
O	4.132096000	-0.509798000	-1.284660000
C	5.311227000	-1.089641000	-1.829253000
H	5.063709000	-1.350162000	-2.856936000
H	6.137927000	-0.373151000	-1.823982000
H	5.593989000	-1.993408000	-1.282146000
C	1.790292000	1.079945000	-3.033398000

H	1.024306000	0.341813000	-3.278750000
H	1.850235000	1.799398000	-3.857045000
H	2.751212000	0.568010000	-2.954119000
C	0.061503000	2.488076000	-1.900015000
H	-0.195898000	3.118445000	-1.044645000
H	0.067189000	3.126129000	-2.789646000
H	-0.724222000	1.738331000	-2.026157000
C	2.509124000	2.906292000	-1.477574000
H	2.340419000	3.441955000	-0.539261000
H	3.511795000	2.471988000	-1.446552000
H	2.484924000	3.643103000	-2.287137000
C	1.444092000	1.838350000	-1.747072000
P	1.347312000	0.629560000	-0.319235000
O	1.716243000	1.447454000	2.207672000
C	0.772024000	1.672965000	1.148711000
H	6.015171000	0.214320000	2.803767000
H	6.186534000	-0.606018000	0.500604000
Ir	0.164292000	-1.241938000	-0.482506000
H	-0.617925000	-0.769123000	-1.875897000
H	1.326228000	-1.859539000	-1.437981000
Cl	-1.042042000	-3.492310000	-0.716500000
H	0.807938000	2.735259000	0.897101000
H	-0.542628000	1.201932000	2.746576000
H	1.018807000	-1.853615000	0.829585000

TS_{I3c-I4c}

Coordinates (Angstroms)			
	X	Y	Z
C	-4.653421000	1.588123000	2.079269000
C	-3.519842000	0.827373000	1.826194000
C	-3.403979000	0.025265000	0.697668000
C	-4.437399000	-0.000315000	-0.241004000

C	-5.582409000	0.765899000	-0.017808000
C	-5.673509000	1.537977000	1.139571000
H	-4.719208000	2.202880000	2.968243000
H	-6.397795000	0.770415000	-0.728484000
H	-6.570272000	2.126010000	1.302014000
O	-4.237803000	-0.786205000	-1.319062000
C	-5.245734000	-0.836106000	-2.321483000
H	-6.183851000	-1.225612000	-1.915421000
H	-5.408646000	0.150831000	-2.764045000
H	-4.869095000	-1.517585000	-3.082187000
O	-2.463440000	0.836838000	2.687714000
P	-1.799606000	-0.808755000	0.674097000
C	-1.265483000	0.341897000	2.065232000
C	-2.090896000	-2.461634000	1.509770000
C	-2.789443000	-2.313600000	2.864419000
H	-3.758720000	-1.816644000	2.768666000
H	-2.968545000	-3.311866000	3.278044000
H	-2.183504000	-1.762131000	3.587300000
C	-2.970505000	-3.297820000	0.571522000
H	-2.520027000	-3.396826000	-0.419174000
H	-3.091363000	-4.299901000	0.997455000
H	-3.966073000	-2.858958000	0.461203000
C	-0.723402000	-3.129248000	1.691551000
H	-0.245269000	-3.325695000	0.729364000
H	-0.045354000	-2.513166000	2.290976000
H	-0.857451000	-4.084604000	2.209848000
C	3.114888000	1.860182000	2.470238000
C	4.281914000	1.900978000	1.725626000
C	4.277837000	1.833737000	0.331926000
C	3.062670000	1.729235000	-0.341482000
C	1.871064000	1.697856000	0.389073000
C	1.915823000	1.744431000	1.775238000

H	3.121320000	1.894059000	3.552409000
O	2.934540000	1.645489000	-1.679475000
C	4.111365000	1.558877000	-2.474114000
H	3.764043000	1.447146000	-3.499833000
H	4.711706000	2.469275000	-2.388223000
H	4.705727000	0.686280000	-2.193201000
C	0.010630000	3.082361000	-2.418929000
H	-0.398427000	2.243990000	-2.986498000
H	-0.357727000	4.011213000	-2.866866000
H	1.098580000	3.064489000	-2.513932000
C	-1.965426000	3.039486000	-0.880809000
H	-2.336954000	3.046489000	0.147997000
H	-2.335927000	3.945598000	-1.370711000
H	-2.394923000	2.177184000	-1.396444000
C	0.142951000	4.241334000	-0.202500000
H	-0.105253000	4.235831000	0.862670000
H	1.230571000	4.291278000	-0.299715000
H	-0.276354000	5.156486000	-0.632831000
C	-0.432317000	3.035044000	-0.951909000
P	0.182853000	1.444797000	-0.183033000
O	0.742523000	1.649229000	2.451003000
C	-0.412823000	1.529016000	1.606721000
H	5.233850000	1.979838000	2.238696000
H	5.214266000	1.859719000	-0.207949000
Ir	-0.297151000	-0.512730000	-1.135848000
H	-1.438902000	0.165213000	-2.050263000
H	0.727595000	-0.154225000	-2.338141000
Cl	-0.683380000	-2.709830000	-2.333602000
H	-1.006871000	2.432672000	1.749488000
H	-0.706495000	-0.213613000	2.818394000
H	1.729681000	-1.268600000	-0.490246000
H	0.824162000	-1.356569000	-0.112995000

C	3.544051000	-1.459479000	0.545607000
O	3.004794000	-1.409382000	-0.603022000
O	3.022231000	-1.403248000	1.648012000
C	5.076270000	-1.695498000	0.493548000
F	5.324605000	-3.016363000	0.423972000
F	5.660335000	-1.127744000	-0.568965000
F	5.687381000	-1.231250000	1.587196000

TS_{15c-II}

Coordinates (Angstroms)			
	X	Y	Z
C	-1.924309000	4.248311000	-1.935405000
C	-1.036953000	3.688792000	-1.024767000
C	-1.436722000	2.754961000	-0.080539000
C	-2.764980000	2.316700000	-0.065732000
C	-3.676557000	2.861680000	-0.969525000
C	-3.242339000	3.820195000	-1.884269000
H	-1.583829000	4.977755000	-2.659577000
H	-4.710755000	2.545042000	-0.973818000
H	-3.959561000	4.234021000	-2.584692000
O	-3.066506000	1.366365000	0.839828000
C	-4.430097000	1.013217000	1.036108000
H	-5.005531000	1.877216000	1.383528000
H	-4.875059000	0.615391000	0.122387000
H	-4.427081000	0.243084000	1.805675000
O	0.280158000	4.033021000	-1.052720000
P	-0.032885000	2.231657000	0.930896000
C	1.094770000	3.268499000	-0.156010000
C	-0.174622000	3.242122000	2.513346000
C	-0.232012000	4.743996000	2.199409000
H	-1.040267000	4.986925000	1.503886000
H	-0.431956000	5.278452000	3.133918000

H	0.706008000	5.135433000	1.800612000
C	-1.463488000	2.867738000	3.255864000
H	-1.523687000	1.798122000	3.454760000
H	-1.476524000	3.400340000	4.213254000
H	-2.349909000	3.173926000	2.693874000
C	1.055600000	2.929958000	3.368840000
H	1.063115000	1.884276000	3.683846000
H	1.986453000	3.132120000	2.828531000
H	1.040933000	3.562661000	4.262573000
C	5.547465000	1.607263000	-0.301087000
C	6.328513000	0.515461000	-0.648177000
C	5.778034000	-0.630361000	-1.217426000
C	4.399204000	-0.708573000	-1.414773000
C	3.583174000	0.358753000	-1.026943000
C	4.180914000	1.508141000	-0.520756000
H	5.974165000	2.516625000	0.103309000
O	3.780841000	-1.756545000	-1.992349000
C	4.567031000	-2.779708000	-2.585513000
H	3.857089000	-3.489225000	-3.008456000
H	5.195956000	-2.372417000	-3.382888000
H	5.191876000	-3.289375000	-1.847275000
C	0.849138000	-1.231065000	-2.900650000
H	0.338454000	-1.619978000	-2.023061000
H	0.203991000	-1.389055000	-3.770955000
H	1.767901000	-1.798390000	-3.040597000
C	-0.174259000	1.053723000	-2.905140000
H	0.002717000	2.131077000	-2.870125000
H	-0.607029000	0.820018000	-3.882922000
H	-0.906411000	0.791925000	-2.137327000
C	2.138930000	0.714893000	-3.809260000
H	2.354284000	1.785324000	-3.763178000
H	3.081049000	0.167878000	-3.732118000

H	1.712580000	0.507533000	-4.796626000
C	1.132292000	0.266460000	-2.745438000
P	1.774779000	0.584336000	-1.009772000
O	3.361487000	2.560195000	-0.246259000
C	2.103109000	2.438767000	-0.927391000
H	7.401469000	0.560049000	-0.497424000
H	6.426792000	-1.444722000	-1.510229000
Ir	0.598280000	0.008335000	0.837695000
H	-0.775215000	-0.316453000	-0.020991000
H	0.888749000	-1.707991000	0.769066000
Cl	-0.617924000	-0.505105000	2.986021000
H	2.213632000	2.852037000	-1.933458000
H	1.662303000	3.971498000	0.452577000
C	-1.925553000	-2.775953000	-1.413341000
C	-0.901549000	-3.789019000	-0.919779000
C	-1.761461000	-3.573106000	1.307089000
C	-2.793702000	-2.569103000	0.818562000
C	-4.184683000	-1.999983000	-1.064276000
C	-4.032503000	-1.011428000	-2.042291000
C	-5.115790000	-0.259006000	-2.487696000
C	-6.380532000	-0.459070000	-1.954082000
C	-6.561442000	-1.432797000	-0.975342000
C	-5.479381000	-2.179536000	-0.562426000
H	-2.182185000	-3.024167000	-2.446009000
H	-0.020361000	-3.747154000	-1.552118000
H	-2.181452000	-4.584363000	1.256481000
H	-2.403429000	-1.552854000	0.951164000
H	-3.053999000	-0.819535000	-2.463608000
H	-4.956490000	0.499206000	-3.246111000
H	-7.225182000	0.128876000	-2.293460000
H	-7.533973000	-1.630344000	-0.539533000
N	-3.132566000	-2.813712000	-0.593635000

N	-0.554914000	-3.556397000	0.478823000
H	-3.685949000	-2.680023000	1.433740000
H	-1.529283000	-3.353681000	2.342552000
H	-1.319846000	-4.799009000	-0.996223000
H	-1.477216000	-1.777284000	-1.395781000
C	0.673041000	-3.223549000	0.921214000
C	0.904292000	-3.402295000	2.412406000
C	1.862891000	-3.602870000	0.049492000
C	2.283956000	-3.007781000	2.921844000
H	0.157216000	-2.855197000	2.979910000
C	3.212413000	-3.185139000	0.629944000
H	1.824724000	-4.697087000	-0.038290000
C	3.393013000	-3.616935000	2.077903000
H	2.373310000	-1.916816000	2.907765000
H	3.302633000	-2.096843000	0.573927000
H	4.372961000	-3.295750000	2.443414000
H	1.760621000	-3.190640000	-0.952604000
H	0.742904000	-4.474592000	2.588124000
H	2.362646000	-3.324382000	3.965998000
H	3.362604000	-4.711813000	2.151053000
H	3.999055000	-3.608563000	0.002468000
F	-5.686289000	-3.141950000	0.366261000
H	1.994789000	0.245913000	1.744766000

A3'

Coordinates (Angstroms)			
	X	Y	Z
C	4.189932000	1.207443000	-0.230626000
C	3.299713000	2.421171000	0.103479000
C	1.820864000	2.024940000	0.247682000
C	1.451335000	0.907018000	-0.726196000
C	3.566309000	-0.089090000	0.283892000

H	4.326197000	1.121876000	-1.312845000
H	3.637144000	2.888118000	1.033037000
H	1.622570000	1.704406000	1.275038000
H	0.379745000	0.701462000	-0.713045000
H	5.184669000	1.330392000	0.202252000
H	3.405143000	3.172747000	-0.684267000
H	1.175522000	2.886925000	0.064537000
H	1.683412000	1.228086000	-1.744415000
C	2.277678000	-0.366850000	-0.492739000
O	2.561595000	-0.918570000	-1.743089000
C	-2.555694000	-0.535405000	-1.303245000
C	-2.281071000	-0.367457000	0.060744000
C	-2.977662000	0.667766000	0.700408000
C	-3.853449000	1.510319000	0.050832000
C	-4.099327000	1.323395000	-1.305065000
C	-3.454062000	0.290389000	-1.969993000
H	-2.060776000	-1.318629000	-1.862418000
H	-4.349009000	2.288268000	0.620244000
H	-4.790771000	1.974655000	-1.826160000
H	-3.635065000	0.124967000	-3.026072000
C	-0.436265000	-0.475629000	1.658617000
C	-0.863359000	-2.372175000	0.175977000
C	0.935800000	-1.128744000	1.634517000
H	-0.358508000	0.570252000	1.359309000
C	0.397219000	-2.084326000	-0.621920000
H	-0.667628000	-3.116511000	0.951091000
H	0.918492000	-2.076014000	2.170966000
H	0.187545000	-1.385415000	-1.427662000
F	-2.802071000	0.839048000	2.033404000
N	-1.403872000	-1.173542000	0.795493000
N	1.462649000	-1.458363000	0.260488000
H	2.155220000	-2.191174000	0.427089000

H	-1.602023000	-2.817833000	-0.488576000
H	-0.753113000	-0.486841000	2.704911000
H	1.649301000	-0.481899000	2.137276000
H	0.815623000	-2.991770000	-1.051367000
H	3.268981000	-1.569014000	-1.663043000
H	3.372589000	0.007712000	1.353793000
H	4.241415000	-0.940897000	0.154352000

TS_{A3'-3'}

Coordinates (Angstroms)			
	X	Y	Z
C	3.380856000	1.426318000	1.236056000
C	3.101372000	2.415445000	0.092780000
C	1.632819000	2.351527000	-0.309406000
C	1.281442000	0.971904000	-0.881729000
C	2.426548000	0.212937000	1.236654000
H	4.416879000	1.079038000	1.187251000
H	3.377684000	3.427354000	0.397073000
H	1.006856000	2.558760000	0.565407000
H	0.207735000	0.806286000	-0.784269000
H	3.268007000	1.924903000	2.201334000
H	3.717794000	2.166487000	-0.778633000
H	1.394021000	3.111211000	-1.056577000
H	1.525821000	0.928645000	-1.944695000
C	1.996707000	-0.166417000	-0.165936000
O	3.244622000	-0.574027000	-0.954879000
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C	-3.494185000	1.425030000	0.766533000
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H	-1.706817000	-0.134521000	-2.270320000
H	-3.992382000	1.830267000	1.639914000
H	-4.163611000	2.945326000	-0.598066000
H	-3.029306000	1.890281000	-2.548739000
C	-0.521074000	-1.658473000	1.248645000
C	-0.836275000	-2.261689000	-1.090379000
C	0.865457000	-2.197009000	0.892739000
H	-0.411804000	-0.686349000	1.730205000
C	0.577953000	-1.829518000	-1.497648000
H	-0.834467000	-3.320204000	-0.818504000
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H	0.546724000	-0.955467000	-2.142997000
F	-2.758355000	-0.338523000	2.118702000
N	-1.346394000	-1.512360000	0.041815000
N	1.427543000	-1.538817000	-0.298388000
H	2.761573000	-1.593333000	-0.741715000
H	-1.508368000	-2.171149000	-1.942446000
H	-0.979073000	-2.339939000	1.973141000
H	1.532306000	-2.088731000	1.743662000
H	1.053817000	-2.637553000	-2.057004000
H	4.077077000	-0.419075000	-0.481675000
H	1.515913000	0.450547000	1.791490000
H	2.909949000	-0.628702000	1.732976000

TS_{A3*-A3'}

Coordinates (Angstroms)			
	X	Y	Z
C	0.793441000	3.062583000	1.394708000
C	-0.093798000	3.924907000	0.474336000
C	-1.330032000	3.150991000	0.027701000
C	-0.959750000	1.893963000	-0.767763000
C	0.542272000	1.549195000	1.254073000

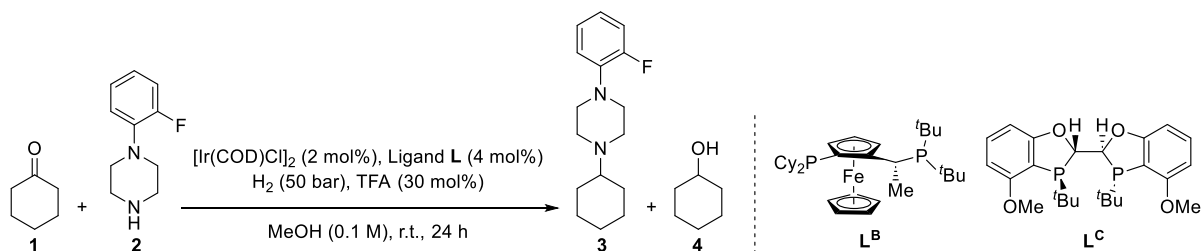
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H	0.608707000	3.322637000	2.437955000
H	0.461346000	4.265512000	-0.411442000
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H	-0.732635000	2.143815000	-1.807045000
C	0.193352000	1.111758000	-0.148226000
O	1.546782000	1.766123000	-1.099561000
C	-4.140833000	-0.134456000	-1.225063000
C	-3.538528000	-0.852926000	-0.183439000
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C	-6.300488000	-0.273575000	-0.175031000
C	-5.499153000	0.139681000	-1.232063000
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H	-6.319564000	-1.335038000	1.709664000
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H	-5.929251000	0.686824000	-2.061903000
C	-1.396193000	-1.358617000	1.003557000
C	-1.511575000	-1.607519000	-1.397652000
C	0.101846000	-1.217564000	0.680032000
H	-1.696191000	-0.640670000	1.770608000
C	-0.235587000	-0.783750000	-1.679412000
H	-1.257528000	-2.669812000	-1.273378000
H	0.506759000	-2.169390000	0.329081000
H	-0.434659000	0.043485000	-2.356778000
F	-3.873665000	-1.994078000	1.869910000
N	-2.152049000	-1.090779000	-0.206179000
N	0.331479000	-0.247633000	-0.417565000
H	2.104347000	-0.799719000	-0.569161000

H	-2.187934000	-1.548999000	-2.247905000
H	-1.563282000	-2.361568000	1.414469000
H	0.668365000	-0.952635000	1.569576000
H	0.521568000	-1.413101000	-2.156409000
H	1.525866000	2.728575000	-1.169483000
H	-0.316744000	1.259522000	1.869856000
H	1.405142000	0.998580000	1.630161000
C	5.270853000	-1.013661000	0.101197000
C	3.896358000	-0.362192000	-0.171448000
O	2.987258000	-1.238248000	-0.495496000
O	3.723274000	0.831966000	-0.058460000
H	2.414994000	1.495153000	-0.678690000
F	6.205853000	-0.086692000	0.168313000
F	5.204937000	-1.659957000	1.264645000
F	5.567607000	-1.877611000	-0.859616000

7. Experimental part.

General methods. All reactions were carried out under an inert atmosphere of nitrogen using Schlenk line techniques with a dual-bank manifold, unless otherwise noted. All reagents were purchased commercially and used as received, unless otherwise noted. Methanol anhydrous 99.8% was dried under argon atmosphere. Analytical thin-layer chromatography (TLC) was performed on 0.25 mm Merck precoated silica gel plates (60-F254). TLC analysis was performed using hexanes/CH₂Cl₂, CH₂Cl₂/MeOH or hexanes/AcOEt as the eluent and stained using permanganate stain, ninhydrin stain, and/or UV light (254 nm). Column chromatography was carried out with the same type of silica gel and a Teledyne Isco Combiflash^(R) using RediSep Rf Gold Normal-Phase Silica^(R) columns (60 Å porosity, 20–40 μm). ¹H NMR, ¹³C NMR and ¹⁹F NMR were recorded with Bruker FT spectrometers at 300 K unless otherwise noted. ¹H (400, 500 or 600 MHz) and ¹³C {¹H} (100, 126 or 151 MHz) NMR chemical shifts are reported relative to internal TMS (δ = 0.00 ppm) CDCl₃ (δ = 7.26 ppm; ¹³C NMR: CDCl₃ at 77.16 ppm) or to residual protiated solvent, and ¹⁹F {¹H} NMR (471 MHz) chemical shifts were referenced to external CFCl₃ (0.0 ppm). Chemical shifts are reported in parts per million (ppm). Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, m = multiplet), coupling constant J (Hz) and integration.

General procedure of the iridium-catalyzed direct reductive amination – synthesis and characterization of amine 3. In an oven dried vial equipped with a stirring bar was added ketone (1.5 mmol, 3 equiv.), amine (0.5 mmol, 1 equiv.), ligand (12.5 mg, 0.022 mmol, 4.4 mol%), [Ir(COD)Cl]₂ (6.7 mg, 0.01 mmol, 2 mol%), anhydrous MeOH (5 mL) and trifluoroacetic acid (17.1 mg, 11.5 μL, 0.15 mmol, 30 mol%) under inert atmosphere. The vial was placed in an autoclave, which was then sealed, and purged (replacing air with 5 bar of H₂, three times). The autoclave was charged with 50 bar of H₂ and the reaction mixture was stirred at room temperature for 24 h. Then, the hydrogen from the autoclave was released. LC- and/or GC-MS analysis were performed to calculate the conversion of amine –limiting reagent-. Next, the solution was poured into NaOH 1 M (30 mL). Extraction with ethyl acetate (3 x 20 mL) and drying the organic layer with MgSO₄ before concentration to dryness under reduced pressure afforded a crude residue that was further purified by column chromatography on silica gel (heptane: ethyl acetate 1:0 to 2:1 with 1% triethylamine) to afford the tertiary amine product **3** (remark: no glovebox was required for this experiment). ¹H NMR (500 MHz, CDCl₃): δ = 7.08–7.04 (m, 1H), 7.06–6.98 (m, 1H), 7.00–6.91 (m, 1H), 6.92 (ddd, J = 7.9, 4.1, 1.4, 1H), 3.16–3.10 (m, 4H), 2.82–2.74 (m, 4H), 2.32 (ddq, J = 11.0, 7.1, 3.4, 1H), 1.93 (dd, J = 9.1, 4.0, 2H), 1.87–1.77 (m, 2H), 1.69–1.61 (m, 1H), 1.26 (td, J = 9.3, 7.1, 4.2, 4H), 1.14 (ddt, J = 16.2, 12.3, 6.1, 1H) ppm. ¹³C {¹H} NMR (126 MHz, CDCl₃): δ = 155.76 (d, J_{C3,F} = 245.9), 140.31 (d, J_{C4,F} = 8.3), 124.43 (d, J_{C6,F} = 3.7), 122.26 (d, J_{C1,F} = 8.0), 118.88 (d, J_{C5,F} = 3.2), 116.03 (d, J_{C2,F} = 20.7), 63.58, 51.06, 49.08, 29.01, 26.35, 25.91 ppm. ¹⁹F {¹H} NMR (471 MHz, CDCl₃): δ = -122.68 ppm. GC: t_R = 12.5 min; MS (EI): m/z = 262 (M⁺, 53), 219 (100), 150 (21). HRMS (ESI): m/z calcd for C₁₆H₂₄N₂F 263.1918 [M+H]⁺, found: 263.1918 (0 ppm). The spectroscopic data match those reported previously.¹



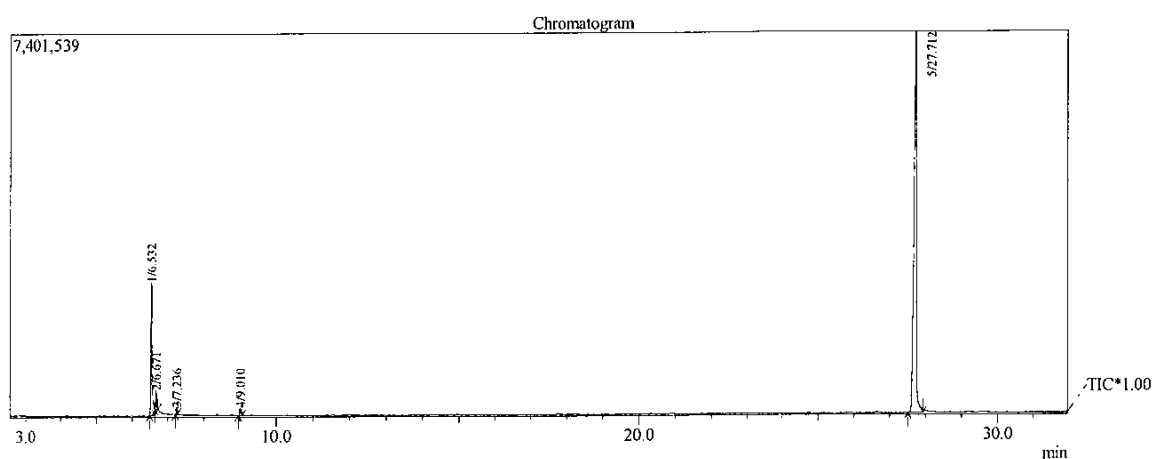
Entry	Ligand	Conversion of 2	Yield of 3
1	L ^B	68	39
2	L ^C	72	41

GC-MS results showing formation of cyclohexanol 4 (ca. 15% yield):

Sample Information

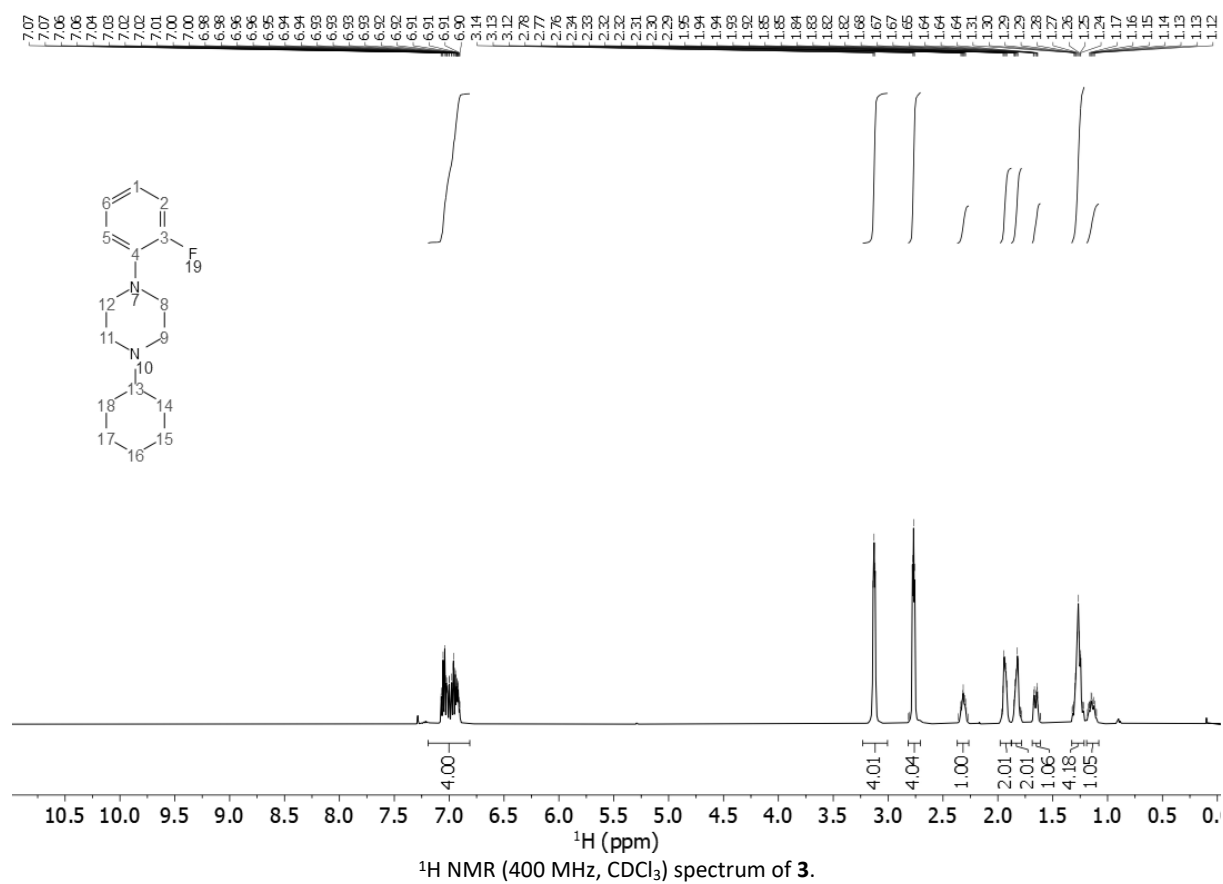
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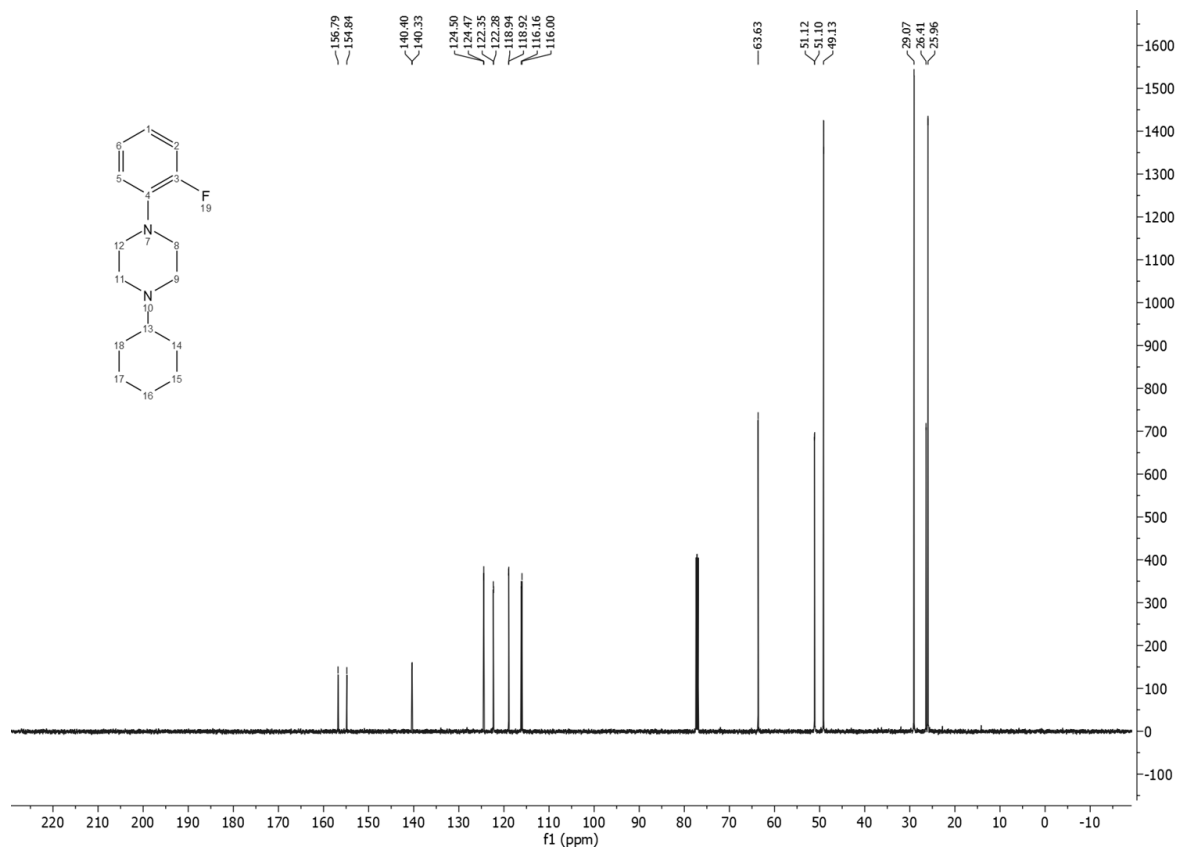
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 Report File :
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Peak#	R. Time	I. Time	F. Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	6.532	6.490	6.637	6350719	14.38	2567673	24.28	2.47	MI	
2	6.671	6.643	6.730	703490	1.59	364737	3.45	1.93	MI	
3	7.236	7.203	7.270	257490	0.58	127984	1.21	2.01	MI	
4	9.010	8.963	9.070	333208	0.75	151060	1.43	2.21	MI	
5	27.712	27.510	27.930	36512624	82.69	7365932	69.64	4.96	MI	
				44157531	100.00	10577386	100.00			

9. NMR data.





¹³C{¹H} NMR (101 MHz, CDCl₃) spectrum of **3**.

tnghuyen2 NTM553sp_P.12.fid

