Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

Improving the Chemical Stability of Blue Heteroleptic Iridium Emitter FIrpic in the Lowest Triplet State through Ancillary Ligand Modification: A Theoretical Perspective

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Benchmark Calculations

All calculations were performed using the Gaussian 16 C.01 package[1]. For the aim to find a better theoretical method for our study, geometry parameters of FIrpic complex in the ground state were optimized with four different functions, including B3LYP,[2-4] M06-2X,[5] PBE0,[6] and ωB97X-D,[7] which were used in previous studies for the iridium complexes.[8-11] Three basis set systems (BS1-3) were employed for calculations here: For BS1, a double-ζ quality basis set LANL2DZ and corresponding effective core potential were used[12,13] for iridium; usual 6-31G(d,p) basis sets were used for carbon, nitrogen, hydrogen, oxygen and sulfur atoms. BS2 is made of a correlation-consistent polarized double-ζ basis set (cc-pVDZ)[14]. BS3 is made of a correlation-consistent polarized double-ζ basis set augmented by multiple diffuse functions (aug-cc-pVDZ)[15]. In addition, solvent effect was considered by conductor-like polarizable continuum model (CPCM)[16] with dichloromethane (CH_2Cl_2) (ε=8.93) and tetrahydrofuran (THF)[18] (ε=7.4257) solvents which were used for experimental studies[17,18] of iridium complexes. It is observed that solvent effect on the geometry parameters of FIrpic is very small.

Optimized geometry parameters of FIrpic in the ground state with different computational methods were collected in Table S1. Experimental determined crystal structures in acetonitrile/ethanol solutions were also listed for comparison. It is found that the PBE0 and ωB97X-D functionals have outperformed the standard B3LYP functional. Moreover, there is a much better description of the Ir-X bond length with PBE0-D3(BJ)[20-22] compared with those from PBE0. Thereby, dispersion correction in functional plays an important role in correctly describing weak interactions.

Table S1. Main geometry parameters of FIrpic in the ground state (S_0) obtained from a number of benchmark calculations. The atom numbering scheme is shown in Figure S1.

	B3LYP /BS1	**B3LYP - D3(BJ) /BS1**	**B3LYP - D3(BJ) /BS2**	**M062X /BS1**	**M062X /BS2**	**PBE0 - D3(BJ) /BS1**	**PBE0 - D3(BJ) /BS2**	**PBE0 - D3(BJ) /BS3**	**ωB97X -D /BS1**	**ωB97X -D /BS2**	**ωB97X -D /BS2 [a]**	**ωB97X -D /BS2 [b]**	***Exptl.*[c]**
Ir-N_1	2.206	2.177	2.156	2.213	2.212	2.149	2.137	2.134	2.175	2.162	2.160	2.161	2.138(4)
Ir-O_1	2.180	2.174	2.152	2.197	2.178	2.155	2.132	2.132	2.170	2.153	2.166	2.165	2.152(3)
Ir-N_2	2.073	2.059	2.053	2.067	2.060	2.040	2.036	2.035	2.060	2.055	2.048	2.048	2.041(4)
Ir-C_2	2.014	2.004	2.006	1.986	1.976	1.992	1.992	1.992	2.002	2.000	1.990	1.990	1.997(5)
Ir-N_3	2.061	2.048	2.043	2.054	2.046	2.030	2.025	2.024	2.025	2.042	2.058	2.058	2.045(4)
Ir-C_3	2.011	1.997	1.996	1.980	1.968	1.994	1.992	1.981	1.992	1.990	2.001	2.001	1.993(4)
α(O_1-Ir-N_1)	76.31	76.90	77.32	75.72	75.88	77.24	77.46	77.56	77.46	77.07	76.72	76.73	77.38(14)
α(C_2-Ir-N_2)	80.22	80.56	80.58	80.63	80.87	80.68	80.01	80.74	80.74	80.50	80.72	80.72	81.53(19)
α(C_3-Ir-N_3)	80.46	80.95	80.85	80.99	81.19	80.99	80.74	81.03	80.01	80.78	80.51	80.51	80.69(18)

[a] from Ref. 17; [b] from Ref. 18; [c] from Ref. 19.

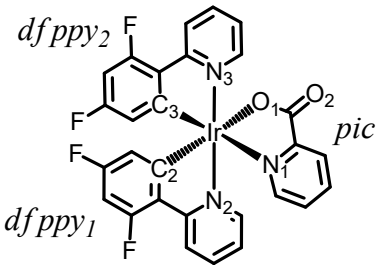

Figure S1. Chemical structure of FIrpic complex.

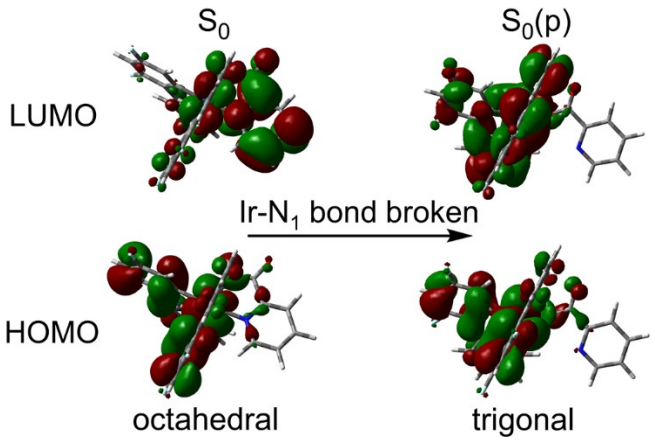

Figure S2. Representations of the HOMO and LUMO of FIrpic as determined at the ωB97X/cc-pVDZ level of theory.

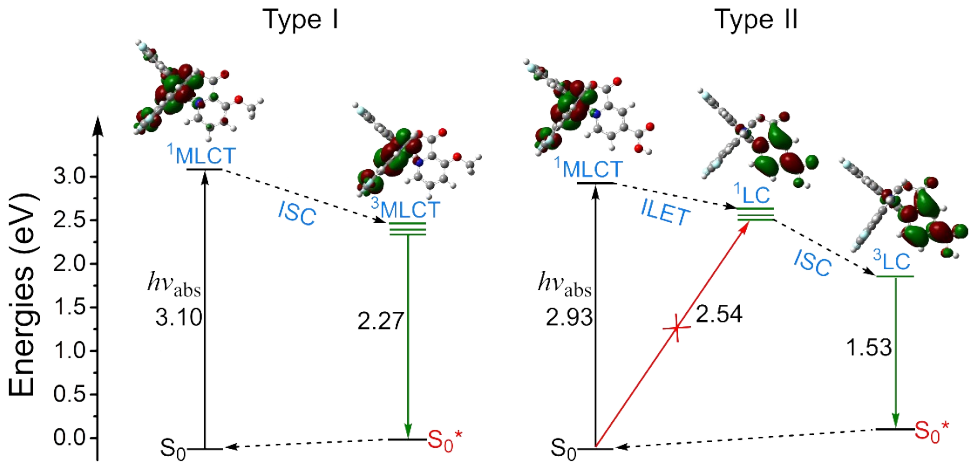

Figure S3. Calculated energy parameters for the degradation pathways of Ir emitters (left: complex **3**; right: complex **17**) in the S_0 and the T_1 states obtained at the ωB97X-D/cc-pVDZ level.

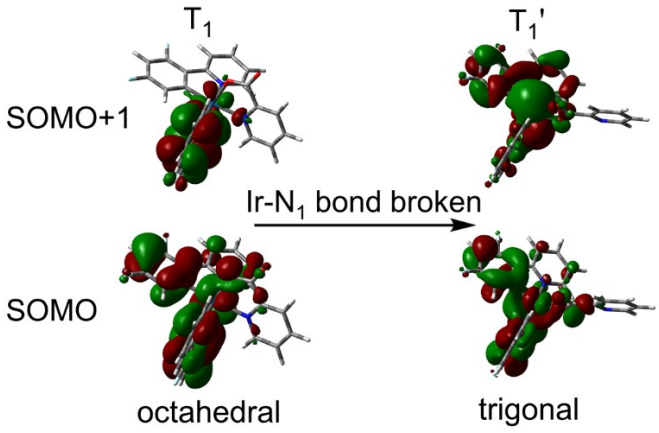

Figure S4. Contour plots of the SOMO (low) and SOMO+1 (high) energy orbitals of FIrpic. isosurface: 1×10^{-5} electrons/bohr^3

Table S2. The main distribution (%) of the frontier molecular orbitals in different states of heteroleptic FIrpic.

	HOMO (SOMO)				LUMO (SOMO+1)			
	Ir	***dfppy*$_1$**	***dfppy*$_2$**	**picolinate**	**Ir**	***dfppy*$_1$**	***dfppy*$_2$**	**picolinate**
S_0	53	18	21	7	2	18	5	74
S_0(p)	66	21	13	0	36	31	32	0
T_1	40	33	19	9	7	87	2	4
T_1'	51	13	19	16	33	36	27	4

Final Products

Losing carbon dioxide (CO_2) unit from the picolinate ligand as final degradation product was observed in experimental studies.[23] According to this, dissociation process between –COO and pyridyl groups of picolinate radical and ion, (1) and (2) in Figure S5, are examined. Calculated E_d results collected in Table S3 show that the dissociation process of picolinate neutral radical is an exothermal reaction and should be much easier to proceed than that of the picolinate ion. The

energy barrier for the dissociation of picolinate radical by losing of the CO_2 unit is only 0.25 eV (Figure S6).

To examine the dissociation process of picolinate ion by the loss of the CO_2 unit, further scan calculations were performed to examine the potential energy variation along with the C-C bond elongation between –COO and pyridyl parts of picolinate anion as shown in Figure S5. It is found that the energy potential surface for the C-C bond stretching is increased continually for the picolinate anion dissociation process and the required energy is about 2.5 eV. It means the loss of the CO_2 unit from picolinate anion is much harder to proceed than that from the picolinate neutral radical.

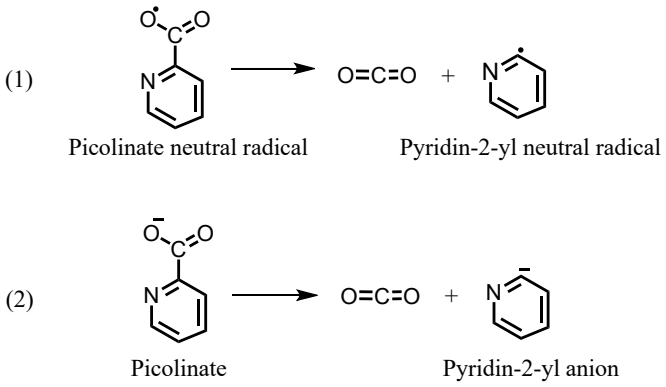

Figure S5. Proposed dissociation pathways for picolinate radical and ion for forming CO_2 product.

Table S3. Calculated dissociation energies (E_d) and energy barriers (E_a) for picolinate particles. (in eV)

	E_d	**E_a**

Radical	-0.10	0.25
Anion	2.64	--

Note: Dissociation energies of picolinate ligand were defined as: $E_d = (E_{CO2} + E_{Pyridine\ ion/radical}) - E_{picolinate}$.

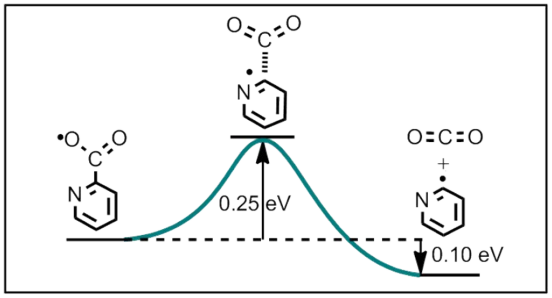

Figure S6. Proposed dissociation pathway for picolinate radical by losing one CO_2 unit.

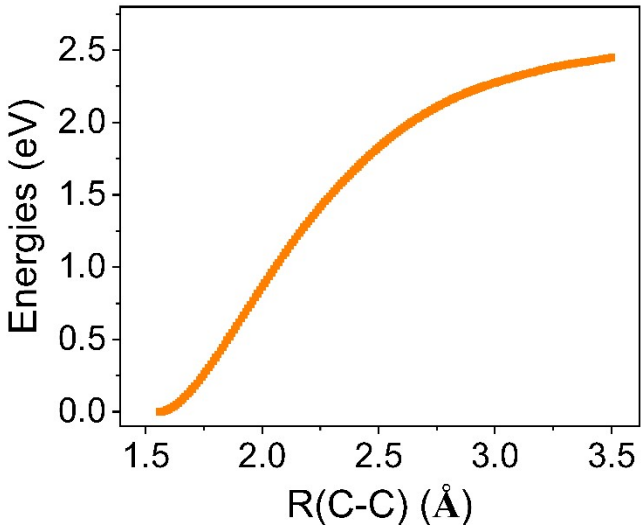

Figure S7. Scan calculation results for the potential energy variation along with the C-C bond stretching between –COO and pyridyl parts of picolinate ion.

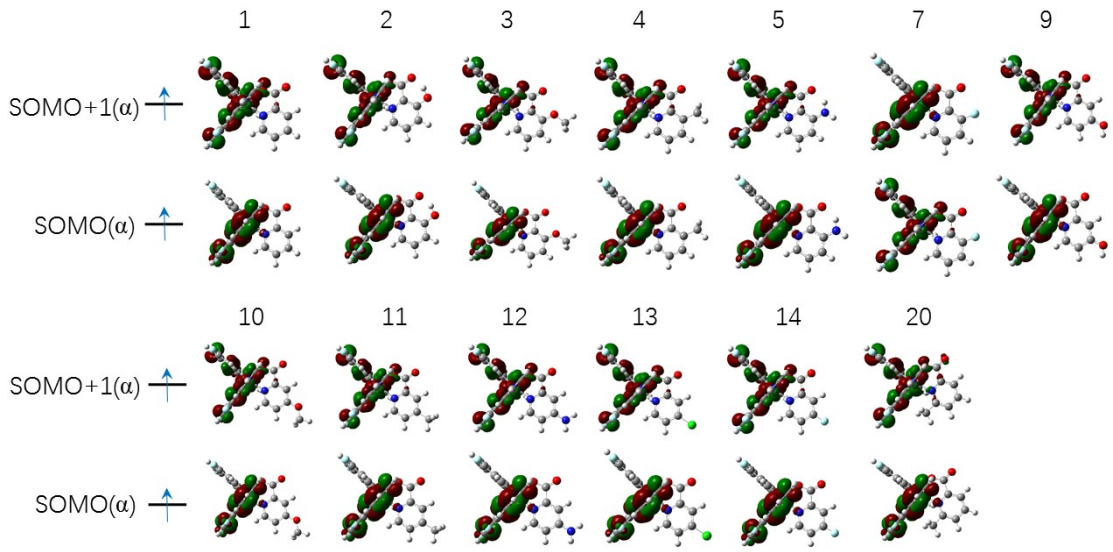

Figure S8. Contour plots of the SOMO (low) and SOMO+1 (high) energy orbitals of Type I emitters.

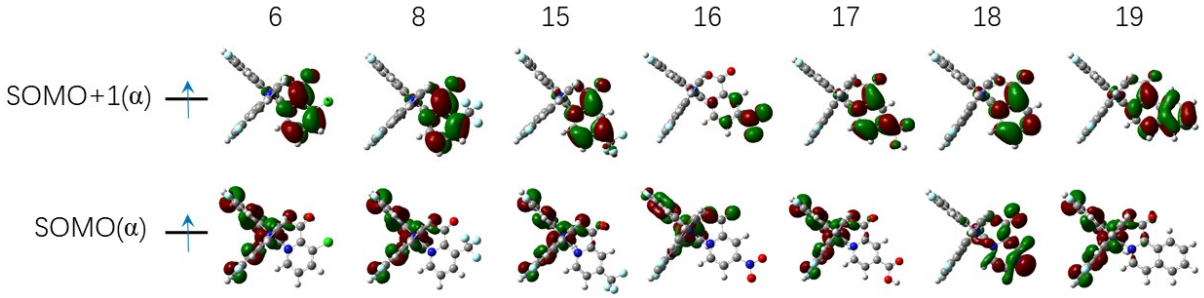

Figure S9. Contour plots of the SOMO (low) and SOMO+1 (high) energy orbitals of Type II emitters.

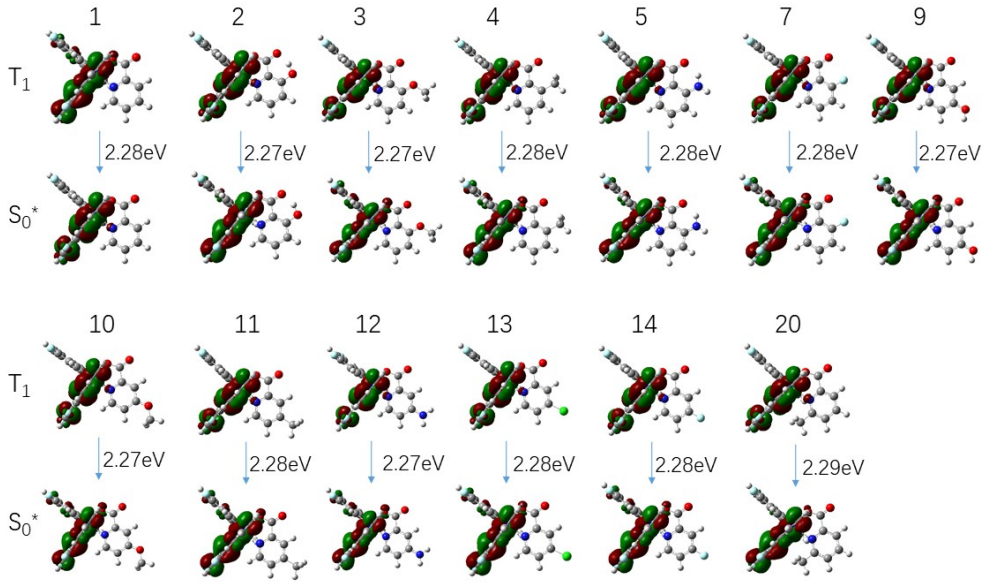

Figure S10. The nature of the orbitals involved in the T_1 to S_0^* transition of Type I emitters.

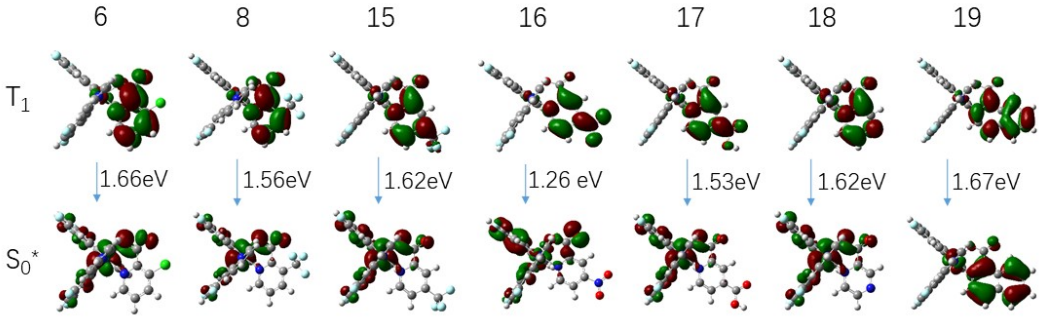

Figure S11. The nature of the orbitals involved in the T_1 to S_0^* transition of Type II emitters.

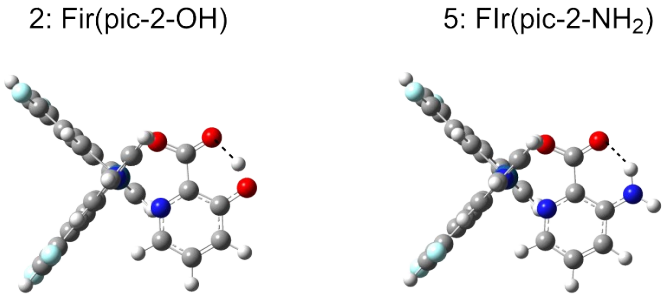

Figure S12. Optimized structures of Fir(pic-2-OH) and Fir(pic-2-NH_2).

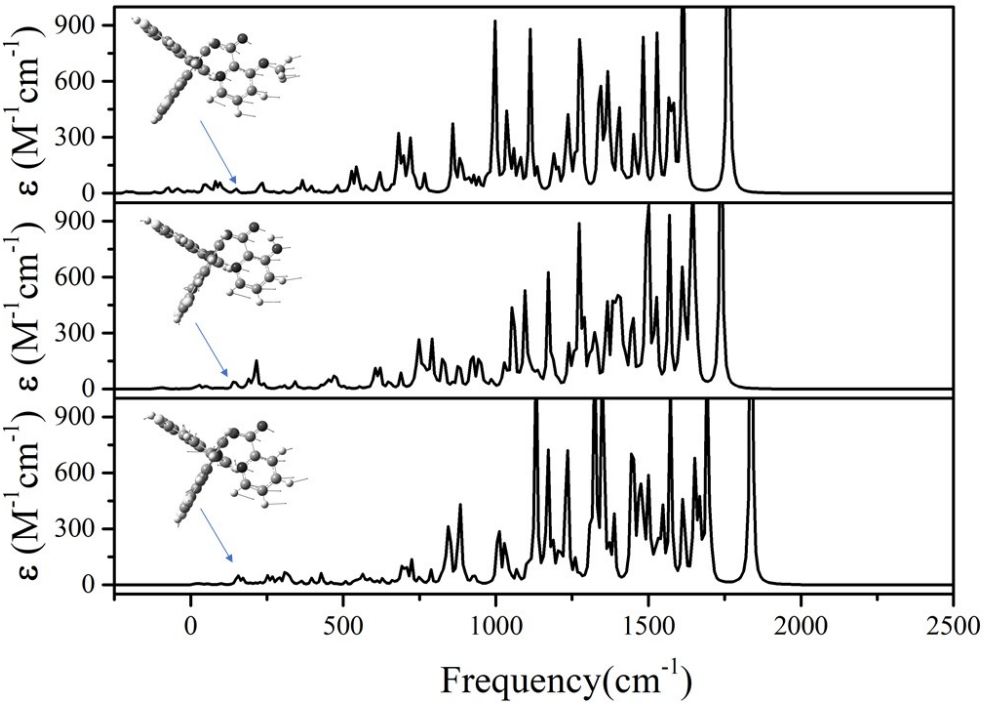

Figure S13. Vibration mode for Ir-N bond stretching in FIrpic, FIr(pic-2-OH) and FIr(pic-2-OMe) complexes.

Table S4. Cartesian coordinates for triplet geometry of complex 1.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.132	-0.323	-0.256	0.215	0.259	-0.115	0.202	0.002	0.000	0.202	0.002	0.000
C	1.648	1.086	-2.410	1.825	1.208	-2.441	-0.012	-1.465	-2.615	-0.012	-1.465	-2.615
C	1.462	2.273	-0.346	3.069	0.166	-0.744	1.316	-2.524	-0.993	1.316	-2.524	-0.993
C	2.371	2.124	-2.986	2.951	1.401	-3.219	0.226	-2.471	-3.535	0.226	-2.471	-3.535
H	1.395	0.186	-2.961	0.832	1.499	-2.765	-0.672	-0.626	-2.810	-0.672	-0.626	-2.810
C	2.207	3.362	-0.927	4.239	0.342	-1.488	1.589	-3.562	-1.886	1.589	-3.562	-1.886
C	2.651	3.289	-2.211	4.177	0.966	-2.725	1.047	-3.530	-3.162	1.047	-3.530	-3.162
H	2.702	2.034	-4.013	2.862	1.877	-4.188	-0.230	-2.420	-4.516	-0.230	-2.420	-4.516
H	2.399	4.235	-0.321	5.177	-0.021	-1.097	2.214	-4.384	-1.571	2.214	-4.384	-1.571
H	3.208	4.111	-2.646	5.084	1.101	-3.305	1.258	-4.336	-3.857	1.258	-4.336	-3.857
C	0.166	0.946	1.246	1.602	-0.674	1.031	1.284	-1.310	1.139	1.284	-1.310	1.139
C	0.922	2.181	0.928	2.933	-0.510	0.548	1.772	-2.419	0.400	1.772	-2.419	0.400
C	-0.394	0.797	2.513	1.405	-1.295	2.270	1.669	-1.143	2.470	1.669	-1.143	2.470
C	1.022	3.165	1.978	3.990	-0.987	1.324	2.627	-3.316	1.041	2.627	-3.316	1.041
C	-0.240	1.790	3.465	2.495	-1.751	2.992	2.514	-2.072	3.056	2.514	-2.072	3.056
H	-0.965	-0.089	2.768	0.416	-1.421	2.694	1.323	-0.302	3.062	1.323	-0.302	3.062
C	0.470	2.985	3.206	3.801	-1.614	2.542	3.010	-3.167	2.364	3.010	-3.167	2.364
H	0.569	3.745	3.972	4.642	-1.970	3.122	3.676	-3.880	2.832	3.676	-3.880	2.832
N	1.205	1.129	-1.158	1.889	0.629	-1.233	0.535	-1.485	-1.389	0.535	-1.485	-1.389
F	-0.773	1.641	4.686	2.293	-2.352	4.172	2.875	-1.916	4.336	2.875	-1.916	4.336
F	1.697	4.308	1.741	5.262	-0.844	0.906	3.126	-4.380	0.384	3.126	-4.380	0.384
C	-0.653	-2.765	1.364	-1.844	-1.394	1.330	-0.870	1.290	2.473	-0.870	1.290	2.473
C	-2.431	-1.555	0.434	-2.332	0.895	1.203	0.397	2.708	1.092	0.397	2.708	1.092
C	-1.504	-3.696	1.928	-3.048	-1.672	1.950	-1.099	2.304	3.385	-1.099	2.304	3.385
H	0.421	-2.832	1.481	-1.131	-2.170	1.076	-1.294	0.298	2.580	-1.294	0.298	2.580
C	-3.337	-2.468	0.984	-3.559	0.670	1.831	0.201	3.764	1.987	0.201	3.764	1.987
C	-2.873	-3.537	1.730	-3.916	-0.616	2.204	-0.543	3.556	3.138	-0.543	3.556	3.138
H	-1.100	-4.520	2.503	-3.293	-2.694	2.213	-1.705	2.111	4.261	-1.705	2.111	4.261
H	-4.394	-2.330	0.816	-4.224	1.501	2.008	0.620	4.733	1.764	0.620	4.733	1.764
H	-3.576	-4.246	2.155	-4.873	-0.793	2.683	-0.699	4.374	3.833	-0.699	4.374	3.833
C	-1.648	0.383	-0.829	-0.591	2.142	0.015	1.029	1.560	-0.974	1.029	1.560	-0.974
C	-1.876	1.515	-1.613	-0.019	3.329	-0.444	1.653	1.531	-2.227	1.653	1.531	-2.227
C	-2.754	-0.382	-0.379	-1.814	2.184	0.730	1.089	2.752	-0.196	1.089	2.752	-0.196
C	-3.174	1.868	-1.940	-0.666	4.533	-0.208	2.312	2.657	-2.687	2.312	2.657	-2.687
H	-1.059	2.128	-1.975	0.922	3.339	-0.983	1.637	0.644	-2.851	1.637	0.644	-2.851
C	-4.041	0.026	-0.740	-2.418	3.424	0.937	1.776	3.851	-0.712	1.776	3.851	-0.712
C	-4.280	1.143	-1.518	-1.868	4.609	0.479	2.392	3.832	-1.951	2.392	3.832	-1.951
H	-5.288	1.433	-1.783	-2.360	5.555	0.658	2.917	4.701	-2.324	2.917	4.701	-2.324
N	-1.098	-1.725	0.644	-1.493	-0.149	0.973	-0.122	1.484	1.375	-0.122	1.484	1.375
F	-3.384	2.955	-2.692	-0.119	5.670	-0.656	2.902	2.626	-3.890	2.902	2.626	-3.890

F	-5.119	-0.672	-0.332	-3.579	3.519	1.613	1.867	4.992	-0.003	1.867	4.992	-0.003
C	2.404	-2.221	-0.683	-1.879	-2.544	-1.733	-4.154	-0.440	-0.315	-4.154	-0.440	-0.315
C	2.830	-1.042	1.271	-0.915	-4.502	-1.055	-5.732	-0.986	1.238	-5.732	-0.986	1.238
C	3.594	-2.926	-0.559	-3.081	-3.186	-2.033	-5.114	-0.310	-1.318	-5.114	-0.310	-1.318
C	4.034	-1.704	1.456	-2.065	-5.235	-1.336	-6.765	-0.890	0.309	-6.765	-0.890	0.309
H	2.468	-0.290	1.965	-0.032	-4.996	-0.655	-5.948	-1.250	2.271	-5.948	-1.250	2.271
C	4.421	-2.665	0.524	-3.173	-4.557	-1.836	-6.445	-0.543	-0.999	-6.445	-0.543	-0.999
H	3.827	-3.657	-1.325	-3.908	-2.592	-2.403	-4.793	-0.028	-2.313	-4.793	-0.028	-2.313
H	4.652	-1.467	2.315	-2.088	-6.305	-1.163	-7.790	-1.081	0.609	-7.790	-1.081	0.609
H	5.358	-3.199	0.644	-4.091	-5.089	-2.066	-7.219	-0.453	-1.755	-7.219	-0.453	-1.755
N	2.036	-1.301	0.224	-0.811	-3.187	-1.249	-4.449	-0.770	0.946	-4.449	-0.770	0.946
O	0.418	-1.713	-1.898	-0.592	-0.533	-1.891	-1.863	-0.459	0.263	-1.863	-0.459	0.263
C	1.464	-2.461	-1.869	-1.795	-1.037	-1.921	-2.702	-0.184	-0.674	-2.702	-0.184	-0.674
O	1.790	-3.315	-2.680	-2.824	-0.405	-2.098	-2.427	0.259	-1.790	-2.427	0.259	-1.790

Table S5. Cartesian coordinates for triplet geometry of complex 2.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.153	-0.199	-0.203	0.481	0.141	-0.087	0.338	0.004	0.034	0.429	0.035	0.038
C	1.121	1.619	-2.370	2.067	0.977	-2.473	-0.141	-1.365	-2.599	-0.139	-1.361	-2.589
C	0.304	2.710	-0.409	3.199	-0.451	-0.993	1.360	-2.469	-1.169	1.354	-2.465	-1.168
C	1.398	2.838	-2.979	3.142	1.013	-3.342	-0.003	-2.337	-3.573	-0.003	-2.333	-3.571
H	1.303	0.674	-2.872	1.136	1.496	-2.674	-0.817	-0.522	-2.695	-0.817	-0.523	-2.694
C	0.583	3.984	-1.025	4.315	-0.444	-1.832	1.537	-3.474	-2.122	1.539	-3.472	-2.121
C	1.116	4.047	-2.274	4.286	0.295	-3.005	0.857	-3.402	-3.329	0.856	-3.402	-3.328
H	1.817	2.850	-3.977	3.076	1.586	-4.258	-0.565	-2.256	-4.496	-0.564	-2.256	-4.496
H	0.353	4.884	-0.473	5.185	-1.024	-1.565	2.195	-4.301	-1.907	2.195	-4.301	-1.908
H	1.321	5.006	-2.736	5.150	0.299	-3.661	0.992	-4.183	-4.071	0.992	-4.183	-4.070
C	-0.455	1.036	1.201	1.737	-1.159	0.845	1.553	-1.331	0.995	1.503	-1.249	0.941
C	-0.248	2.458	0.837	3.029	-1.209	0.251	1.966	-2.408	0.168	1.947	-2.400	0.183
C	-1.009	0.724	2.437	1.512	-1.844	2.043	2.084	-1.204	2.280	2.077	-1.219	2.263
C	-0.641	3.441	1.818	4.024	-1.956	0.882	2.894	-3.315	0.678	2.893	-3.307	0.676
C	-1.352	1.733	3.323	2.539	-2.571	2.620	2.998	-2.141	2.735	2.995	-2.134	2.733
H	-1.186	-0.306	2.724	0.552	-1.814	2.546	1.801	-0.387	2.936	1.801	-0.390	2.935
C	-1.171	3.103	3.022	3.807	-2.648	2.060	3.422	-3.207	1.954	3.419	-3.208	1.954
H	-1.453	3.867	3.736	4.601	-3.216	2.527	4.141	-3.927	2.320	4.141	-3.928	2.320
N	0.603	1.527	-1.150	2.106	0.284	-1.325	0.536	-1.422	-1.441	0.538	-1.422	-1.430
F	-1.876	1.428	4.518	2.312	-3.231	3.763	3.499	-2.024	3.971	3.499	-2.024	3.970
F	-0.473	4.748	1.537	5.263	-2.024	0.358	3.325	-4.350	-0.067	3.326	-4.350	-0.065
C	0.316	-2.666	1.552	-1.772	-1.218	1.363	-0.461	1.163	2.671	-0.463	1.161	2.657
C	-1.726	-2.344	0.448	-1.812	1.126	1.456	0.567	2.678	1.199	0.574	2.672	1.195
C	-0.120	-3.837	2.142	-2.989	-1.318	2.011	-0.621	2.137	3.639	-0.618	2.133	3.638
H	1.311	-2.276	1.728	-1.241	-2.089	0.997	-0.824	0.150	2.796	-0.823	0.149	2.795
C	-2.219	-3.523	1.019	-3.039	1.081	2.121	0.438	3.696	2.147	0.438	3.694	2.145
C	-1.415	-4.268	1.865	-3.629	-0.144	2.393	-0.152	3.420	3.371	-0.153	3.420	3.370
H	0.540	-4.392	2.796	-3.426	-2.294	2.183	-1.106	1.890	4.575	-1.106	1.891	4.575
H	-3.224	-3.841	0.790	-3.527	2.003	2.396	0.787	4.690	1.911	0.787	4.690	1.911
H	-1.797	-5.182	2.307	-4.591	-0.179	2.893	-0.258	4.209	4.108	-0.258	4.209	4.108
C	-1.713	-0.315	-0.912	0.076	2.115	0.247	0.995	1.626	-0.969	0.986	1.526	-0.930
C	-2.326	0.585	-1.784	0.845	3.208	-0.157	1.473	1.661	-2.284	1.460	1.674	-2.263
C	-2.440	-1.448	-0.463	-1.072	2.327	1.053	1.100	2.792	-0.160	1.080	2.787	-0.167
C	-3.627	0.355	-2.199	0.464	4.486	0.220	2.031	2.828	-2.776	2.032	2.824	-2.773
H	-1.808	1.465	-2.148	1.738	3.085	-0.760	1.420	0.794	-2.933	1.420	0.795	-2.932
C	-3.749	-1.625	-0.916	-1.406	3.635	1.400	1.680	3.935	-0.711	1.679	3.924	-0.708
C	-4.367	-0.743	-1.782	-0.659	4.729	0.997	2.149	3.981	-2.011	2.147	3.981	-2.013
H	-5.382	-0.907	-2.117	-0.942	5.732	1.286	2.595	4.883	-2.410	2.595	4.883	-2.410
N	-0.460	-1.939	0.735	-1.200	-0.033	1.097	0.137	1.424	1.498	0.130	1.407	1.488
F	-4.207	1.224	-3.036	1.200	5.532	-0.175	2.481	2.858	-4.037	2.480	2.859	-4.036

F	-4.473	-2.687	-0.513	-2.485	3.888	2.164	1.808	5.056	0.024	1.809	5.056	0.022
C	3.015	-1.030	-0.373	-2.743	-1.601	-1.611	-4.029	-0.540	0.138	-4.026	-0.539	0.134
C	2.776	0.304	1.516	-2.882	-3.846	-1.166	-5.417	-1.375	1.759	-5.416	-1.375	1.759
C	4.390	-1.207	-0.136	-4.147	-1.449	-1.559	-5.112	-0.266	-0.726	-5.112	-0.266	-0.726
C	4.132	0.175	1.812	-4.279	-3.798	-1.100	-6.552	-1.151	0.973	-6.552	-1.151	0.973
H	2.094	0.878	2.134	-2.353	-4.783	-1.012	-5.508	-1.811	2.751	-5.508	-1.811	2.751
C	4.946	-0.581	0.989	-4.919	-2.589	-1.296	-6.401	-0.591	-0.280	-6.400	-0.591	-0.280
H	4.537	0.670	2.687	-4.848	-4.699	-0.894	-7.536	-1.413	1.348	-7.536	-1.413	1.348
H	6.005	-0.705	1.188	-5.998	-2.491	-1.250	-7.244	-0.391	-0.932	-7.244	-0.391	-0.932
N	2.249	-0.292	0.447	-2.137	-2.777	-1.410	-4.191	-1.078	1.353	-4.191	-1.078	1.353
O	1.107	-1.434	-1.734	-0.605	-0.549	-1.789	-1.692	-0.524	0.493	-1.671	-0.519	0.499
C	2.350	-1.663	-1.573	-1.884	-0.382	-1.800	-2.635	-0.215	-0.310	-2.621	-0.215	-0.311
O	3.066	-2.349	-2.323	-2.438	0.725	-1.923	-2.467	0.336	-1.422	-2.470	0.337	-1.419
O	5.145	-1.939	-0.940	-4.757	-0.278	-1.728	-4.963	0.281	-1.933	-4.963	0.281	-1.932
H	4.520	-2.267	-1.656	-4.022	0.380	-1.862	-3.989	0.446	-2.027	-3.988	0.446	-2.027

Table S6. Cartesian coordinates for triplet geometry of complex 3.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.022	-0.176	-0.184	0.506	-0.145	-0.085	0.478	-0.020	0.553	-0.058	0.070	0.553
C	0.883	1.705	-2.339	0.062	-1.881	-2.479	-1.191	-0.376	-1.187	-0.370	-2.405	-1.187
C	-0.154	2.725	-0.444	-0.786	-2.749	-0.472	-1.071	-2.264	-1.072	-2.252	-1.032	-1.072
C	1.045	2.936	-2.961	-0.404	-2.962	-3.205	-2.012	-1.030	-2.006	-1.025	-3.313	-2.006
H	1.200	0.777	-2.803	0.575	-1.047	-2.943	-0.907	0.665	-0.911	0.661	-2.531	-0.911
C	-0.002	4.010	-1.077	-1.270	-3.867	-1.155	-1.893	-2.970	-1.894	-2.972	-1.906	-1.894
C	0.582	4.114	-2.301	-1.072	-3.975	-2.523	-2.357	-2.352	-2.357	-2.352	-3.057	-2.357
H	1.508	2.980	-3.939	-0.247	-3.001	-4.275	-2.369	-0.505	-2.370	-0.506	-4.194	-2.370
H	-0.367	4.885	-0.558	-1.806	-4.631	-0.612	-2.160	-3.991	-2.160	-3.991	-1.682	-2.160
H	0.691	5.082	-2.776	-1.448	-4.842	-3.056	-2.994	-2.900	-2.993	-2.901	-3.746	-2.993
C	-0.771	1.002	1.178	-0.489	-1.163	1.370	0.225	-1.822	0.246	-1.722	0.942	0.246
C	-0.723	2.431	0.788	-0.961	-2.436	0.949	-0.519	-2.756	-0.510	-2.733	0.266	-0.510
C	-1.320	0.649	2.411	-0.633	-0.793	2.711	0.790	-2.219	0.772	-2.220	2.204	0.772
C	-1.272	3.375	1.729	-1.561	-3.272	1.892	-0.671	-4.050	-0.665	-4.045	0.739	-0.665
C	-1.813	1.623	3.259	-1.243	-1.662	3.599	0.603	-3.517	0.606	-3.509	2.668	0.606
H	-1.379	-0.390	2.715	-0.278	0.163	3.078	1.377	-1.536	1.374	-1.540	2.828	1.374
C	-1.794	2.998	2.925	-1.717	-2.910	3.218	-0.125	-4.454	-0.127	-4.452	1.951	-0.127
H	-2.193	3.737	3.610	-2.185	-3.580	3.927	-0.259	-5.466	-0.259	-5.466	2.309	-0.259
N	0.315	1.576	-1.143	-0.101	-1.793	-1.151	-0.719	-0.983	-0.705	-0.995	-1.291	-0.705
F	-2.334	1.284	4.448	-1.389	-1.295	4.879	1.137	-3.893	1.136	-3.894	3.838	1.136
F	-1.261	4.688	1.421	-2.017	-4.489	1.538	-1.367	-4.977	-1.366	-4.978	0.059	-1.366
C	0.401	-2.596	1.600	0.261	2.309	1.646	1.237	1.199	1.238	1.203	2.672	1.238
C	-1.633	-2.505	0.441	2.429	1.858	0.873	2.861	1.396	2.861	1.389	0.993	2.861
C	0.078	-3.802	2.191	0.681	3.456	2.296	2.020	1.887	2.018	1.884	3.593	2.018
H	1.345	-2.102	1.794	-0.782	1.998	1.631	0.243	0.840	0.238	0.837	2.925	0.238
C	-2.012	-3.725	1.013	2.902	3.004	1.511	3.695	2.092	3.693	2.091	1.877	3.693
C	-1.156	-4.371	1.888	2.024	3.803	2.228	3.273	2.332	3.274	2.330	3.177	3.274
H	0.777	-4.279	2.867	-0.041	4.063	2.827	1.650	2.072	1.650	2.073	4.591	1.650
H	-2.971	-4.152	0.762	3.946	3.264	1.431	4.654	2.445	4.653	2.446	1.534	4.653
H	-1.450	-5.317	2.331	2.389	4.699	2.721	3.917	2.875	3.917	2.875	3.862	3.917
C	-1.794	-0.505	-0.952	2.487	-0.115	-0.580	2.036	0.482	1.979	0.441	-1.073	1.979
C	-2.468	0.310	-1.862	3.169	-1.060	-1.350	2.198	0.168	2.192	0.181	-2.439	2.192
C	-2.410	-1.702	-0.504	3.215	0.923	0.057	3.110	1.097	3.089	1.092	-0.413	3.089
C	-3.722	-0.065	-2.312	4.543	-0.959	-1.497	3.392	0.468	3.393	0.468	-3.095	3.393
H	-2.033	1.233	-2.227	2.654	-1.881	-1.836	1.411	-0.308	1.414	-0.307	-3.039	1.414
C	-3.678	-2.025	-0.994	4.597	0.971	-0.125	4.291	1.370	4.279	1.366	-1.097	4.279
C	-4.356	-1.228	-1.896	5.283	0.049	-0.897	4.458	1.070	4.455	1.070	-2.445	4.455
H	-5.336	-1.504	-2.260	6.356	0.113	-1.016	5.386	1.293	5.387	1.292	-2.950	5.387
N	-0.427	-1.963	0.757	1.114	1.524	0.969	1.655	0.944	1.617	0.925	1.413	1.617
F	-4.364	0.723	-3.185	5.191	-1.863	-2.244	3.539	0.171	3.539	0.172	-4.396	3.539

F	-4.299	-3.151	-0.592	5.335	1.933	0.461	5.334	1.943	5.334	1.943	-0.473	5.334
C	2.994	-0.644	-0.256	-2.653	1.846	-0.605	-3.047	2.461	-3.046	2.462	0.249	-3.046
C	2.465	0.716	1.579	-3.951	1.317	1.215	-4.469	4.063	-4.469	4.063	1.045	-4.469
C	4.374	-0.536	0.036	-3.783	1.967	-1.433	-4.103	1.550	-4.104	1.552	0.060	-4.104
C	3.797	0.851	1.921	-5.117	1.414	0.477	-5.571	3.239	-5.571	3.239	0.891	-5.571
H	1.663	1.179	2.143	-3.971	1.055	2.269	-4.578	5.071	-4.578	5.071	1.436	-4.578
C	4.762	0.225	1.144	-5.038	1.749	-0.876	-5.392	1.951	-5.392	1.950	0.384	-5.392
H	4.080	1.444	2.783	-6.080	1.232	0.942	-6.562	3.590	-6.562	3.590	1.159	-6.562
H	5.808	0.332	1.401	-2.741	1.530	0.681	-6.243	1.291	-6.243	1.291	0.253	-6.243
N	2.099	-0.013	0.516	-0.683	0.916	-1.489	-3.224	3.685	-3.224	3.684	0.728	-3.224
O	1.154	-1.291	-1.625	-1.247	2.047	-1.153	-1.139	1.200	-1.120	1.171	0.743	-1.120
C	2.420	-1.462	-1.429	-0.757	3.156	-1.214	-1.650	2.019	-1.637	2.022	-0.114	-1.637
O	3.156	-2.184	-2.076	-5.941	1.828	-1.470	-1.130	2.397	-1.131	2.390	-1.167	-1.131
O	5.239	-1.160	-0.770	-3.538	2.281	-2.724	-3.757	0.344	-3.756	0.343	-0.452	-3.756
C	6.620	-1.050	-0.499	-4.642	2.435	-3.586	-4.771	-0.616	-4.771	-0.615	-0.633	-4.771
H	7.117	-1.629	-1.277	-5.308	3.239	-3.248	-5.526	-0.275	-5.526	-0.275	-1.354	-5.526
H	6.961	-0.009	-0.549	-4.230	2.698	-4.560	-4.276	-1.505	-4.276	-1.505	-1.023	-4.276
H	6.875	-1.471	0.481	-5.217	1.505	-3.676	-5.265	-0.862	-5.265	-0.862	0.316	-5.265

Table S7. Cartesian coordinates for triplet geometry of complex 4.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.151	-0.202	-0.202	0.349	-0.212	-0.097	0.302	-0.010	0.011	0.938	0.252	0.255
C	1.115	1.616	-2.368	0.408	-1.866	-2.584	0.300	-1.776	-2.406	0.296	-1.744	-2.347
C	0.264	2.705	-0.420	-0.661	-2.880	-0.758	1.805	-2.418	-0.720	1.781	-2.392	-0.722
C	1.379	2.834	-2.981	0.143	-2.945	-3.406	0.684	-2.831	-3.215	0.678	-2.809	-3.204
H	1.315	0.669	-2.859	0.917	-0.976	-2.936	-0.487	-1.076	-2.671	-0.482	-1.078	-2.670
C	0.526	3.979	-1.041	-0.948	-4.000	-1.543	2.231	-3.494	-1.501	2.230	-3.478	-1.487
C	1.070	4.043	-2.286	-0.539	-4.033	-2.867	1.673	-3.694	-2.754	1.671	-3.696	-2.755
H	1.805	2.847	-3.976	0.462	-2.927	-4.440	0.211	-2.968	-4.180	0.214	-2.968	-4.181
H	0.275	4.878	-0.497	-1.497	-4.824	-1.112	2.985	-4.165	-1.117	2.986	-4.165	-1.119
H	1.262	5.002	-2.752	-0.763	-4.900	-3.479	2.002	-4.530	-3.363	2.002	-4.530	-3.363
C	-0.479	1.029	1.197	-0.758	-1.360	1.160	1.574	-1.004	1.271	1.122	-0.399	0.641
C	-0.293	2.451	0.826	-1.063	-2.645	0.631	2.243	-2.088	0.643	2.140	-1.988	0.638
C	-1.027	0.714	2.439	-1.114	-1.069	2.481	1.920	-0.636	2.572	1.920	-0.648	2.444
C	-0.709	3.432	1.798	-1.716	-3.568	1.450	3.237	-2.754	1.360	3.171	-2.713	1.365
C	-1.390	1.721	3.317	-1.766	-2.023	3.242	2.909	-1.343	3.237	2.852	-1.343	3.194
H	-1.187	-0.318	2.730	-0.889	-0.110	2.933	1.432	0.192	3.077	1.432	0.184	3.079
C	-1.234	3.091	3.004	-2.082	-3.283	2.753	3.586	-2.405	2.653	3.597	-2.407	2.653
H	-1.532	3.856	3.711	-2.585	-4.021	3.364	4.362	-2.942	3.183	4.364	-2.945	3.181
N	0.586	1.524	-1.151	0.038	-1.846	-1.295	0.864	-1.568	-1.206	0.838	-1.520	-1.122
F	-1.910	1.417	4.515	-2.114	-1.730	4.503	3.236	-0.997	4.489	3.238	-1.000	4.486
F	-0.566	4.741	1.509	-2.016	-4.798	0.990	3.909	-3.782	0.808	3.914	-3.780	0.816
C	0.332	-2.672	1.548	-0.360	2.133	1.650	-1.075	1.380	2.271	-1.057	1.341	2.195
C	-1.712	-2.364	0.445	1.927	1.909	1.185	0.083	2.797	0.795	0.078	2.765	0.805
C	-0.095	-3.847	2.136	-0.152	3.294	2.373	-1.484	2.448	3.048	-1.471	2.437	3.044
H	1.326	-2.276	1.722	-1.349	1.721	1.477	-1.392	0.361	2.461	-1.390	0.360	2.462
C	-2.196	-3.547	1.015	2.192	3.074	1.906	-0.293	3.907	1.555	-0.281	3.891	1.538
C	-1.386	-4.287	1.861	1.149	3.766	2.503	-1.071	3.728	2.689	-1.078	3.721	2.698
H	0.571	-4.399	2.789	-0.996	3.813	2.810	-2.118	2.273	3.909	-2.118	2.277	3.909
H	-3.198	-3.873	0.786	3.207	3.432	1.982	0.012	4.894	1.241	0.012	4.894	1.243
H	-1.762	-5.204	2.301	1.353	4.675	3.058	-1.369	4.588	3.279	-1.369	4.588	3.279
C	-1.712	-0.338	-0.918	2.379	-0.002	-0.282	0.937	1.529	-1.116	0.863	0.865	-0.704
C	-2.327	0.554	-1.796	3.250	-0.855	-0.962	1.599	1.450	-2.348	1.578	1.442	-2.256
C	-2.430	-1.475	-0.468	2.906	1.075	0.476	0.820	2.793	-0.469	0.822	2.639	-0.437
C	-3.625	0.312	-2.215	4.615	-0.627	-0.902	2.130	2.597	-2.910	2.080	2.574	-2.869
H	-1.814	1.436	-2.162	2.888	-1.700	-1.537	1.711	0.509	-2.874	1.696	0.522	-2.879
C	-3.737	-1.663	-0.925	4.289	1.253	0.502	1.386	3.910	-1.083	1.334	3.846	-1.102
C	-4.358	-0.789	-1.796	5.163	0.422	-0.178	2.041	3.842	-2.300	2.058	3.847	-2.303
H	-5.371	-0.962	-2.134	6.232	0.586	-0.137	2.470	4.727	-2.752	2.469	4.730	-2.751
N	-0.449	-1.949	0.733	0.650	1.454	1.085	-0.289	1.552	1.196	-0.245	1.403	1.101
F	-4.209	1.173	-3.058	5.447	-1.443	-1.563	2.758	2.518	-4.091	2.757	2.522	-4.091

F	-4.455	-2.730	-0.520	4.841	2.257	1.210	1.314	5.120	-0.497	1.319	5.121	-0.505
C	3.059	-0.992	-0.356	-2.534	2.076	-1.162	-3.969	-0.765	-0.037	-3.949	-0.759	-0.070
C	2.720	0.366	1.517	-4.178	1.196	0.181	-5.399	-0.530	1.738	-5.392	-0.528	1.738
C	4.433	-1.104	-0.083	-3.432	2.939	-1.812	-4.979	-1.271	-0.874	-4.975	-1.271	-0.868
C	4.061	0.309	1.853	-5.155	1.984	-0.413	-6.470	-1.033	1.009	-6.469	-1.034	1.004
H	1.992	0.916	2.104	-4.424	0.504	0.982	-5.529	-0.218	2.772	-5.529	-0.218	2.770
C	4.911	-0.432	1.044	-4.768	2.861	-1.420	-6.246	-1.409	-0.309	-6.248	-1.410	-0.305
H	4.426	0.834	2.727	-6.190	1.916	-0.094	-7.451	-1.128	1.463	-7.451	-1.128	1.462
N	2.247	-0.272	0.441	-2.899	1.232	-0.192	-4.172	-0.408	1.236	-4.174	-0.415	1.227
O	1.125	-1.405	-1.699	-0.552	0.877	-1.673	-1.650	-0.798	0.334	-1.622	-0.850	0.295
C	2.379	-1.659	-1.563	-1.051	2.069	-1.505	-2.558	-0.556	-0.549	-2.374	-0.423	-0.549
O	3.055	-2.357	-2.305	-0.446	3.123	-1.619	-2.359	-0.173	-1.702	-2.416	-0.236	-1.612
H	5.969	-0.493	1.286	-5.505	3.495	-1.906	-7.058	-1.811	-0.909	-7.058	-1.810	-0.909
C	5.389	-1.896	-0.934	-2.990	3.899	-2.884	-4.736	-1.658	-2.309	-4.735	-1.658	-2.304
H	5.082	-2.941	-0.998	-2.294	4.634	-2.474	-4.523	-0.775	-2.914	-4.521	-0.774	-2.914
H	5.395	-1.528	-1.961	-2.457	3.380	-3.686	-3.868	-2.315	-2.405	-3.868	-2.314	-2.405
H	6.398	-1.835	-0.517	-3.850	4.414	-3.318	-5.610	-2.174	-2.717	-5.609	-2.173	-2.718

Table S8. Cartesian coordinates for triplet geometry of complex 5.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.157	-0.195	-0.208	0.463	0.156	-0.092	0.307	-0.004	0.010	0.407	0.030	0.017
C	1.086	1.645	-2.371	2.071	0.664	-2.555	0.118	-1.553	-2.553	0.118	-1.550	-2.542
C	0.241	2.715	-0.410	3.105	-0.736	-0.980	1.608	-2.444	-0.969	1.605	-2.439	-0.969
C	1.334	2.869	-2.979	3.128	0.539	-3.437	0.406	-2.560	-3.458	0.405	-2.555	-3.457
H	1.291	0.703	-2.870	1.185	1.245	-2.785	-0.623	-0.781	-2.736	-0.622	-0.781	-2.735
C	0.488	3.995	-1.026	4.202	-0.890	-1.831	1.936	-3.477	-1.849	1.937	-3.475	-1.848
C	1.020	4.071	-2.275	4.213	-0.246	-3.059	1.337	-3.528	-3.100	1.337	-3.528	-3.099
H	1.752	2.891	-3.978	3.094	1.043	-4.395	-0.098	-2.579	-4.417	-0.098	-2.579	-4.417
H	0.234	4.889	-0.475	5.024	-1.521	-1.529	2.646	-4.230	-1.544	2.646	-4.230	-1.545
H	1.200	5.035	-2.737	5.063	-0.367	-3.723	1.589	-4.331	-3.785	1.590	-4.331	-3.785
C	-0.473	1.023	1.202	1.624	-1.171	0.924	1.537	-1.190	1.138	1.482	-1.122	1.080
C	-0.302	2.449	0.838	2.895	-1.379	0.321	2.104	-2.264	0.402	2.087	-2.255	0.414
C	-1.011	0.697	2.444	1.362	-1.744	2.173	1.946	-0.960	2.453	1.941	-0.974	2.435
C	-0.717	3.421	1.820	3.834	-2.160	0.995	3.062	-3.061	1.028	3.059	-3.053	1.025
C	-1.376	1.695	3.331	2.333	-2.514	2.791	2.895	-1.792	3.024	2.893	-1.787	3.021
H	-1.160	-0.338	2.731	0.417	-1.595	2.682	1.538	-0.145	3.040	1.540	-0.147	3.041
C	-1.232	3.069	3.027	3.580	-2.741	2.225	3.472	-2.849	2.334	3.469	-2.850	2.334
H	-1.531	3.826	3.742	4.330	-3.340	2.723	4.218	-3.485	2.791	4.218	-3.486	2.791
N	0.568	1.541	-1.152	2.072	0.062	-1.356	0.720	-1.489	-1.355	0.715	-1.483	-1.341
F	-1.886	1.379	4.530	2.071	-3.065	3.984	3.281	-1.578	4.289	3.281	-1.579	4.288
F	-0.585	4.733	1.539	5.053	-2.376	0.463	3.639	-4.085	0.372	3.640	-4.085	0.374
C	0.378	-2.668	1.532	-1.871	-0.890	1.475	-0.847	1.256	2.461	-0.847	1.253	2.447
C	-1.678	-2.377	0.447	-1.689	1.449	1.424	0.324	2.728	1.050	0.328	2.723	1.047
C	-0.033	-3.849	2.120	-3.070	-0.834	2.161	-1.136	2.269	3.355	-1.134	2.265	3.355
H	1.369	-2.262	1.700	-1.435	-1.828	1.151	-1.216	0.243	2.581	-1.216	0.243	2.580
C	-2.146	-3.567	1.017	-2.889	1.561	2.128	0.067	3.784	1.927	0.068	3.782	1.925
C	-1.322	-4.300	1.853	-3.581	0.416	2.492	-0.658	3.549	3.086	-0.658	3.548	3.086
H	0.643	-4.395	2.766	-3.590	-1.752	2.406	-1.729	2.055	4.236	-1.729	2.056	4.236
H	-3.147	-3.902	0.795	-3.278	2.540	2.362	0.424	4.774	1.686	0.423	4.774	1.687
H	-1.685	-5.223	2.294	-4.522	0.502	3.025	-0.862	4.367	3.769	-0.862	4.367	3.769
C	-1.711	-0.345	-0.908	0.240	2.175	0.099	1.001	1.587	-1.007	0.986	1.494	-0.955
C	-2.344	0.545	-1.777	1.088	3.165	-0.403	1.604	1.577	-2.272	1.588	1.589	-2.255
C	-2.414	-1.491	-0.458	-0.857	2.547	0.920	0.997	2.793	-0.248	0.982	2.781	-0.259
C	-3.642	0.291	-2.185	0.836	4.495	-0.106	2.182	2.735	-2.759	2.183	2.730	-2.757
H	-1.843	1.433	-2.143	1.946	2.922	-1.020	1.632	0.681	-2.880	1.632	0.683	-2.880
C	-3.722	-1.692	-0.904	-1.060	3.900	1.184	1.606	3.923	-0.792	1.605	3.914	-0.789
C	-4.360	-0.820	-1.765	-0.233	4.892	0.684	2.201	3.924	-2.041	2.198	3.924	-2.042
H	-5.374	-1.002	-2.095	-0.415	5.934	0.910	2.665	4.818	-2.436	2.666	4.818	-2.435
N	-0.417	-1.951	0.725	-1.198	0.218	1.125	-0.114	1.478	1.358	-0.117	1.461	1.344
F	-4.243	1.150	-3.019	1.647	5.442	-0.596	2.752	2.723	-3.972	2.751	2.723	-3.971

F	-4.425	-2.768	-0.498	-2.085	4.303	1.960	1.638	5.079	-0.101	1.638	5.079	-0.103
C	3.044	-0.986	-0.381	-2.828	-1.648	-1.474	-4.012	-0.664	-0.023	-4.008	-0.664	-0.028
C	2.737	0.368	1.502	-2.884	-3.904	-1.009	-5.368	-1.092	1.784	-5.368	-1.092	1.784
C	4.428	-1.131	-0.110	-4.245	-1.556	-1.496	-5.107	-0.661	-0.924	-5.107	-0.662	-0.923
C	4.088	0.285	1.821	-4.281	-3.928	-1.047	-6.511	-1.120	0.982	-6.511	-1.120	0.982
H	2.025	0.926	2.099	-2.315	-4.808	-0.808	-5.437	-1.251	2.858	-5.437	-1.251	2.858
C	4.932	-0.460	1.023	-4.961	-2.752	-1.289	-6.379	-0.904	-0.374	-6.379	-0.903	-0.374
H	4.468	0.804	2.695	-4.821	-4.855	-0.881	-7.487	-1.305	1.421	-7.487	-1.305	1.421
N	2.255	-0.257	0.427	-2.188	-2.797	-1.220	-4.158	-0.871	1.290	-4.159	-0.871	1.290
O	1.124	-1.386	-1.732	-0.684	-0.634	-1.681	-1.689	-0.657	0.350	-1.669	-0.653	0.352
C	2.379	-1.612	-1.598	-1.968	-0.428	-1.684	-2.610	-0.392	-0.505	-2.598	-0.387	-0.502
O	3.068	-2.269	-2.383	-2.481	0.685	-1.833	-2.404	0.068	-1.641	-2.405	0.067	-1.638
H	5.989	-0.540	1.260	-6.047	-2.732	-1.309	-7.247	-0.919	-1.028	-7.247	-0.919	-1.028
N	5.217	-1.900	-0.894	-4.902	-0.374	-1.662	-4.950	-0.478	-2.273	-4.949	-0.478	-2.273
H	4.775	-2.264	-1.738	-4.317	0.419	-1.905	-4.055	-0.079	-2.536	-4.055	-0.079	-2.536
H	6.215	-1.858	-0.793	-5.869	-0.394	-1.935	-5.764	-0.194	-2.792	-5.764	-0.194	-2.792

Table S9. Cartesian coordinates for triplet geometry of complex 6.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	-0.020	-0.307	-0.195	-0.492	0.158	-0.068	-0.447	0.009	0.074	-0.547	0.037	0.068
C	1.598	1.239	-2.199	-0.062	2.025	-2.367	0.842	1.485	-2.201	0.833	1.484	-2.189
C	0.696	2.504	-0.432	0.887	2.732	-0.343	-0.393	2.831	-0.724	-0.399	2.822	-0.722
C	2.230	2.348	-2.734	0.426	3.128	-3.042	1.196	2.577	-2.974	1.199	2.572	-2.972
H	1.677	0.257	-2.652	-0.626	1.243	-2.863	1.196	0.479	-2.402	1.196	0.479	-2.400
C	1.312	3.651	-0.934	1.396	3.869	-0.973	-0.068	3.962	-1.473	-0.069	3.961	-1.473
C	2.080	3.569	-2.087	1.158	4.069	-2.324	0.725	3.832	-2.604	0.724	3.833	-2.604
H	2.824	2.244	-3.633	0.237	3.239	-4.103	1.833	2.436	-3.839	1.829	2.436	-3.839
H	1.190	4.591	-0.419	1.982	4.575	-0.405	-0.429	4.930	-1.160	-0.429	4.930	-1.160
H	2.562	4.459	-2.476	1.555	4.950	-2.817	0.981	4.711	-3.187	0.981	4.711	-3.186
C	-0.615	1.112	1.112	0.592	1.047	1.412	-1.275	1.531	1.162	-1.236	1.449	1.099
C	-0.131	2.403	0.779	1.097	2.325	1.051	-1.178	2.793	0.518	-1.171	2.779	0.535
C	-1.384	0.936	2.260	0.764	0.590	2.721	-2.004	1.415	2.347	-1.994	1.427	2.333
C	-0.464	3.468	1.618	1.759	3.079	2.021	-1.817	3.885	1.105	-1.816	3.876	1.100
C	-1.671	2.030	3.061	1.436	1.380	3.638	-2.611	2.537	2.886	-2.611	2.533	2.884
H	-1.765	-0.038	2.546	0.384	-0.372	3.043	-2.110	0.464	2.859	-2.109	0.467	2.859
C	-1.226	3.309	2.763	1.945	2.631	3.316	-2.535	3.785	2.285	-2.533	3.785	2.286
H	-1.464	4.155	3.394	2.460	3.240	4.047	-3.021	4.652	2.714	-3.021	4.652	2.713
N	0.855	1.325	-1.087	0.140	1.848	-1.053	0.056	1.610	-1.120	0.069	1.604	-1.114
F	-2.407	1.856	4.163	1.610	0.931	4.888	-3.301	2.426	4.028	-3.302	2.427	4.028
F	-0.043	4.714	1.341	2.248	4.299	1.725	-1.763	5.102	0.532	-1.764	5.102	0.534
C	-0.397	-2.613	1.672	-0.281	-2.403	1.508	-0.457	-1.728	2.507	-0.454	-1.733	2.499
C	-2.293	-2.040	0.405	-2.453	-1.835	0.831	-1.673	-2.576	0.686	-1.682	-2.569	0.682
C	-1.071	-3.638	2.309	-0.721	-3.572	2.103	-0.749	-2.835	3.282	-0.749	-2.826	3.279
H	0.643	-2.381	1.869	0.771	-2.130	1.480	0.172	-0.919	2.858	0.172	-0.920	2.857
C	-3.020	-3.060	1.025	-2.947	-3.001	1.416	-2.004	-3.712	1.430	-2.001	-3.706	1.428
C	-2.406	-3.856	1.979	-2.077	-3.869	2.058	-1.544	-3.837	2.731	-1.545	-3.838	2.731
H	-0.556	-4.248	3.040	-0.005	-4.233	2.575	-0.355	-2.907	4.288	-0.354	-2.907	4.288
H	-4.051	-3.222	0.748	-4.002	-3.221	1.354	-2.604	-4.487	0.977	-2.603	-4.487	0.977
H	-2.967	-4.650	2.459	-2.458	-4.779	2.509	-1.795	-4.719	3.310	-1.795	-4.719	3.310
C	-1.812	-0.182	-1.101	-2.484	0.223	-0.499	-1.439	-1.124	-1.268	-1.408	-1.067	-1.225
C	-2.175	0.726	-2.095	-3.156	1.238	-1.186	-1.711	-0.796	-2.601	-1.711	-0.813	-2.586
C	-2.765	-1.122	-0.632	-3.229	-0.827	0.097	-2.015	-2.299	-0.709	-1.995	-2.294	-0.715
C	-3.459	0.687	-2.615	-4.536	1.192	-1.295	-2.530	-1.620	-3.352	-2.525	-1.613	-3.347
H	-1.477	1.464	-2.473	-2.626	2.070	-1.637	-1.297	0.092	-3.064	-1.298	0.089	-3.065
C	-4.043	-1.112	-1.192	-4.617	-0.818	-0.043	-2.837	-3.086	-1.516	-2.834	-3.076	-1.513
C	-4.415	-0.221	-2.182	-5.293	0.174	-0.735	-3.108	-2.773	-2.836	-3.108	-2.776	-2.835
H	-5.413	-0.237	-2.600	-6.371	0.152	-0.824	-3.751	-3.403	-3.437	-3.751	-3.403	-3.436
N	-0.999	-1.834	0.762	-1.125	-1.552	0.905	-0.925	-1.595	1.256	-0.901	-1.583	1.253
F	-3.803	1.558	-3.570	-5.174	2.162	-1.964	-2.783	-1.306	-4.629	-2.782	-1.307	-4.626

F	-4.976	-1.987	-0.776	-5.371	-1.788	0.507	-3.411	-4.200	-1.024	-3.409	-4.199	-1.026
C	2.825	-1.131	-0.058	2.633	-1.902	-0.814	3.801	-0.921	0.446	3.797	-0.924	0.438
C	2.303	0.068	1.938	4.009	-1.601	1.002	5.201	-1.973	1.924	5.199	-1.973	1.923
C	4.197	-1.089	0.319	3.732	-1.928	-1.673	4.875	-0.223	-0.114	4.879	-0.205	-0.124
C	3.611	0.089	2.339	5.154	-1.617	0.217	6.325	-1.326	1.423	6.326	-1.322	1.418
H	1.521	0.526	2.536	4.074	-1.467	2.079	5.293	-2.684	2.742	5.293	-2.684	2.742
C	4.595	-0.503	1.488	5.012	-1.788	-1.156	6.156	-0.421	0.381	6.146	-0.423	0.385
H	3.890	0.554	3.276	6.134	-1.498	0.664	7.307	-1.518	1.839	7.307	-1.518	1.840
N	1.894	-0.512	0.791	2.781	-1.742	0.504	3.968	-1.773	1.459	3.970	-1.771	1.457
O	0.892	-1.757	-1.225	0.679	-0.839	-1.544	1.583	-0.231	0.763	1.572	-0.233	0.758
C	2.268	-1.744	-1.239	1.191	-2.011	-1.292	2.388	-0.774	-0.081	2.380	-0.766	-0.076
O	2.840	-2.209	-2.215	0.644	-3.093	-1.360	2.116	-1.169	-1.211	2.111	-1.170	-1.203
H	5.644	-0.494	1.759	5.873	-1.807	-1.816	6.995	0.122	-0.040	6.997	0.122	-0.043
Cl	5.415	-1.804	-0.702	3.502	-2.125	-3.388	4.626	0.926	-1.403	4.627	0.904	-1.382

Table S10. Cartesian coordinates for triplet geometry of complex 7.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.141	-0.220	-0.207	0.371	-0.167	-0.100	0.315	0.003	0.031	0.415	0.021	0.029
C	1.184	1.554	-2.372	0.092	-2.037	-2.414	0.030	-1.746	-2.387	0.030	-1.743	-2.375
C	0.413	2.679	-0.411	-1.030	-2.714	-0.467	1.537	-2.540	-0.768	1.536	-2.536	-0.765
C	1.509	2.759	-2.983	-0.354	-3.141	-3.116	0.270	-2.833	-3.210	0.270	-2.829	-3.209
H	1.326	0.600	-2.870	0.705	-1.266	-2.866	-0.694	-0.971	-2.620	-0.694	-0.971	-2.620
C	0.740	3.940	-1.030	-1.500	-3.851	-1.128	1.818	-3.651	-1.564	1.819	-3.649	-1.563
C	1.274	3.979	-2.280	-1.155	-4.066	-2.453	1.187	-3.792	-2.792	1.186	-3.791	-2.792
H	1.926	2.753	-3.982	-0.079	-3.265	-4.156	-0.257	-2.919	-4.151	-0.257	-2.919	-4.152
H	0.544	4.849	-0.479	-2.139	-4.545	-0.603	2.518	-4.394	-1.213	2.518	-4.394	-1.214
H	1.515	4.929	-2.743	-1.521	-4.947	-2.970	1.403	-4.655	-3.412	1.403	-4.655	-3.412
C	-0.408	1.037	1.204	-0.836	-1.022	1.292	1.546	-1.112	1.227	1.493	-1.044	1.171
C	-0.147	2.450	0.837	-1.340	-2.293	0.902	2.070	-2.257	0.572	2.054	-2.249	0.581
C	-0.961	0.749	2.449	-1.101	-0.551	2.582	1.994	-0.781	2.508	1.990	-0.797	2.492
C	-0.499	3.448	1.818	-2.090	-3.025	1.823	3.026	-3.022	1.242	3.022	-3.015	1.239
C	-1.259	1.770	3.335	-1.858	-1.320	3.449	2.939	-1.584	3.126	2.937	-1.579	3.123
H	-1.177	-0.275	2.738	-0.727	0.406	2.926	1.622	0.092	3.032	1.622	0.090	3.032
C	-1.031	3.131	3.027	-2.367	-2.564	3.097	3.473	-2.710	2.515	3.471	-2.711	2.515
H	-1.279	3.907	3.741	-2.950	-3.156	3.790	4.216	-3.323	3.008	4.217	-3.323	3.007
N	0.663	1.486	-1.152	-0.217	-1.845	-1.123	0.664	-1.599	-1.212	0.658	-1.588	-1.204
F	-1.784	1.489	4.536	-2.119	-0.857	4.679	3.362	-1.273	4.358	3.362	-1.273	4.357
F	-0.285	4.748	1.533	-2.580	-4.237	1.496	3.562	-4.113	0.663	3.563	-4.112	0.664
C	0.202	-2.708	1.526	0.088	2.421	1.414	-0.747	1.495	2.394	-0.748	1.491	2.380
C	-1.831	-2.281	0.444	2.296	1.797	0.933	0.372	2.821	0.811	0.375	2.814	0.809
C	-0.282	-3.863	2.109	0.498	3.598	2.013	-1.013	2.590	3.195	-1.010	2.585	3.194
H	1.216	-2.368	1.696	-0.960	2.153	1.305	-1.102	0.498	2.629	-1.101	0.498	2.628
C	-2.373	-3.441	1.008	2.762	2.970	1.529	0.138	3.958	1.588	0.139	3.956	1.587
C	-1.598	-4.231	1.840	1.859	3.871	2.072	-0.550	3.838	2.786	-0.550	3.837	2.785
H	0.358	-4.456	2.750	-0.241	4.284	2.410	-1.576	2.462	4.111	-1.576	2.462	4.111
H	-3.394	-3.712	0.784	3.822	3.170	1.550	0.482	4.920	1.240	0.482	4.920	1.240
H	-2.019	-5.131	2.276	2.219	4.786	2.530	-0.737	4.719	3.391	-0.737	4.719	3.390
C	-1.731	-0.249	-0.906	2.399	-0.288	-0.350	0.991	1.490	-1.147	0.977	1.406	-1.088
C	-2.304	0.683	-1.772	3.104	-1.327	-0.961	1.559	1.358	-2.420	1.545	1.372	-2.406
C	-2.508	-1.347	-0.457	3.111	0.758	0.291	1.008	2.761	-0.506	0.992	2.750	-0.517
C	-3.617	0.516	-2.180	4.490	-1.312	-0.948	2.126	2.462	-3.030	2.126	2.457	-3.027
H	-1.747	1.537	-2.137	2.598	-2.155	-1.445	1.569	0.408	-2.942	1.569	0.410	-2.942
C	-3.827	-1.459	-0.902	4.505	0.717	0.275	1.602	3.834	-1.171	1.602	3.826	-1.167
C	-4.407	-0.546	-1.761	5.217	-0.300	-0.338	2.164	3.714	-2.429	2.161	3.714	-2.430
H	-5.431	-0.659	-2.090	6.299	-0.303	-0.331	2.618	4.565	-2.919	2.618	4.565	-2.919
N	-0.546	-1.937	0.724	0.961	1.541	0.902	-0.051	1.607	1.252	-0.056	1.597	1.243
F	-4.160	1.415	-3.011	5.163	-2.306	-1.542	2.664	2.333	-4.250	2.664	2.333	-4.249

F	-4.599	-2.486	-0.496	5.228	1.683	0.873	1.653	5.050	-0.594	1.653	5.050	-0.595
C	2.990	-1.147	-0.404	-2.421	2.071	-1.232	-4.007	-0.511	0.048	-4.004	-0.510	0.046
C	2.769	0.215	1.488	-3.994	1.553	0.366	-5.561	-0.175	1.702	-5.561	-0.175	1.702
C	4.353	-1.288	-0.133	-3.420	2.549	-2.077	-4.977	-1.101	-0.763	-4.977	-1.101	-0.762
C	4.117	0.103	1.794	-5.042	2.002	-0.429	-6.582	-0.751	0.952	-6.582	-0.751	0.952
H	2.080	0.793	2.096	-4.178	1.146	1.356	-5.762	0.212	2.698	-5.762	0.212	2.698
C	4.926	-0.663	0.967	-4.747	2.515	-1.689	-6.281	-1.234	-0.315	-6.280	-1.234	-0.315
H	4.523	0.609	2.662	-6.065	1.951	-0.075	-7.587	-0.825	1.352	-7.587	-0.825	1.352
N	2.242	-0.395	0.422	-2.720	1.582	-0.027	-4.305	-0.064	1.271	-4.305	-0.065	1.271
O	1.037	-1.468	-1.722	-0.441	0.898	-1.753	-1.700	-0.590	0.449	-1.685	-0.585	0.444
C	2.276	-1.796	-1.603	-0.952	2.091	-1.631	-2.588	-0.313	-0.442	-2.580	-0.311	-0.433
O	2.915	-2.534	-2.331	-0.388	3.153	-1.806	-2.384	0.095	-1.582	-2.380	0.095	-1.578
H	5.987	-0.787	1.152	-5.516	2.879	-2.361	-7.023	-1.704	-0.951	-7.023	-1.704	-0.951
F	5.140	-2.014	-0.912	-3.096	3.020	-3.285	-4.656	-1.574	-1.969	-4.656	-1.574	-1.969

Table S11. Cartesian coordinates for triplet geometry of complex 8.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	-0.461	-0.263	-0.361	1.029	-0.011	-0.069	-0.919	0.000	-0.030	0.809	0.152	-0.056
C	0.741	1.571	-2.413	2.108	0.971	-2.655	-0.076	-1.446	2.469	-1.043	0.913	2.209
C	0.326	2.535	-0.308	3.627	-0.294	-1.380	-1.656	-2.581	1.153	-0.466	2.597	0.728
C	1.302	2.741	-2.892	3.032	1.141	-3.671	-0.056	-2.464	3.407	-1.764	1.786	3.018
H	0.657	0.677	-3.021	1.092	1.353	-2.704	0.561	-0.570	2.531	-0.984	-0.135	2.456
C	0.883	3.738	-0.744	4.597	-0.144	-2.372	-1.675	-3.632	2.072	-1.197	3.542	1.472
C	1.372	3.837	-2.039	4.297	0.582	-3.516	-0.876	-3.568	3.204	-1.850	3.132	2.627
H	1.678	2.780	-3.906	2.757	1.694	-4.560	0.594	-2.385	4.269	-2.293	1.432	3.899
H	0.935	4.578	-0.069	5.565	-0.604	-2.246	-2.305	-4.489	1.888	-1.255	4.572	1.153
H	1.810	4.770	-2.378	5.047	0.699	-4.291	-0.888	-4.385	3.919	-2.423	3.846	3.213
C	-0.669	0.920	1.254	2.545	-1.176	0.636	-2.149	-1.369	-0.923	0.849	1.474	-0.984
C	-0.213	2.243	1.028	3.732	-1.074	-0.140	-2.405	-2.504	-0.109	0.272	2.831	-0.537
C	-1.162	0.556	2.504	2.561	-1.907	1.826	-2.821	-1.224	-2.137	1.535	1.933	-2.277
C	-0.300	3.155	2.081	4.880	-1.719	0.316	-3.328	-3.447	-0.562	0.411	4.114	-1.117
C	-1.212	1.504	3.514	3.732	-2.532	2.225	-3.721	-2.199	-2.538	1.666	3.189	-2.876
H	-1.509	-0.451	2.708	1.679	-1.994	2.451	-2.659	-0.365	-2.779	2.040	1.118	-2.849
C	-0.790	2.812	3.329	4.907	-2.454	1.489	-3.994	-3.320	-1.769	1.109	4.327	-2.302
H	-0.840	3.542	4.125	5.814	-2.943	1.818	-4.705	-4.070	-2.091	1.203	5.314	-2.736
N	0.267	1.481	-1.163	2.414	0.296	-1.536	-0.868	-1.499	1.386	-0.308	1.314	1.120
F	-1.687	1.155	4.713	3.743	-3.240	3.361	-4.358	-2.063	-3.708	2.358	3.375	-4.027
F	0.103	4.426	1.917	6.029	-1.644	-0.381	-3.614	-4.538	0.174	-0.129	5.241	-0.564
C	-0.470	-2.860	1.121	-1.008	-1.526	1.522	-0.491	1.324	-2.674	1.335	-1.517	-2.496
C	-2.584	-2.110	0.418	-1.071	0.804	1.803	-1.465	2.694	-1.033	2.754	-1.882	-0.695
C	-1.011	-3.996	1.695	-2.157	-1.698	2.271	-0.512	2.344	-3.607	2.032	-2.397	-3.332
H	0.592	-2.644	1.128	-0.502	-2.353	1.039	-0.069	0.348	-2.884	0.457	-0.978	-2.887
C	-3.179	-3.238	0.986	-2.230	0.685	2.573	-1.517	3.755	-1.941	3.502	-2.798	-1.468
C	-2.389	-4.179	1.628	-2.775	-0.570	2.802	-1.045	3.574	-3.232	3.142	-3.058	-2.787
H	-0.362	-4.716	2.178	-2.563	-2.692	2.412	-0.115	2.173	-4.600	1.712	-2.594	-4.350
H	-4.249	-3.368	0.915	-2.705	1.574	2.959	-1.913	4.707	-1.623	4.349	-3.313	-1.028
H	-2.848	-5.057	2.068	-3.687	-0.663	3.382	-1.081	4.397	-3.938	3.710	-3.768	-3.379
C	-2.402	-0.006	-0.811	0.610	1.914	0.410	-1.576	1.526	1.115	1.791	-0.533	1.074
C	-2.952	1.059	-1.525	1.283	3.052	-0.039	-1.906	1.472	2.474	2.118	-0.308	2.541
C	-3.250	-1.031	-0.315	-0.410	2.045	1.390	-1.854	2.712	0.378	2.933	-1.511	0.691
C	-4.319	1.092	-1.750	0.939	4.292	0.475	-2.491	2.572	3.077	3.173	-0.781	3.335
H	-2.334	1.863	-1.909	2.071	2.993	-0.781	-1.718	0.588	3.072	1.414	0.360	3.079
C	-4.618	-0.942	-0.570	-0.710	3.319	1.870	-2.451	3.784	1.041	3.991	-1.978	1.484
C	-5.175	0.104	-1.284	-0.053	4.456	1.431	-2.777	3.743	2.385	4.155	-1.620	2.826
H	-6.241	0.146	-1.468	-0.306	5.431	1.826	-3.240	4.590	2.872	4.980	-1.984	3.420
N	-1.239	-1.945	0.516	-0.477	-0.313	1.304	-0.977	1.491	-1.434	1.716	-1.172	-1.277

F	-4.844	2.110	-2.438	1.583	5.382	0.040	-2.799	2.519	4.379	3.297	-0.416	4.629
F	-5.459	-1.890	-0.121	-1.664	3.489	2.805	-2.741	4.920	0.379	4.971	-2.797	0.998
C	2.311	-1.128	-0.914	-2.620	-1.216	-1.431	3.432	-0.250	-0.614	-3.159	-2.003	-0.546
C	2.316	-0.158	1.240	-3.695	-3.157	-0.896	4.700	-0.792	-2.431	-4.298	-3.490	-1.875
C	3.706	-1.174	-0.913	-3.798	-0.477	-1.329	4.562	-0.040	0.175	-4.362	-1.361	-0.196
C	3.677	-0.201	1.301	-4.917	-2.511	-0.739	5.890	-0.618	-1.731	-5.532	-2.935	-1.562
C	4.411	-0.724	0.179	-3.625	-4.232	-0.748	4.723	-1.087	-3.478	-4.233	-4.345	-2.546
H	4.197	-1.575	-1.792	-4.960	-1.138	-0.956	5.811	-0.232	-0.398	-5.559	-1.840	-0.707
H	4.191	0.159	2.184	-3.770	0.588	-1.525	4.434	0.274	1.204	-6.444	-3.341	-1.982
N	1.601	-0.615	0.177	-5.806	-3.064	-0.459	6.847	-0.771	-2.216	-3.140	-3.036	-1.399
O	0.187	-1.510	-1.813	-2.561	-2.532	-1.212	3.492	-0.617	-1.897	-1.013	-0.870	-0.870
C	1.520	-1.580	-2.046	-0.250	-1.110	-1.417	1.074	-0.351	-0.728	-1.802	-1.516	0.002
O	1.956	-1.985	-3.112	-1.329	-0.454	-1.689	2.069	-0.037	0.023	-1.549	-1.842	1.170
H	1.733	0.242	2.064	-1.396	0.722	-2.040	2.013	0.407	1.169	-6.495	-1.359	-0.446
C	5.897	-0.746	0.232	-6.229	-0.364	-0.717	7.059	-0.074	0.431	-4.353	-0.172	0.731
F	6.355	-1.462	1.284	-7.320	-1.129	-0.882	6.926	0.896	1.347	-5.555	0.446	0.744
F	6.415	0.495	0.384	-6.265	0.111	0.541	7.345	-1.209	1.091	-3.449	0.747	0.350
F	6.448	-1.270	-0.875	-6.337	0.686	-1.542	8.125	0.225	-0.328	-4.077	-0.502	2.000

Table S12. Cartesian coordinates for triplet geometry of complex 9.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.062	-0.230	-0.277	0.487	0.066	-0.109	0.374	0.000	0.009	0.474	0.013	0.007
C	1.001	1.601	-2.443	2.099	-0.370	-2.582	-0.117	-1.503	-2.547	-0.117	-1.500	-2.535
C	0.533	2.648	-0.347	2.462	-1.948	-0.881	1.302	-2.586	-1.020	1.300	-2.582	-1.018
C	1.353	2.816	-3.015	2.985	-1.006	-3.431	0.004	-2.534	-3.462	0.004	-2.530	-3.461
H	1.015	0.673	-3.006	1.538	0.510	-2.874	-0.759	-0.642	-2.703	-0.759	-0.642	-2.702
C	0.891	3.919	-0.925	3.372	-2.625	-1.698	1.459	-3.650	-1.911	1.460	-3.647	-1.909
C	1.291	4.002	-2.221	3.636	-2.148	-2.972	0.813	-3.618	-3.138	0.812	-3.617	-3.138
H	1.661	2.846	-4.053	3.153	-0.614	-4.427	-0.532	-2.482	-4.402	-0.532	-2.482	-4.402
H	0.826	4.802	-0.305	3.851	-3.520	-1.331	2.077	-4.490	-1.633	2.077	-4.490	-1.633
H	1.555	4.960	-2.654	4.340	-2.673	-3.609	0.933	-4.443	-3.832	0.933	-4.443	-3.832
C	-0.237	0.968	1.252	0.979	-1.539	1.027	1.494	-1.336	1.082	1.446	-1.258	1.031
C	0.094	2.378	0.942	2.023	-2.328	0.463	1.876	-2.476	0.328	1.861	-2.467	0.337
C	-0.677	0.636	2.532	0.527	-1.839	2.318	1.993	-1.163	2.374	1.987	-1.177	2.357
C	-0.071	3.330	2.011	2.546	-3.381	1.215	2.747	-3.395	0.915	2.745	-3.387	0.912
C	-0.798	1.614	3.503	1.083	-2.900	3.012	2.848	-2.114	2.907	2.846	-2.108	2.904
H	-0.941	-0.386	2.782	-0.247	-1.254	2.801	1.729	-0.299	2.975	1.729	-0.301	2.975
C	-0.496	2.973	3.252	2.094	-3.692	2.485	3.244	-3.239	2.198	3.241	-3.240	2.198
H	-0.605	3.715	4.032	2.522	-4.513	3.043	3.918	-3.970	2.624	3.918	-3.970	2.624
N	0.608	1.491	-1.177	1.864	-0.817	-1.339	0.530	-1.523	-1.371	0.528	-1.515	-1.361
F	-1.213	1.292	4.738	0.635	-3.183	4.243	3.319	-1.952	4.150	3.320	-1.952	4.149
F	0.214	4.628	1.782	3.538	-4.146	0.721	3.150	-4.489	0.240	3.151	-4.489	0.242
C	0.122	-2.821	1.297	-2.010	0.273	1.556	-0.443	1.376	2.532	-0.444	1.374	2.517
C	-1.974	-2.198	0.458	-0.835	2.284	1.291	0.779	2.710	1.032	0.782	2.703	1.029
C	-0.381	-3.978	1.860	-3.027	0.896	2.254	-0.551	2.413	3.440	-0.549	2.408	3.439
H	1.170	-2.558	1.377	-2.034	-0.785	1.318	-0.907	0.409	2.687	-0.907	0.409	2.686
C	-2.537	-3.354	1.009	-1.833	2.961	1.996	0.706	3.786	1.920	0.707	3.784	1.918
C	-1.739	-4.243	1.710	-2.931	2.265	2.476	0.045	3.632	3.129	0.045	3.632	3.128
H	0.278	-4.650	2.397	-3.875	0.317	2.600	-1.096	2.263	4.364	-1.096	2.263	4.364
H	-3.591	-3.544	0.878	-1.745	4.027	2.145	1.153	4.730	1.648	1.153	4.730	1.649
H	-2.176	-5.140	2.136	-3.711	2.793	3.014	-0.016	4.466	3.820	-0.016	4.466	3.820
C	-1.868	-0.096	-0.781	1.176	1.999	-0.077	1.189	1.503	-1.057	1.167	1.411	-1.006
C	-2.460	0.922	-1.531	2.354	2.476	-0.653	1.707	1.426	-2.356	1.696	1.441	-2.339
C	-2.671	-1.168	-0.314	0.372	2.871	0.699	1.368	2.701	-0.307	1.349	2.693	-0.318
C	-3.815	0.866	-1.807	2.712	3.802	-0.472	2.379	2.513	-2.887	2.379	2.508	-2.884
H	-1.882	1.759	-1.904	3.001	1.835	-1.242	1.598	0.533	-2.960	1.598	0.535	-2.959
C	-4.033	-1.167	-0.623	0.784	4.195	0.847	2.062	3.758	-0.896	2.061	3.749	-0.893
C	-4.631	-0.167	-1.366	1.944	4.685	0.273	2.574	3.693	-2.180	2.572	3.693	-2.181
H	-5.688	-0.195	-1.591	2.238	5.718	0.409	3.109	4.530	-2.610	3.109	4.530	-2.609
N	-0.647	-1.954	0.623	-0.944	0.944	1.095	0.227	1.517	1.376	0.220	1.505	1.368
F	-4.375	1.846	-2.526	3.840	4.260	-1.031	2.868	2.437	-4.132	2.868	2.437	-4.131

F	-4.831	-2.166	-0.196	0.058	5.064	1.577	2.265	4.903	-0.217	2.265	4.903	-0.219
C	2.795	-1.333	-0.812	-3.095	-0.614	-1.396	-4.005	-0.265	0.081	-4.002	-0.265	0.078
C	2.909	-0.099	1.143	-3.659	-2.687	-0.643	-5.459	-0.672	1.778	-5.459	-0.672	1.778
C	4.141	-1.637	-0.754	-4.424	-0.262	-1.595	-5.030	-0.151	-0.850	-5.030	-0.151	-0.850
C	4.263	-0.351	1.275	-5.019	-2.449	-0.817	-6.564	-0.588	0.937	-6.564	-0.588	0.937
H	2.368	0.500	1.869	-3.328	-3.647	-0.253	-5.608	-0.875	2.837	-5.608	-0.875	2.837
C	4.897	-1.137	0.307	-5.410	-1.203	-1.307	-6.342	-0.320	-0.413	-6.341	-0.320	-0.413
H	4.576	-2.250	-1.534	-4.673	0.727	-1.960	-4.802	0.071	-1.884	-4.802	0.071	-1.884
H	4.809	0.062	2.118	-5.748	-3.217	-0.574	-7.567	-0.727	1.331	-7.567	-0.727	1.331
N	2.188	-0.580	0.124	-2.702	-1.805	-0.923	-4.198	-0.520	1.381	-4.198	-0.520	1.381
O	0.707	-1.447	-1.954	-0.807	-0.022	-1.767	-1.676	-0.370	0.455	-1.657	-0.365	0.449
C	1.932	-1.842	-1.973	-2.027	0.432	-1.690	-2.581	-0.079	-0.414	-2.572	-0.079	-0.404
O	2.470	-2.550	-2.810	-2.363	1.596	-1.844	-2.387	0.324	-1.561	-2.383	0.323	-1.558
O	6.205	-1.439	0.348	-6.700	-0.858	-1.510	-7.337	-0.214	-1.322	-7.337	-0.214	-1.322
H	6.618	-1.030	1.115	-7.271	-1.600	-1.290	-8.184	-0.348	-0.889	-8.184	-0.348	-0.889

Table S13. Cartesian coordinates for triplet geometry of complex 10.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	-0.108	-0.210	-0.309	0.672	0.021	-0.109	0.574	-0.001	0.010	0.674	0.009	0.005
C	0.592	1.701	-2.495	2.102	-0.612	-2.650	-0.028	-1.513	-2.517	-0.027	-1.509	-2.506
C	0.192	2.691	-0.358	2.366	-2.210	-0.949	1.412	-2.615	-1.025	1.411	-2.611	-1.022
C	0.839	2.942	-3.067	2.869	-1.351	-3.532	0.043	-2.553	-3.427	0.044	-2.549	-3.426
H	0.627	0.783	-3.073	1.631	0.324	-2.925	-0.656	-0.639	-2.661	-0.656	-0.639	-2.660
C	0.440	3.988	-0.934	3.152	-2.991	-1.799	1.519	-3.689	-1.911	1.521	-3.686	-1.909
C	0.756	4.111	-2.251	3.408	-2.556	-3.090	0.837	-3.652	-3.119	0.837	-3.651	-3.118
H	1.082	3.003	-4.120	3.032	-0.987	-4.539	-0.520	-2.496	-4.351	-0.519	-2.496	-4.351
H	0.363	4.857	-0.297	3.544	-3.933	-1.445	2.127	-4.540	-1.645	2.127	-4.540	-1.645
H	0.938	5.089	-2.683	4.016	-3.162	-3.753	0.919	-4.485	-3.809	0.919	-4.485	-3.809
C	-0.382	0.948	1.256	1.030	-1.623	1.021	1.694	-1.354	1.061	1.647	-1.277	1.011
C	-0.151	2.378	0.950	1.950	-2.530	0.419	2.029	-2.508	0.305	2.014	-2.498	0.315
C	-0.722	0.574	2.555	0.607	-1.863	2.334	2.234	-1.183	2.336	2.227	-1.196	2.320
C	-0.305	3.305	2.043	2.385	-3.630	1.157	2.896	-3.441	0.873	2.894	-3.434	0.870
C	-0.839	1.530	3.548	1.070	-2.976	3.013	3.084	-2.148	2.851	3.082	-2.143	2.849
H	-0.911	-0.465	2.803	-0.072	-1.191	2.845	2.007	-0.309	2.938	2.007	-0.311	2.938
C	-0.632	2.907	3.301	1.960	-3.881	2.450	3.433	-3.287	2.140	3.431	-3.288	2.141
H	-0.735	3.632	4.099	2.318	-4.742	2.997	4.104	-4.030	2.552	4.104	-4.030	2.552
N	0.283	1.551	-1.211	1.879	-1.021	-1.392	0.654	-1.538	-1.361	0.651	-1.529	-1.351
F	-1.159	1.168	4.800	0.651	-3.200	4.266	3.594	-1.988	4.079	3.594	-1.989	4.078
F	-0.109	4.620	1.820	3.260	-4.506	0.627	3.255	-4.549	0.196	3.256	-4.549	0.197
C	0.197	-2.814	1.216	-1.702	0.523	1.668	-0.141	1.417	2.540	-0.143	1.414	2.526
C	-1.979	-2.303	0.515	-0.318	2.384	1.327	1.078	2.705	0.998	1.080	2.698	0.996
C	-0.203	-4.005	1.788	-2.606	1.263	2.407	-0.197	2.463	3.442	-0.195	2.458	3.441
H	1.231	-2.490	1.237	-1.860	-0.525	1.442	-0.629	0.464	2.715	-0.628	0.464	2.714
C	-2.439	-3.498	1.079	-1.195	3.176	2.071	1.057	3.789	1.879	1.058	3.787	1.877
C	-1.550	-4.347	1.716	-2.341	2.613	2.610	0.424	3.663	3.105	0.424	3.662	3.105
H	0.525	-4.644	2.273	-3.497	0.788	2.798	-0.722	2.335	4.381	-0.722	2.336	4.381
H	-3.487	-3.748	1.008	-0.979	4.225	2.206	1.522	4.719	1.587	1.522	4.719	1.588
H	-1.908	-5.275	2.152	-3.029	3.230	3.179	0.403	4.504	3.791	0.403	4.504	3.790
C	-2.070	-0.183	-0.694	1.579	1.862	-0.132	1.397	1.471	-1.091	1.373	1.382	-1.038
C	-2.763	0.808	-1.390	2.774	2.198	-0.769	1.877	1.371	-2.403	1.866	1.386	-2.387
C	-2.780	-1.306	-0.197	0.919	2.825	0.672	1.630	2.670	-0.356	1.611	2.661	-0.366
C	-4.128	0.677	-1.585	3.291	3.476	-0.619	2.563	2.434	-2.961	2.563	2.430	-2.959
H	-2.259	1.683	-1.784	3.315	1.484	-1.380	1.726	0.477	-2.997	1.726	0.479	-2.996
C	-4.156	-1.381	-0.424	1.486	4.094	0.786	2.336	3.702	-0.972	2.335	3.694	-0.969
C	-4.854	-0.408	-1.113	2.666	4.445	0.152	2.811	3.614	-2.269	2.808	3.614	-2.270
H	-5.920	-0.494	-1.275	3.082	5.437	0.262	3.356	4.432	-2.720	3.356	4.432	-2.719
N	-0.660	-1.985	0.604	-0.589	1.065	1.150	0.502	1.530	1.367	0.495	1.519	1.359
F	-4.786	1.632	-2.253	4.435	3.798	-1.236	3.014	2.336	-4.219	3.014	2.337	-4.218

F	-4.868	-2.430	0.034	0.901	5.045	1.540	2.590	4.846	-0.308	2.590	4.846	-0.310
C	2.646	-1.145	-1.024	-3.028	-0.223	-1.227	-3.804	-0.170	0.223	-3.802	-0.170	0.220
C	2.806	0.065	0.941	-3.820	-2.196	-0.418	-5.208	-0.521	1.972	-5.208	-0.521	1.971
C	4.006	-1.368	-1.046	-4.307	0.287	-1.383	-4.858	-0.050	-0.670	-4.858	-0.050	-0.670
C	4.180	-0.106	0.995	-5.149	-1.795	-0.546	-6.345	-0.429	1.169	-6.345	-0.429	1.169
C	4.800	-0.841	-0.023	-3.599	-3.185	-0.023	-5.327	-0.705	3.038	-5.327	-0.705	3.038
H	4.431	-1.943	-1.860	-5.398	-0.516	-1.044	-6.163	-0.187	-0.192	-6.162	-0.187	-0.192
H	4.734	0.331	1.816	-4.446	1.294	-1.756	-4.663	0.150	-1.716	-4.663	0.150	-1.716
N	2.053	-0.441	-0.038	-5.944	-2.473	-0.259	-7.326	-0.545	1.614	-7.326	-0.545	1.614
O	0.502	-1.364	-2.040	-2.770	-1.450	-0.747	-3.959	-0.401	1.535	-3.959	-0.401	1.535
C	1.745	-1.687	-2.140	-0.702	0.067	-1.701	-1.467	-0.320	0.521	-1.449	-0.316	0.515
O	2.270	-2.349	-3.020	-1.850	0.675	-1.579	-2.395	-0.020	-0.321	-2.386	-0.020	-0.313
H	2.276	0.620	1.710	-2.039	1.870	-1.737	-2.230	0.365	-1.479	-2.227	0.364	-1.477
O	6.116	-1.084	-0.097	-6.622	0.021	-1.222	-7.155	-0.069	-1.099	-7.155	-0.069	-1.099
C	6.959	-0.555	0.911	-7.747	-0.772	-0.903	-8.486	-0.198	-0.644	-8.486	-0.198	-0.644
H	7.969	-0.866	0.648	-7.760	-1.042	0.160	-8.734	0.573	0.095	-8.734	0.573	0.095
H	6.910	0.539	0.935	-8.621	-0.160	-1.128	-9.119	-0.071	-1.522	-9.119	-0.071	-1.522
H	6.701	-0.957	1.897	-7.779	-1.685	-1.509	-8.667	-1.188	-0.208	-8.667	-1.188	-0.208

Table S14. Cartesian coordinates for triplet geometry of complex 11.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.060	-0.225	-0.277	0.492	0.076	-0.110	0.378	-0.001	0.009	0.478	0.011	0.006
C	0.965	1.627	-2.439	2.107	-0.252	-2.596	-0.103	-1.519	-2.540	-0.103	-1.517	-2.529
C	0.483	2.661	-0.341	2.569	-1.820	-0.910	1.348	-2.572	-1.021	1.346	-2.567	-1.019
C	1.297	2.849	-3.009	3.022	-0.832	-3.456	0.032	-2.550	-3.455	0.032	-2.546	-3.453
H	0.994	0.700	-3.005	1.496	0.597	-2.877	-0.763	-0.671	-2.692	-0.763	-0.671	-2.692
C	0.820	3.939	-0.915	3.509	-2.439	-1.737	1.519	-3.634	-1.911	1.520	-3.632	-1.910
C	1.217	4.031	-2.212	3.738	-1.939	-3.009	0.864	-3.617	-3.134	0.863	-3.616	-3.134
H	1.602	2.886	-4.047	3.161	-0.424	-4.449	-0.511	-2.510	-4.391	-0.511	-2.510	-4.391
H	0.743	4.818	-0.293	4.039	-3.310	-1.381	2.155	-4.462	-1.636	2.155	-4.462	-1.636
H	1.466	4.995	-2.643	4.466	-2.419	-3.655	0.995	-4.441	-3.827	0.996	-4.441	-3.827
C	-0.261	0.964	1.255	1.078	-1.507	1.011	1.529	-1.314	1.077	1.480	-1.240	1.027
C	0.048	2.380	0.947	2.160	-2.233	0.435	1.929	-2.448	0.322	1.914	-2.439	0.332
C	-0.697	0.624	2.533	0.652	-1.841	2.302	2.033	-1.128	2.366	2.027	-1.142	2.348
C	-0.134	3.328	2.018	2.747	-3.259	1.175	2.821	-3.348	0.905	2.818	-3.341	0.902
C	-0.835	1.599	3.506	1.272	-2.873	2.986	2.910	-2.062	2.894	2.908	-2.057	2.892
H	-0.945	-0.402	2.781	-0.149	-1.303	2.795	1.757	-0.269	2.967	1.757	-0.271	2.967
C	-0.555	2.962	3.257	2.322	-3.603	2.446	3.322	-3.181	2.185	3.320	-3.181	2.186
H	-0.677	3.702	4.039	2.800	-4.403	2.997	4.013	-3.898	2.608	4.014	-3.898	2.608
N	0.576	1.507	-1.174	1.906	-0.720	-1.355	0.553	-1.525	-1.369	0.549	-1.515	-1.359
F	-1.248	1.268	4.738	0.850	-3.189	4.218	3.386	-1.888	4.134	3.386	-1.889	4.133
F	0.131	4.631	1.791	3.777	-3.964	0.670	3.240	-4.436	0.230	3.240	-4.436	0.232
C	0.163	-2.815	1.298	-2.001	0.135	1.575	-0.450	1.367	2.531	-0.452	1.365	2.517
C	-1.943	-2.229	0.455	-0.940	2.209	1.316	0.743	2.717	1.023	0.745	2.711	1.021
C	-0.321	-3.980	1.861	-3.046	0.696	2.285	-0.572	2.403	3.438	-0.569	2.399	3.437
H	1.205	-2.532	1.382	-1.969	-0.921	1.331	-0.899	0.393	2.690	-0.898	0.393	2.690
C	-2.486	-3.396	1.005	-1.968	2.826	2.033	0.656	3.794	1.909	0.657	3.792	1.908
C	-1.674	-4.269	1.708	-3.022	2.067	2.516	0.004	3.631	3.122	0.003	3.631	3.121
H	0.348	-4.639	2.400	-3.857	0.069	2.633	-1.110	2.247	4.364	-1.110	2.247	4.365
H	-3.536	-3.604	0.871	-1.938	3.893	2.190	1.087	4.745	1.634	1.087	4.745	1.634
H	-2.095	-5.174	2.133	-3.825	2.548	3.064	-0.068	4.466	3.811	-0.068	4.466	3.811
C	-1.873	-0.124	-0.781	1.076	2.044	-0.066	1.162	1.513	-1.065	1.140	1.424	-1.011
C	-2.481	0.886	-1.528	2.222	2.589	-0.645	1.675	1.442	-2.367	1.663	1.456	-2.351
C	-2.656	-1.211	-0.317	0.229	2.865	0.720	1.326	2.715	-0.319	1.308	2.705	-0.331
C	-3.835	0.806	-1.806	2.508	3.932	-0.456	2.326	2.538	-2.903	2.326	2.533	-2.901
H	-1.919	1.734	-1.899	2.900	1.989	-1.242	1.577	0.546	-2.969	1.577	0.548	-2.968
C	-4.018	-1.234	-0.629	0.569	4.209	0.876	1.999	3.782	-0.914	1.998	3.774	-0.911
C	-4.633	-0.243	-1.369	1.697	4.766	0.299	2.506	3.723	-2.200	2.503	3.723	-2.200
H	-5.689	-0.289	-1.597	1.935	5.812	0.440	3.024	4.567	-2.634	3.024	4.567	-2.633
N	-0.620	-1.962	0.621	-0.976	0.866	1.110	0.211	1.517	1.373	0.207	1.506	1.363
F	-4.412	1.778	-2.524	3.606	4.454	-1.019	2.809	2.467	-4.151	2.809	2.468	-4.150

F	-4.799	-2.248	-0.205	-0.199	5.032	1.615	2.186	4.932	-0.238	2.187	4.932	-0.240
C	2.805	-1.282	-0.817	-3.066	-0.735	-1.386	-3.995	-0.319	0.122	-3.992	-0.319	0.119
C	2.902	-0.062	1.149	-3.559	-2.826	-0.629	-5.428	-0.726	1.839	-5.428	-0.726	1.838
C	4.160	-1.566	-0.745	-4.414	-0.436	-1.568	-5.044	-0.207	-0.788	-5.043	-0.207	-0.788
C	4.259	-0.307	1.277	-4.926	-2.623	-0.790	-6.540	-0.641	1.006	-6.540	-0.641	1.006
C	4.921	-1.075	0.314	-3.189	-3.774	-0.243	-5.559	-0.927	2.900	-5.559	-0.927	2.900
H	4.584	-2.175	-1.537	-5.380	-1.397	-1.276	-6.356	-0.375	-0.351	-6.355	-0.375	-0.351
H	4.796	0.101	2.127	-4.679	0.552	-1.928	-4.809	0.018	-1.823	-4.809	0.018	-1.823
N	2.190	-0.543	0.121	-5.626	-3.413	-0.534	-7.536	-0.776	1.415	-7.536	-0.776	1.415
O	0.720	-1.426	-1.960	-2.633	-1.912	-0.921	-4.172	-0.573	1.423	-4.172	-0.573	1.422
C	1.952	-1.798	-1.980	-0.802	-0.059	-1.764	-1.661	-0.405	0.468	-1.642	-0.401	0.465
O	2.504	-2.490	-2.821	-2.039	0.348	-1.683	-2.580	-0.127	-0.391	-2.569	-0.125	-0.385
H	2.348	0.521	1.878	-2.418	1.498	-1.838	-2.402	0.271	-1.543	-2.401	0.270	-1.540
C	6.398	-1.337	0.403	-6.845	-1.127	-1.495	-7.516	-0.294	-1.307	-7.516	-0.294	-1.306
H	6.654	-2.305	-0.035	-7.081	-0.073	-1.332	-7.335	0.453	-2.084	-7.335	0.453	-2.084
H	6.949	-0.568	-0.149	-7.127	-1.372	-2.525	-7.668	-1.257	-1.805	-7.668	-1.257	-1.805
H	6.747	-1.317	1.438	-7.467	-1.731	-0.829	-8.444	-0.038	-0.789	-8.444	-0.038	-0.789

Table S15. Cartesian coordinates for triplet geometry of complex 12.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.062	-0.221	-0.278	0.486	0.042	-0.114	0.370	-0.002	0.004	0.470	0.010	0.003
C	0.969	1.622	-2.445	1.985	-0.572	-2.619	-0.050	-1.544	-2.540	-0.050	-1.542	-2.530
C	0.490	2.661	-0.347	2.264	-2.144	-0.897	1.389	-2.567	-0.992	1.389	-2.561	-0.989
C	1.302	2.842	-3.017	2.791	-1.295	-3.478	0.112	-2.579	-3.445	0.112	-2.574	-3.444
H	0.996	0.695	-3.008	1.491	0.346	-2.913	-0.720	-0.706	-2.708	-0.720	-0.706	-2.707
C	0.827	3.937	-0.924	3.091	-2.909	-1.723	1.589	-3.632	-1.871	1.590	-3.631	-1.870
C	1.223	4.027	-2.222	3.358	-2.478	-3.014	0.954	-3.632	-3.104	0.954	-3.632	-3.103
H	1.607	2.877	-4.055	2.963	-0.937	-4.486	-0.417	-2.553	-4.390	-0.417	-2.553	-4.390
H	0.751	4.818	-0.304	3.504	-3.835	-1.352	2.231	-4.450	-1.580	2.231	-4.450	-1.580
H	1.472	4.989	-2.655	3.998	-3.072	-3.658	1.107	-4.459	-3.789	1.107	-4.459	-3.789
C	-0.250	0.969	1.253	0.870	-1.582	1.039	1.517	-1.294	1.102	1.468	-1.224	1.051
C	0.060	2.383	0.944	1.830	-2.464	0.465	1.946	-2.427	0.361	1.931	-2.417	0.372
C	-0.681	0.629	2.535	0.424	-1.824	2.344	1.994	-1.095	2.399	1.988	-1.107	2.381
C	-0.116	3.331	2.014	2.282	-3.545	1.222	2.839	-3.311	0.966	2.836	-3.304	0.962
C	-0.814	1.603	3.507	0.906	-2.917	3.043	2.873	-2.013	2.949	2.871	-2.008	2.946
H	-0.929	-0.397	2.783	-0.288	-1.170	2.833	1.694	-0.236	2.989	1.694	-0.238	2.990
C	-0.532	2.966	3.256	1.836	-3.798	2.507	3.314	-3.130	2.253	3.312	-3.130	2.254
H	-0.649	3.706	4.037	2.208	-4.644	3.070	4.007	-3.835	2.694	4.007	-3.835	2.693
N	0.579	1.506	-1.178	1.750	-0.975	-1.361	0.588	-1.533	-1.359	0.581	-1.522	-1.349
F	-1.221	1.275	4.743	0.466	-3.144	4.288	3.323	-1.827	4.196	3.324	-1.827	4.196
F	0.150	4.633	1.787	3.195	-4.398	0.719	3.285	-4.397	0.304	3.286	-4.397	0.306
C	0.168	-2.809	1.300	-1.935	0.487	1.613	-0.535	1.378	2.493	-0.536	1.376	2.479
C	-1.940	-2.223	0.461	-0.587	2.380	1.305	0.694	2.724	1.010	0.694	2.719	1.009
C	-0.316	-3.974	1.865	-2.862	1.201	2.349	-0.683	2.420	3.390	-0.681	2.416	3.389
H	1.210	-2.526	1.379	-2.070	-0.562	1.371	-0.986	0.404	2.645	-0.986	0.404	2.645
C	-2.482	-3.389	1.014	-1.489	3.147	2.046	0.580	3.806	1.887	0.582	3.804	1.885
C	-1.669	-4.262	1.716	-2.627	2.554	2.569	-0.104	3.648	3.082	-0.104	3.647	3.082
H	0.355	-4.632	2.403	-3.746	0.703	2.727	-1.246	2.267	4.302	-1.246	2.268	4.302
H	-3.533	-3.597	0.884	-1.296	4.198	2.193	1.015	4.757	1.617	1.015	4.757	1.617
H	-2.090	-5.166	2.143	-3.332	3.151	3.139	-0.196	4.486	3.765	-0.196	4.486	3.765
C	-1.872	-0.120	-0.779	1.340	1.907	-0.131	1.168	1.509	-1.061	1.144	1.424	-1.004
C	-2.482	0.887	-1.528	2.535	2.275	-0.753	1.711	1.433	-2.350	1.698	1.446	-2.336
C	-2.655	-1.206	-0.311	0.647	2.853	0.666	1.309	2.717	-0.318	1.294	2.704	-0.331
C	-3.836	0.807	-1.803	3.017	3.564	-0.594	2.370	2.529	-2.877	2.370	2.524	-2.875
H	-1.919	1.734	-1.903	3.101	1.576	-1.359	1.630	0.534	-2.949	1.631	0.536	-2.949
C	-4.018	-1.229	-0.619	1.182	4.135	0.790	1.993	3.782	-0.903	1.992	3.775	-0.899
C	-4.633	-0.240	-1.361	2.360	4.516	0.171	2.529	3.718	-2.176	2.527	3.718	-2.177
H	-5.691	-0.285	-1.586	2.750	5.518	0.288	3.055	4.562	-2.603	3.055	4.562	-2.602
N	-0.617	-1.958	0.625	-0.827	1.057	1.115	0.158	1.523	1.353	0.156	1.515	1.341
F	-4.415	1.778	-2.522	4.160	3.916	-1.198	2.882	2.454	-4.114	2.882	2.455	-4.113

F	-4.798	-2.241	-0.192	0.564	5.069	1.539	2.161	4.937	-0.229	2.162	4.937	-0.230
C	2.803	-1.296	-0.812	-3.174	-0.425	-1.324	-3.999	-0.346	0.071	-3.997	-0.346	0.068
C	2.914	-0.065	1.140	-3.882	-2.395	-0.439	-5.442	-0.709	1.781	-5.442	-0.709	1.781
C	4.148	-1.594	-0.752	-4.471	-0.033	-1.622	-5.030	-0.268	-0.855	-5.030	-0.268	-0.855
C	4.264	-0.310	1.274	-5.214	-2.112	-0.708	-6.549	-0.657	0.945	-6.550	-0.657	0.945
C	4.921	-1.097	0.309	-5.534	-0.893	-1.323	-5.588	-0.880	2.846	-5.588	-0.880	2.846
H	4.562	-2.207	-1.544	-4.629	0.939	-2.077	-6.351	-0.428	-0.422	-6.351	-0.428	-0.422
H	4.805	0.102	2.119	-5.989	-2.827	-0.448	-4.785	-0.077	-1.894	-4.785	-0.077	-1.894
N	2.188	-0.547	0.122	-2.862	-1.588	-0.736	-7.548	-0.794	1.349	-7.548	-0.794	1.349
O	0.718	-1.428	-1.958	-0.858	0.009	-1.727	-4.180	-0.561	1.380	-4.180	-0.561	1.379
C	1.949	-1.808	-1.977	-2.046	0.544	-1.647	-1.668	-0.429	0.430	-1.648	-0.426	0.430
O	2.494	-2.504	-2.820	-2.305	1.723	-1.830	-2.582	-0.160	-0.438	-2.569	-0.157	-0.436
H	2.372	0.532	1.867	-3.622	-3.333	0.047	-2.394	0.225	-1.593	-2.397	0.225	-1.590
N	6.248	-1.394	0.418	-6.831	-0.570	-1.652	-7.405	-0.404	-1.313	-7.405	-0.404	-1.313
H	6.720	-1.790	-0.379	-7.568	-1.061	-1.175	-8.318	-0.212	-0.931	-8.318	-0.212	-0.931
H	6.820	-0.860	1.050	-7.028	0.399	-1.843	-7.233	0.045	-2.198	-7.233	0.045	-2.198

Table S16. Cartesian coordinates for triplet geometry of complex 13.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	-0.079	-0.202	-0.286	0.671	0.082	-0.103	0.573	0.002	0.022	0.673	0.011	0.012
C	0.631	1.736	-2.448	2.301	-0.053	-2.599	-0.133	-1.436	-2.522	-0.132	-1.434	-2.511
C	0.096	2.712	-0.335	2.856	-1.655	-0.974	1.382	-2.572	-1.132	1.381	-2.566	-1.129
C	0.847	2.987	-3.014	3.246	-0.545	-3.480	-0.099	-2.449	-3.465	-0.099	-2.445	-3.464
H	0.729	0.820	-3.022	1.642	0.771	-2.848	-0.770	-0.563	-2.613	-0.770	-0.562	-2.613
C	0.313	4.018	-0.905	3.828	-2.187	-1.824	1.453	-3.618	-2.053	1.454	-3.616	-2.052
C	0.679	4.152	-2.208	4.025	-1.625	-3.076	0.714	-3.551	-3.226	0.714	-3.551	-3.225
H	1.131	3.056	-4.057	3.360	-0.092	-4.456	-0.705	-2.369	-4.359	-0.705	-2.370	-4.359
H	0.171	4.884	-0.275	4.408	-3.038	-1.501	2.077	-4.473	-1.841	2.077	-4.473	-1.841
H	0.838	5.136	-2.635	4.778	-2.039	-3.739	0.767	-4.364	-3.943	0.767	-4.364	-3.942
C	-0.477	0.948	1.259	1.354	-1.504	0.959	1.760	-1.368	0.972	1.709	-1.290	0.927
C	-0.295	2.388	0.956	2.475	-2.142	0.355	2.063	-2.497	0.168	2.050	-2.488	0.179
C	-0.865	0.566	2.539	0.956	-1.907	2.239	2.367	-1.226	2.221	2.360	-1.239	2.204
C	-0.542	3.312	2.037	3.126	-3.157	1.057	2.965	-3.439	0.664	2.962	-3.431	0.661
C	-1.072	1.521	3.521	1.640	-2.924	2.884	3.249	-2.199	2.664	3.247	-2.194	2.662
H	-1.021	-0.479	2.785	0.128	-1.434	2.755	2.168	-0.370	2.857	2.168	-0.373	2.858
C	-0.912	2.905	3.279	2.728	-3.571	2.316	3.567	-3.316	1.905	3.564	-3.316	1.906
H	-1.086	3.627	4.067	3.256	-4.359	2.835	4.262	-4.065	2.261	4.262	-4.065	2.261
N	0.275	1.575	-1.178	2.129	-0.579	-1.377	0.602	-1.491	-1.400	0.599	-1.482	-1.390
F	-1.437	1.149	4.756	1.244	-3.307	4.105	3.822	-2.067	3.867	3.822	-2.068	3.866
F	-0.392	4.633	1.814	4.194	-3.779	0.524	3.294	-4.525	-0.061	3.295	-4.525	-0.059
C	0.262	-2.783	1.271	-1.819	-0.081	1.583	0.002	1.314	2.646	-0.001	1.312	2.632
C	-1.897	-2.369	0.461	-0.911	2.070	1.373	1.055	2.693	1.063	1.057	2.687	1.061
C	-0.115	-3.988	1.832	-2.908	0.388	2.292	-0.032	2.330	3.582	-0.030	2.326	3.581
H	1.279	-2.417	1.343	-1.707	-1.127	1.323	-0.427	0.335	2.829	-0.426	0.335	2.829
C	-2.333	-3.580	1.010	-1.987	2.596	2.090	1.053	3.751	1.975	1.054	3.750	1.973
C	-1.442	-4.387	1.696	-2.988	1.753	2.547	0.514	3.565	3.239	0.514	3.564	3.238
H	0.614	-4.592	2.358	-3.675	-0.303	2.620	-0.480	2.154	4.552	-0.480	2.154	4.552
H	-3.365	-3.874	0.890	-2.037	3.659	2.267	1.459	4.707	1.682	1.459	4.707	1.682
H	-1.781	-5.327	2.121	-3.831	2.163	3.093	0.508	4.385	3.949	0.508	4.385	3.949
C	-2.020	-0.258	-0.759	1.121	2.081	0.004	1.284	1.534	-1.080	1.265	1.446	-1.025
C	-2.721	0.703	-1.488	2.231	2.718	-0.550	1.686	1.487	-2.420	1.676	1.501	-2.404
C	-2.704	-1.409	-0.293	0.213	2.821	0.802	1.517	2.719	-0.325	1.500	2.709	-0.337
C	-4.068	0.513	-1.747	2.421	4.073	-0.327	2.297	2.592	-2.987	2.297	2.587	-2.985
H	-2.237	1.599	-1.860	2.954	2.181	-1.155	1.534	0.605	-3.030	1.534	0.606	-3.030
C	-4.063	-1.543	-0.585	0.455	4.182	0.992	2.144	3.795	-0.953	2.144	3.787	-0.949
C	-4.769	-0.602	-1.309	1.547	4.829	0.439	2.541	3.761	-2.277	2.538	3.761	-2.278
H	-5.822	-0.733	-1.521	1.708	5.886	0.607	3.026	4.612	-2.736	3.026	4.612	-2.736
N	-0.598	-1.995	0.610	-0.848	0.733	1.139	0.552	1.487	1.433	0.545	1.478	1.423
F	-4.734	1.440	-2.448	3.483	4.684	-0.865	2.674	2.544	-4.272	2.674	2.545	-4.271

F	-4.750	-2.622	-0.160	-0.375	4.930	1.742	2.395	4.930	-0.272	2.395	4.930	-0.273
C	2.739	-1.015	-0.879	-2.893	-0.730	-1.364	-3.799	-0.272	0.389	-3.797	-0.271	0.385
C	2.764	0.200	1.095	-3.401	-2.864	-0.738	-5.152	-0.814	2.139	-5.153	-0.815	2.139
C	4.116	-1.184	-0.844	-4.236	-0.352	-1.361	-4.886	-0.078	-0.464	-4.889	-0.079	-0.460
C	4.139	0.083	1.205	-4.767	-2.601	-0.702	-6.309	-0.658	1.381	-6.308	-0.656	1.377
C	4.817	-0.624	0.214	-5.176	-1.312	-1.023	-5.230	-1.105	3.184	-5.230	-1.105	3.184
H	4.587	-1.743	-1.644	-4.500	0.669	-1.606	-6.155	-0.280	0.054	-6.170	-0.278	0.043
H	4.667	0.531	2.038	-5.481	-3.370	-0.434	-4.711	0.225	-1.488	-4.712	0.225	-1.488
N	2.083	-0.340	0.076	-2.474	-1.961	-1.057	-7.290	-0.822	1.812	-7.290	-0.822	1.811
O	0.657	-1.335	-1.990	-0.627	-0.076	-1.765	-3.919	-0.632	1.670	-3.919	-0.631	1.669
C	1.914	-1.597	-2.035	-1.855	0.343	-1.670	-1.450	-0.361	0.616	-1.432	-0.357	0.612
O	2.517	-2.232	-2.887	-2.229	1.499	-1.799	-2.409	-0.052	-0.183	-2.397	-0.051	-0.178
H	2.174	0.731	1.835	-3.037	-3.859	-0.491	-2.298	0.394	-1.325	-2.297	0.393	-1.322
Cl	6.540	-0.802	0.311	-6.871	-0.904	-0.986	-7.558	-0.062	-0.958	-7.539	-0.065	-0.944

Table S17. Cartesian coordinates for triplet geometry of complex 14.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.065	-0.233	-0.275	0.484	0.082	-0.107	0.385	0.002	0.016	0.485	0.014	0.013
C	1.018	1.596	-2.437	2.146	-0.217	-2.567	-0.138	-1.448	-2.565	-0.138	-1.444	-2.553
C	0.552	2.644	-0.342	2.591	-1.792	-0.882	1.293	-2.566	-1.076	1.291	-2.562	-1.073
C	1.380	2.810	-3.008	3.080	-0.784	-3.414	-0.032	-2.462	-3.502	-0.031	-2.458	-3.501
H	1.027	0.669	-3.003	1.533	0.630	-2.854	-0.778	-0.581	-2.699	-0.777	-0.581	-2.698
C	0.921	3.913	-0.917	3.550	-2.398	-1.697	1.436	-3.612	-1.989	1.437	-3.610	-1.986
C	1.325	3.995	-2.213	3.797	-1.888	-2.962	0.776	-3.555	-3.208	0.774	-3.554	-3.208
H	1.688	2.839	-4.045	3.234	-0.368	-4.402	-0.578	-2.389	-4.435	-0.577	-2.389	-4.435
H	0.863	4.796	-0.296	4.081	-3.266	-1.336	2.053	-4.460	-1.734	2.053	-4.460	-1.735
H	1.598	4.952	-2.644	4.540	-2.358	-3.597	0.885	-4.367	-3.918	0.885	-4.367	-3.918
C	-0.239	0.968	1.252	1.065	-1.502	1.015	1.517	-1.356	1.046	1.467	-1.272	0.996
C	0.104	2.376	0.943	2.162	-2.216	0.453	1.885	-2.483	0.266	1.869	-2.473	0.276
C	-0.692	0.641	2.528	0.622	-1.845	2.298	2.037	-1.207	2.334	2.031	-1.222	2.317
C	-0.063	3.331	2.012	2.745	-3.242	1.198	2.760	-3.416	0.824	2.758	-3.408	0.822
C	-0.814	1.621	3.497	1.239	-2.875	2.986	2.896	-2.171	2.837	2.894	-2.165	2.835
H	-0.965	-0.379	2.777	-0.191	-1.315	2.781	1.786	-0.353	2.954	1.787	-0.355	2.954
C	-0.500	2.978	3.249	2.303	-3.595	2.460	3.276	-3.285	2.103	3.273	-3.286	2.103
H	-0.610	3.721	4.028	2.778	-4.394	3.014	3.953	-4.026	2.506	3.953	-4.026	2.506
N	0.624	1.486	-1.173	1.926	-0.695	-1.333	0.522	-1.494	-1.397	0.521	-1.485	-1.387
F	-1.242	1.303	4.727	0.800	-3.200	4.210	3.386	-2.032	4.075	3.386	-2.032	4.074
F	0.233	4.626	1.783	3.789	-3.936	0.705	3.148	-4.499	0.125	3.149	-4.499	0.127
C	0.102	-2.820	1.308	-2.038	0.110	1.538	-0.378	1.318	2.588	-0.380	1.316	2.573
C	-1.986	-2.189	0.452	-0.997	2.196	1.296	0.777	2.699	1.079	0.781	2.691	1.075
C	-0.411	-3.973	1.871	-3.103	0.659	2.226	-0.482	2.337	3.516	-0.480	2.332	3.515
H	1.150	-2.562	1.396	-1.987	-0.946	1.299	-0.815	0.338	2.743	-0.814	0.339	2.741
C	-2.558	-3.342	1.003	-2.046	2.802	1.991	0.706	3.759	1.986	0.707	3.757	1.985
C	-1.770	-4.232	1.712	-3.101	2.031	2.454	0.081	3.573	3.209	0.081	3.573	3.208
H	0.240	-4.645	2.416	-3.913	0.023	2.561	-0.997	2.161	4.452	-0.997	2.161	4.453
H	-3.612	-3.527	0.865	-2.032	3.870	2.147	1.128	4.716	1.719	1.128	4.716	1.719
H	-2.214	-5.125	2.138	-3.921	2.503	2.985	0.022	4.394	3.915	0.022	4.394	3.915
C	-1.862	-0.089	-0.787	1.048	2.055	-0.045	1.160	1.535	-1.039	1.140	1.439	-0.992
C	-2.443	0.932	-1.539	2.200	2.612	-0.599	1.654	1.487	-2.349	1.643	1.503	-2.330
C	-2.672	-1.157	-0.326	0.177	2.866	0.725	1.335	2.723	-0.274	1.314	2.715	-0.283
C	-3.797	0.883	-1.824	2.469	3.958	-0.402	2.296	2.594	-2.875	2.296	2.589	-2.873
H	-1.860	1.768	-1.909	2.898	2.020	-1.182	1.549	0.602	-2.965	1.549	0.603	-2.964
C	-4.032	-1.150	-0.644	0.498	4.213	0.889	1.997	3.802	-0.860	1.997	3.792	-0.857
C	-4.620	-0.147	-1.390	1.633	4.782	0.337	2.484	3.766	-2.154	2.481	3.766	-2.155
H	-5.677	-0.169	-1.623	1.856	5.831	0.484	2.995	4.619	-2.581	2.995	4.619	-2.580
N	-0.658	-1.952	0.624	-1.014	0.853	1.090	0.255	1.491	1.417	0.247	1.477	1.410
F	-4.348	1.867	-2.546	3.572	4.493	-0.940	2.761	2.545	-4.131	2.761	2.546	-4.130

F	-4.837	-2.146	-0.223	-0.294	5.026	1.613	2.193	4.939	-0.167	2.194	4.939	-0.168
C	2.796	-1.341	-0.804	-3.039	-0.753	-1.437	-3.999	-0.293	0.102	-3.996	-0.292	0.099
C	2.907	-0.114	1.162	-3.507	-2.869	-0.720	-5.455	-0.818	1.774	-5.455	-0.818	1.774
C	4.146	-1.650	-0.743	-4.390	-0.447	-1.596	-5.030	-0.114	-0.819	-5.030	-0.114	-0.819
C	4.261	-0.368	1.301	-4.880	-2.683	-0.851	-6.565	-0.676	0.946	-6.565	-0.676	0.946
C	4.869	-1.149	0.325	-5.304	-1.441	-1.300	-5.595	-1.096	2.816	-5.595	-1.096	2.816
H	4.584	-2.261	-1.523	-4.688	0.538	-1.931	-6.322	-0.317	-0.370	-6.321	-0.317	-0.370
H	4.828	0.025	2.135	-5.592	-3.465	-0.615	-4.807	0.176	-1.838	-4.807	0.176	-1.838
N	2.193	-0.592	0.134	-2.596	-1.938	-1.004	-7.574	-0.836	1.305	-7.574	-0.836	1.305
O	0.712	-1.455	-1.952	-0.782	-0.044	-1.791	-4.195	-0.636	1.378	-4.195	-0.636	1.378
C	1.936	-1.847	-1.970	-2.022	0.345	-1.726	-1.668	-0.377	0.474	-1.650	-0.370	0.464
O	2.484	-2.550	-2.805	-2.422	1.488	-1.885	-2.576	-0.074	-0.384	-2.569	-0.075	-0.369
H	2.360	0.481	1.886	-3.123	-3.823	-0.366	-2.394	0.366	-1.520	-2.387	0.365	-1.518
F	6.168	-1.416	0.428	-6.611	-1.204	-1.437	-7.349	-0.163	-1.211	-7.349	-0.163	-1.211

Table S18. Cartesian coordinates for triplet geometry of complex 15.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	-0.242	-0.276	-0.145	-0.691	0.141	-0.076	0.666	0.037	-0.075	-1.017	0.013	-0.015
C	1.328	1.341	-2.135	-0.279	1.167	-2.853	-1.041	0.925	2.243	-0.078	-1.442	2.455
C	0.211	2.581	-0.476	0.075	2.753	-1.162	-0.468	2.623	0.730	-1.653	-2.579	1.149
C	1.883	2.484	-2.683	0.053	2.072	-3.844	-1.778	1.800	3.021	-0.057	-2.461	3.406
H	1.524	0.355	-2.540	-0.538	0.137	-3.069	-0.980	-0.137	2.454	0.561	-0.570	2.530
C	0.744	3.762	-0.995	0.411	3.710	-2.123	-1.198	3.545	1.480	-1.677	-3.629	2.069
C	1.582	3.709	-2.099	0.393	3.368	-3.466	-1.851	3.131	2.632	-0.874	-3.567	3.204
H	2.537	2.402	-3.542	0.047	1.762	-4.881	-2.293	1.430	3.899	0.594	-2.386	4.269
H	0.504	4.705	-0.529	0.694	4.703	-1.809	-1.255	4.572	1.151	-2.305	-4.489	1.888
H	2.001	4.626	-2.501	0.655	4.108	-4.215	-2.423	3.846	3.213	-0.889	-4.385	3.919
C	-1.045	1.131	1.060	-0.152	1.741	1.056	0.850	1.767	-1.156	-2.092	-1.281	-0.877
C	-0.671	2.449	0.694	0.105	2.914	0.295	0.258	2.889	-0.521	-2.388	-2.492	-0.120
C	-1.858	0.927	2.173	-0.128	1.816	2.452	1.568	1.942	-2.341	-2.814	-1.241	-2.121
C	-1.152	3.509	1.464	0.381	4.102	0.973	0.407	4.141	-1.119	-3.325	-3.439	-0.560
C	-2.294	2.020	2.906	0.158	3.022	3.068	1.678	3.210	-2.890	-3.719	-2.192	-2.536
H	-2.160	-0.066	2.483	-0.331	0.950	3.072	2.047	1.110	-2.845	-2.659	-0.367	-2.778
C	-1.959	3.323	2.573	0.418	4.184	2.353	1.107	4.327	-2.300	-3.992	-3.321	-1.769
H	-2.313	4.167	3.150	0.631	5.121	2.850	1.205	5.313	-2.736	-4.705	-4.070	-2.091
N	0.517	1.398	-1.068	-0.292	1.506	-1.555	-0.394	1.329	1.139	-0.871	-1.491	1.377
F	-3.072	1.819	3.975	0.192	3.083	4.406	2.359	3.375	-4.031	-4.358	-2.064	-3.707
F	-0.837	4.778	1.152	0.624	5.238	0.291	-0.131	5.240	-0.558	-3.615	-4.538	0.172
C	-0.499	-2.527	1.808	-0.178	-1.592	2.333	1.346	-1.511	-2.541	-0.487	1.323	-2.660
C	-2.367	-2.197	0.419	-2.260	-1.921	1.307	2.771	-1.894	-0.716	-1.470	2.685	-1.028
C	-1.107	-3.584	2.458	-0.424	-2.585	3.264	2.037	-2.409	-3.333	-0.515	2.339	-3.606
H	0.502	-2.189	2.047	0.759	-1.042	2.298	0.466	-0.984	-2.889	-0.070	0.349	-2.882
C	-3.027	-3.256	1.050	-2.559	-2.929	2.224	3.508	-2.806	-1.475	-1.517	3.752	-1.939
C	-2.395	-3.945	2.071	-1.638	-3.259	3.207	3.142	-3.058	-2.788	-1.045	3.575	-3.231
H	-0.578	-4.110	3.243	0.329	-2.825	4.004	1.710	-2.594	-4.349	-0.115	2.173	-4.601
H	-4.021	-3.528	0.728	-3.501	-3.451	2.152	4.348	-3.314	-1.027	-1.913	4.707	-1.623
H	-2.904	-4.769	2.560	-1.866	-4.047	3.917	3.710	-3.768	-3.380	-1.081	4.397	-3.938
C	-1.981	-0.369	-1.149	-2.535	-0.506	-0.676	1.997	-0.678	1.262	-1.562	1.426	1.069
C	-2.372	0.454	-2.205	-3.288	-0.009	-1.742	2.124	-0.298	2.603	-1.898	1.490	2.452
C	-2.865	-1.376	-0.684	-3.107	-1.470	0.195	2.973	-1.543	0.691	-1.830	2.706	0.383
C	-3.614	0.267	-2.789	-4.576	-0.479	-1.945	3.186	-0.776	3.350	-2.491	2.568	3.075
H	-1.726	1.239	-2.582	-2.895	0.742	-2.418	1.411	0.367	3.076	-1.718	0.589	3.070
C	-4.105	-1.516	-1.310	-4.408	-1.902	-0.058	4.023	-1.987	1.494	-2.451	3.774	1.039
C	-4.502	-0.710	-2.361	-5.161	-1.427	-1.119	4.152	-1.623	2.823	-2.774	3.743	2.386
H	-5.469	-0.842	-2.829	-6.169	-1.781	-1.287	4.979	-1.983	3.421	-3.240	4.591	2.872
N	-1.120	-1.850	0.831	-1.075	-1.260	1.392	1.717	-1.247	-1.279	-0.967	1.475	-1.429
F	-3.984	1.056	-3.803	-5.291	-0.006	-2.974	3.298	-0.415	4.635	-2.799	2.519	4.378

F	-4.973	-2.458	-0.900	-4.999	-2.810	0.740	4.972	-2.799	0.991	-2.741	4.919	0.381
C	2.663	-0.773	0.152	2.843	-1.129	0.187	-3.169	-1.998	-0.563	3.428	-0.249	-0.612
C	1.918	0.412	2.075	3.636	0.375	1.734	-4.298	-3.491	-1.874	4.700	-0.792	-2.431
C	4.020	-0.540	0.558	4.128	-1.327	-0.332	-4.361	-1.360	-0.192	4.562	-0.040	0.175
C	3.199	0.600	2.532	4.941	0.255	1.276	-5.532	-2.935	-1.562	5.890	-0.618	-1.732
H	1.061	0.796	2.622	3.391	1.041	2.558	-4.233	-4.345	-2.546	4.723	-1.087	-3.478
C	4.272	0.124	1.726	5.187	-0.618	0.223	-5.559	-1.840	-0.707	5.810	-0.232	-0.398
H	3.381	1.121	3.463	5.741	0.829	1.729	-6.444	-3.341	-1.982	4.434	0.274	1.204
N	1.635	-0.239	0.937	2.612	-0.295	1.205	-3.137	-3.036	-1.398	6.847	-0.771	-2.216
O	0.862	-1.668	-1.059	0.828	-1.016	-1.020	-1.105	-0.916	-0.849	3.492	-0.617	-1.896
C	2.228	-1.503	-1.009	1.598	-1.826	-0.353	-1.830	-1.558	-0.004	1.058	-0.342	-0.712
O	2.899	-1.953	-1.929	1.416	-3.005	-0.123	-1.552	-1.831	1.159	2.062	-0.041	0.002
H	5.296	0.293	2.033	6.188	-0.745	-0.172	-6.495	-1.359	-0.446	2.001	0.407	1.170
C	5.188	-0.998	-0.280	4.376	-2.300	-1.456	-4.357	-0.170	0.732	7.058	-0.074	0.431
F	6.363	-0.667	0.304	5.580	-2.086	-2.023	-5.554	0.446	0.743	6.926	0.896	1.347
F	5.196	-0.420	-1.490	3.457	-2.186	-2.425	-3.448	0.746	0.351	7.346	-1.209	1.091
F	5.213	-2.325	-0.446	4.363	-3.568	-1.030	-4.076	-0.502	2.000	8.126	0.225	-0.328

Table S19. Cartesian coordinates for triplet geometry of complex 16.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	-0.184	-0.181	-0.300	0.377	-0.140	-0.296	-0.713	0.001	-0.027	-0.974	0.068	0.029
C	0.310	1.791	-2.500	0.722	-2.416	-2.217	0.071	-1.399	2.517	-0.020	-1.374	2.382
C	-0.213	2.731	-0.408	1.985	-2.572	-0.238	-1.458	-2.570	1.175	-1.392	-2.541	1.066
C	0.416	3.037	-3.090	1.242	-3.602	-2.701	0.075	-2.402	3.471	0.080	-2.368	3.435
H	0.450	0.864	-3.045	-0.014	-1.829	-2.754	0.697	-0.515	2.586	0.722	-0.528	2.542
C	-0.114	4.013	-0.958	2.538	-3.776	-0.682	-1.492	-3.608	2.108	-1.511	-3.564	2.068
C	0.201	4.163	-2.299	2.166	-4.287	-1.917	-0.728	-3.518	3.262	-0.723	-3.515	3.261
H	0.656	3.116	-4.143	0.926	-3.975	-3.667	0.699	-2.304	4.350	0.694	-2.307	4.355
H	-0.293	4.875	-0.332	3.251	-4.295	-0.060	-2.109	-4.473	1.919	-2.110	-4.473	1.926
H	0.273	5.157	-2.728	2.598	-5.219	-2.265	-0.752	-4.324	3.988	-0.752	-4.326	3.985
C	-0.651	0.986	1.245	1.592	-0.636	1.200	-1.907	-1.393	-0.931	-1.771	-0.794	-0.570
C	-0.562	2.379	0.970	2.259	-1.878	1.021	-2.173	-2.519	-0.109	-2.043	-2.205	-0.140
C	-0.992	0.578	2.538	1.803	0.084	2.379	-2.549	-1.272	-2.165	-2.262	-1.278	-1.923
C	-0.812	3.288	2.001	3.091	-2.344	2.041	-3.073	-3.478	-0.573	-2.991	-3.379	-0.558
C	-1.230	1.527	3.519	2.640	-0.433	3.353	-3.428	-2.261	-2.575	-3.382	-2.274	-2.518
H	-1.083	-0.472	2.793	1.332	1.044	2.550	-2.380	-0.419	-2.814	-2.374	-0.449	-2.818
C	-1.145	2.893	3.283	3.300	-1.647	3.216	-3.709	-3.376	-1.798	-3.704	-3.374	-1.822
H	-1.334	3.619	4.062	3.950	-2.034	3.989	-4.403	-4.137	-2.129	-4.403	-4.143	-2.125
N	0.010	1.649	-1.200	1.091	-1.917	-1.027	-0.688	-1.476	1.413	-0.808	-1.313	1.299
F	-1.552	1.121	4.754	2.833	0.264	4.480	-4.035	-2.148	-3.763	-4.031	-2.133	-3.717
F	-0.727	4.613	1.775	3.730	-3.522	1.908	-3.367	-4.562	0.171	-3.360	-4.545	0.127
C	0.377	-2.696	1.283	-1.369	1.779	1.234	-0.238	1.285	-2.684	-0.263	1.384	-2.571
C	-1.819	-2.465	0.502	0.545	2.720	0.258	-1.245	2.678	-1.083	-1.301	2.501	-0.952
C	0.105	-3.917	1.868	-1.764	2.996	1.756	-0.240	2.291	-3.633	-0.239	2.218	-3.625
H	1.363	-2.251	1.335	-1.935	0.868	1.391	0.188	0.306	-2.872	0.187	0.294	-2.824
C	-2.149	-3.699	1.074	0.187	3.976	0.755	-1.278	3.725	-2.007	-1.247	3.699	-1.984
C	-1.187	-4.424	1.756	-0.972	4.112	1.501	-0.780	3.527	-3.285	-0.804	3.543	-3.254
H	0.887	-4.452	2.391	-2.673	3.062	2.341	0.176	2.106	-4.615	0.174	2.114	-4.619
H	-3.155	-4.074	0.975	0.822	4.826	0.555	-1.681	4.682	-1.711	-1.680	4.682	-1.722
H	-1.444	-5.381	2.198	-1.253	5.086	1.887	-0.803	4.339	-4.005	-0.801	4.340	-4.002
C	-2.130	-0.376	-0.715	1.895	1.002	-0.820	-1.401	1.542	1.079	-1.271	0.859	1.005
C	-2.929	0.530	-1.416	3.026	0.576	-1.520	-1.764	1.507	2.431	-1.733	1.560	2.088
C	-2.714	-1.576	-0.237	1.744	2.376	-0.500	-1.664	2.716	0.319	-1.582	2.478	0.264
C	-4.263	0.237	-1.640	3.968	1.512	-1.910	-2.364	2.615	3.004	-2.307	2.613	2.989
H	-2.533	1.465	-1.795	3.186	-0.466	-1.768	-1.589	0.632	3.046	-1.563	0.651	3.030
C	-4.067	-1.817	-0.495	2.732	3.267	-0.926	-2.278	3.797	0.952	-2.194	3.741	0.972
C	-4.864	-0.931	-1.193	3.850	2.867	-1.631	-2.635	3.774	2.289	-2.653	3.777	2.290
H	-5.908	-1.144	-1.378	4.598	3.581	-1.948	-3.110	4.629	2.752	-3.112	4.632	2.749
N	-0.551	-1.987	0.621	-0.255	1.647	0.498	-0.747	1.469	-1.456	-0.721	1.127	-1.542
F	-5.017	1.115	-2.316	5.047	1.099	-2.585	-2.703	2.579	4.298	-2.696	2.577	4.250

F	-4.654	-2.949	-0.058	2.616	4.579	-0.652	-2.554	4.922	0.267	-2.549	4.890	0.306
C	2.651	-0.836	-0.946	-3.511	-0.366	-0.505	3.658	-0.244	-0.492	3.543	-0.244	-0.468
C	2.638	0.399	1.022	-4.012	-1.552	1.388	4.977	-0.790	-2.278	4.984	-0.785	-2.260
C	4.032	-0.941	-0.926	-4.851	-0.091	-0.757	4.765	-0.048	0.336	4.799	-0.043	0.347
C	4.015	0.349	1.123	-5.378	-1.368	1.225	6.151	-0.632	-1.549	6.164	-0.639	-1.575
C	4.712	-0.342	0.129	-5.788	-0.613	0.127	5.025	-1.083	-3.324	5.026	-1.084	-3.328
H	4.524	-1.485	-1.724	-5.127	0.520	-1.607	6.011	-0.254	-0.223	5.984	-0.250	-0.211
H	4.535	0.819	1.948	-6.096	-1.775	1.926	4.632	0.256	1.366	4.632	0.255	1.364
N	1.972	-0.183	0.013	-3.089	-1.077	0.548	7.129	-0.791	-1.983	7.127	-0.791	-1.983
O	0.575	-1.268	-2.030	-1.329	-0.420	-1.442	3.757	-0.606	-1.773	3.769	-0.613	-1.795
C	1.843	-1.462	-2.092	-2.465	0.206	-1.457	1.305	-0.342	-0.669	0.870	-0.252	-0.534
O	2.472	-2.057	-2.953	-2.772	1.149	-2.165	2.278	-0.024	0.107	2.369	-0.079	-0.228
H	2.030	0.909	1.762	-3.640	-2.113	2.242	2.197	0.429	1.248	1.956	0.496	1.463
N	6.115	-0.371	0.166	-7.163	-0.431	-0.116	7.218	-0.070	0.604	7.195	-0.074	0.586
O	6.787	-0.075	1.234	-8.060	-0.625	0.801	8.298	-0.248	0.064	8.309	-0.246	0.070
O	6.810	-1.220	-0.530	-7.609	0.500	-0.906	7.058	0.247	1.769	7.067	0.250	1.780

Table S20. Cartesian coordinates for triplet geometry of complex 17.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	-0.245	-0.120	-0.421	0.805	0.069	-0.101	0.714	-0.001	0.026	0.881	-0.084	-0.375
C	-0.309	1.953	-2.582	2.404	-0.088	-2.614	-0.079	-1.436	-2.494	0.064	-1.437	-2.429
C	-0.605	2.779	-0.402	2.935	-1.716	-1.006	1.460	-2.586	-1.143	1.397	-2.476	-1.036
C	-0.414	3.221	-3.125	3.328	-0.598	-3.508	-0.082	-2.452	-3.435	-0.081	-2.430	-3.420
H	-0.131	1.065	-3.177	1.763	0.753	-2.849	-0.708	-0.555	-2.570	-0.726	-0.562	-2.493
C	-0.715	4.079	-0.901	3.885	-2.266	-1.871	1.494	-3.635	-2.063	1.493	-3.584	-2.028
C	-0.621	4.296	-2.267	4.084	-1.700	-3.121	0.725	-3.562	-3.215	0.729	-3.557	-3.218
H	-0.328	3.354	-4.196	3.443	-0.140	-4.483	-0.711	-2.366	-4.313	-0.710	-2.372	-4.312
H	-0.870	4.899	-0.217	4.447	-3.134	-1.560	2.113	-4.496	-1.865	2.114	-4.495	-1.874
H	-0.706	5.304	-2.659	4.819	-2.127	-3.795	0.749	-4.377	-3.931	0.746	-4.379	-3.927
C	-0.536	0.975	1.236	1.458	-1.541	0.943	1.909	-1.383	0.948	1.623	-0.536	0.503
C	-0.683	2.361	0.999	2.557	-2.203	0.323	2.177	-2.517	0.138	2.116	-2.271	0.085
C	-0.572	0.480	2.538	1.065	-1.942	2.225	2.550	-1.246	2.181	2.277	-1.319	1.997
C	-0.876	3.201	2.096	3.189	-3.239	1.011	3.080	-3.469	0.613	2.999	-3.371	0.641
C	-0.776	1.362	3.587	1.729	-2.980	2.856	3.432	-2.229	2.602	3.369	-2.235	2.528
H	-0.447	-0.575	2.751	0.255	-1.452	2.754	2.378	-0.387	2.820	2.375	-0.385	2.805
C	-0.928	2.728	3.395	2.795	-3.651	2.271	3.716	-3.351	1.837	3.721	-3.361	1.851
H	-1.079	3.404	4.227	3.307	-4.457	2.780	4.412	-4.107	2.176	4.415	-4.111	2.169
N	-0.408	1.746	-1.261	2.232	-0.620	-1.394	0.686	-1.497	-1.392	0.784	-0.902	-1.122
F	-0.823	0.890	4.836	1.337	-3.361	4.079	4.039	-2.102	3.789	4.032	-2.087	3.744
F	-1.021	4.525	1.921	4.235	-3.885	0.462	3.376	-4.560	-0.118	3.370	-4.549	-0.079
C	0.914	-2.586	0.903	-1.671	-0.043	1.611	0.229	1.328	2.659	0.292	1.364	2.476
C	-1.399	-2.643	0.500	-0.718	2.087	1.396	1.266	2.685	1.047	1.230	2.611	1.110
C	0.901	-3.862	1.439	-2.746	0.449	2.326	0.237	2.346	3.593	0.234	2.367	3.587
H	1.825	-2.005	0.823	-1.583	-1.091	1.351	-0.213	0.357	2.855	-0.214	0.346	2.836
C	-1.465	-3.930	1.032	-1.779	2.637	2.118	1.306	3.745	1.957	1.254	3.693	1.869
C	-0.310	-4.540	1.501	-2.796	1.816	2.580	0.796	3.570	3.234	0.773	3.526	3.265
H	1.824	-4.303	1.793	-3.524	-0.226	2.659	-0.190	2.180	4.575	-0.182	2.189	4.579
H	-2.414	-4.442	1.072	-1.806	3.701	2.294	1.723	4.692	1.651	1.725	4.689	1.652
H	-0.360	-5.542	1.913	-3.628	2.244	3.129	0.824	4.391	3.942	0.828	4.391	3.942
C	-2.205	-0.563	-0.526	1.306	2.056	0.015	1.420	1.518	-1.098	1.168	0.498	-0.838
C	-3.220	0.255	-1.025	2.427	2.669	-0.544	1.786	1.461	-2.448	1.766	1.355	-2.143
C	-2.522	-1.854	-0.031	0.420	2.814	0.820	1.693	2.700	-0.353	1.646	2.293	-0.286
C	-4.523	-0.216	-1.049	2.649	4.018	-0.317	2.400	2.554	-3.034	2.369	2.605	-2.946
H	-3.015	1.250	-1.401	3.134	2.118	-1.155	1.602	0.580	-3.052	1.586	0.593	-3.059
C	-3.851	-2.272	-0.077	0.694	4.168	1.013	2.321	3.764	-0.999	2.200	3.612	-0.975
C	-4.866	-1.476	-0.581	1.797	4.792	0.456	2.682	3.720	-2.333	2.690	3.711	-2.383
H	-5.888	-1.830	-0.604	1.985	5.845	0.626	3.169	4.562	-2.807	3.172	4.568	-2.803
N	-0.202	-1.999	0.449	-0.685	0.749	1.160	0.751	1.488	1.433	0.934	1.347	1.501
F	-5.493	0.565	-1.535	3.723	4.607	-0.860	2.742	2.498	-4.327	2.734	2.492	-4.300

F	-4.207	-3.486	0.377	-0.114	4.933	1.771	2.608	4.896	-0.328	2.600	4.870	-0.361
C	2.606	-0.548	-1.144	-2.790	-0.609	-1.327	-3.648	-0.214	0.505	-3.478	-0.241	0.458
C	2.577	0.678	0.867	-3.347	-2.750	-0.745	-4.960	-0.694	2.311	-4.983	-0.680	2.282
C	3.967	-0.711	-1.060	-4.120	-0.197	-1.266	-4.759	-0.052	-0.321	-4.813	-0.052	-0.328
C	3.928	0.558	1.000	-4.700	-2.442	-0.658	-6.133	-0.565	1.574	-6.146	-0.574	1.621
H	1.989	1.212	1.605	-3.002	-3.761	-0.540	-5.006	-0.947	3.368	-5.007	-0.949	3.372
C	4.685	-0.171	0.019	-5.092	-1.130	-0.925	-6.024	-0.236	0.224	-5.990	-0.223	0.202
H	4.478	-1.261	-1.843	-4.374	0.836	-1.471	-4.626	0.214	-1.363	-4.625	0.211	-1.360
H	4.427	1.015	1.845	-5.427	-3.198	-0.387	-7.101	-0.715	2.037	-7.099	-0.718	2.037
N	1.876	0.135	-0.173	-2.405	-1.863	-1.068	-3.740	-0.528	1.801	-3.746	-0.534	1.824
O	0.515	-0.799	-2.175	-0.508	-0.024	-1.753	-1.295	-0.335	0.677	-0.820	-0.255	0.721
C	1.821	-1.105	-2.261	-1.723	0.432	-1.636	-2.269	-0.014	-0.099	-2.355	-0.073	0.151
O	2.271	-1.750	-3.187	-2.058	1.601	-1.744	-2.178	0.426	-1.245	-1.898	0.534	-1.489
C	6.120	-0.364	0.089	-6.515	-0.688	-0.846	-7.215	-0.072	-0.659	-7.173	-0.076	-0.636
O	6.802	-0.978	-0.716	-6.893	0.443	-1.035	-7.165	0.195	-1.837	-7.182	0.199	-1.854
O	6.687	0.217	1.183	-7.355	-1.691	-0.532	-8.377	-0.255	-0.007	-8.398	-0.255	-0.010
H	7.628	0.018	1.106	-8.241	-1.305	-0.511	-9.077	-0.129	-0.662	-9.072	-0.129	-0.662

Table S21. Cartesian coordinates for triplet geometry of complex 18.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.034	-0.387	-0.302	0.246	0.238	-0.112	0.211	0.004	0.011	0.311	0.018	0.014
C	1.915	0.730	-2.357	1.885	1.248	-2.390	-0.095	-1.435	-2.612	-0.096	-1.431	-2.599
C	1.756	1.954	-0.356	3.097	0.097	-0.740	1.257	-2.530	-1.036	1.254	-2.527	-1.032
C	2.877	1.587	-2.861	3.018	1.445	-3.157	0.100	-2.437	-3.546	0.100	-2.435	-3.545
H	1.554	-0.129	-2.912	0.901	1.580	-2.702	-0.744	-0.582	-2.785	-0.744	-0.582	-2.784
C	2.722	2.848	-0.819	4.272	0.274	-1.475	1.487	-3.566	-1.943	1.489	-3.562	-1.941
C	3.282	2.660	-2.075	4.231	0.954	-2.682	0.911	-3.514	-3.204	0.909	-3.513	-3.204
H	3.296	1.407	-3.843	2.944	1.967	-4.103	-0.382	-2.370	-4.514	-0.382	-2.370	-4.514
H	3.031	3.672	-0.194	5.200	-0.131	-1.099	2.106	-4.401	-1.652	2.106	-4.401	-1.653
H	4.037	3.351	-2.435	5.142	1.091	-3.255	1.088	-4.317	-3.911	1.088	-4.318	-3.911
C	0.175	0.924	1.217	1.604	-0.776	0.997	1.308	-1.332	1.105	1.259	-1.248	1.053
C	1.079	1.982	0.948	2.939	-0.629	0.522	1.755	-2.444	0.344	1.738	-2.434	0.352
C	-0.479	0.858	2.444	1.389	-1.437	2.213	1.738	-1.181	2.425	1.735	-1.197	2.407
C	1.265	2.951	1.935	3.982	-1.162	1.280	2.615	-3.359	0.953	2.612	-3.351	0.950
C	-0.245	1.844	3.389	2.465	-1.948	2.918	2.587	-2.127	2.977	2.585	-2.121	2.975
H	-1.167	0.054	2.680	0.396	-1.549	2.634	1.427	-0.338	3.032	1.428	-0.340	3.032
C	0.620	2.904	3.159	3.775	-1.830	2.474	3.042	-3.226	2.263	3.039	-3.227	2.263
H	0.789	3.669	3.905	4.605	-2.231	3.040	3.709	-3.953	2.706	3.710	-3.953	2.705
N	1.374	0.918	-1.146	1.930	0.613	-1.209	0.483	-1.474	-1.402	0.483	-1.466	-1.392
F	-0.874	1.783	4.566	2.245	-2.586	4.075	2.990	-1.985	4.246	2.991	-1.986	4.245
F	2.098	3.985	1.729	5.258	-1.038	0.869	3.075	-4.427	0.274	3.076	-4.426	0.276
C	-0.967	-2.690	1.323	-1.859	-1.424	1.265	-0.747	1.273	2.541	-0.749	1.272	2.526
C	-2.641	-1.322	0.399	-2.307	0.875	1.197	0.448	2.704	1.112	0.453	2.696	1.109
C	-1.904	-3.520	1.911	-3.082	-1.703	1.845	-0.943	2.281	3.467	-0.940	2.276	3.466
H	0.102	-2.849	1.410	-1.151	-2.205	1.012	-1.157	0.277	2.665	-1.156	0.278	2.664
C	-3.626	-2.127	0.977	-3.553	0.650	1.787	0.285	3.755	2.019	0.286	3.752	2.018
C	-3.252	-3.226	1.736	-3.941	-0.641	2.108	-0.406	3.538	3.201	-0.406	3.538	3.200
H	-1.576	-4.376	2.489	-3.350	-2.727	2.070	-1.506	2.080	4.370	-1.506	2.080	4.370
H	-4.667	-1.889	0.821	-4.210	1.486	1.974	0.690	4.727	1.783	0.690	4.727	1.783
H	-4.014	-3.854	2.184	-4.914	-0.817	2.554	-0.536	4.352	3.906	-0.536	4.352	3.906
C	-1.665	0.482	-0.928	-0.519	2.134	0.093	1.002	1.570	-0.984	0.983	1.471	-0.940
C	-1.766	1.609	-1.746	0.086	3.325	-0.306	1.580	1.548	-2.259	1.568	1.564	-2.240
C	-2.844	-0.145	-0.448	-1.755	2.170	0.783	1.088	2.757	-0.203	1.067	2.749	-0.213
C	-3.019	2.090	-2.088	-0.542	4.531	-0.036	2.216	2.679	-2.739	2.216	2.674	-2.737
H	-0.885	2.118	-2.122	1.039	3.336	-0.825	1.544	0.664	-2.885	1.544	0.665	-2.884
C	-4.078	0.386	-0.823	-2.341	3.413	1.026	1.749	3.862	-0.740	1.748	3.852	-0.737
C	-4.192	1.498	-1.639	-1.758	4.603	0.627	2.318	3.852	-2.001	2.315	3.851	-2.002
H	-5.163	1.888	-1.914	-2.236	5.552	0.833	2.825	4.725	-2.390	2.825	4.725	-2.390
N	-1.332	-1.620	0.603	-1.481	-0.175	0.950	-0.052	1.476	1.411	-0.059	1.463	1.404
F	-3.115	3.166	-2.875	0.037	5.673	-0.426	2.761	2.655	-3.962	2.761	2.655	-3.961

F	-5.222	-0.174	-0.393	-3.515	3.505	1.679	1.861	5.000	-0.030	1.862	5.000	-0.032
C	2.355	-2.206	-0.532	-1.988	-2.350	-1.797	-4.155	-0.417	-0.226	-4.151	-0.416	-0.229
C	2.605	-1.099	1.506	-1.151	-4.393	-1.290	-5.745	-1.003	1.273	-5.745	-1.002	1.272
C	3.647	-2.704	-0.375	-3.265	-2.910	-1.904	-5.142	-0.270	-1.205	-5.143	-0.270	-1.205
C	3.857	-1.630	1.613	-2.425	-4.946	-1.396	-6.725	-0.863	0.293	-6.725	-0.863	0.294
H	4.038	-3.340	-1.167	-4.108	-2.273	-2.151	-4.861	0.039	-2.207	-4.861	0.039	-2.207
H	4.464	-1.403	2.485	-2.587	-6.007	-1.226	-7.771	-1.052	0.522	-7.771	-1.052	0.522
N	1.793	-1.380	0.444	-0.925	-3.095	-1.486	-4.455	-0.783	1.021	-4.455	-0.783	1.021
O	0.310	-1.903	-1.617	-0.598	-0.411	-1.939	-1.862	-0.433	0.324	-1.844	-0.424	0.313
C	1.535	-2.471	-1.708	-1.823	-0.850	-1.978	-2.711	-0.145	-0.597	-2.706	-0.147	-0.578
O	1.867	-3.116	-2.688	-2.822	-0.168	-2.144	-2.461	0.318	-1.710	-2.451	0.317	-1.708
H	2.200	-0.443	2.270	-0.294	-5.012	-1.036	-6.009	-1.299	2.285	-6.009	-1.299	2.285
N	4.428	-2.456	0.666	-3.493	-4.207	-1.703	-6.432	-0.495	-0.955	-6.431	-0.495	-0.955

Table S22. Cartesian coordinates for triplet geometry of complex 19.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	-0.174	-0.135	-0.235	0.889	-0.004	-0.109	0.822	-0.003	0.010	0.922	0.007	0.011
C	0.246	1.782	-2.491	2.373	-0.631	-2.620	0.295	-1.380	-2.609	0.296	-1.376	-2.596
C	-0.643	2.726	-0.528	2.514	-2.283	-0.956	1.635	-2.591	-1.107	1.631	-2.588	-1.104
C	0.223	3.000	-3.146	3.136	-1.379	-3.498	0.378	-2.381	-3.562	0.378	-2.378	-3.560
H	0.589	0.863	-2.953	1.952	0.332	-2.884	-0.299	-0.481	-2.740	-0.300	-0.482	-2.739
C	-0.682	3.980	-1.146	3.294	-3.075	-1.803	1.751	-3.627	-2.036	1.753	-3.624	-2.033
C	-0.249	4.113	-2.456	3.609	-2.617	-3.073	1.126	-3.516	-3.269	1.124	-3.515	-3.269
H	0.564	3.066	-4.172	3.347	-0.997	-4.489	-0.140	-2.265	-4.506	-0.140	-2.266	-4.506
H	-1.059	4.831	-0.598	3.633	-4.041	-1.463	2.321	-4.508	-1.782	2.321	-4.508	-1.782
H	-0.284	5.084	-2.938	4.212	-3.232	-3.733	1.214	-4.319	-3.992	1.214	-4.320	-3.992
C	-0.978	1.015	1.184	1.140	-1.693	0.987	1.860	-1.432	1.044	1.814	-1.342	0.993
C	-1.082	2.389	0.829	2.041	-2.620	0.389	2.195	-2.561	0.252	2.177	-2.550	0.261
C	-1.388	0.621	2.462	0.666	-1.948	2.279	2.350	-1.333	2.347	2.344	-1.349	2.330
C	-1.583	3.293	1.768	2.407	-3.757	1.110	3.010	-3.544	0.813	3.008	-3.537	0.811
C	-1.878	1.564	3.350	1.062	-3.097	2.942	3.149	-2.346	2.853	3.147	-2.339	2.852
H	-1.336	-0.416	2.776	-0.001	-1.262	2.788	2.123	-0.480	2.977	2.123	-0.482	2.977
C	-1.986	2.912	3.034	1.931	-4.023	2.381	3.496	-3.463	2.107	3.493	-3.463	2.107
H	-2.373	3.635	3.740	2.235	-4.913	2.916	4.126	-4.243	2.513	4.126	-4.243	2.513
N	-0.171	1.657	-1.222	2.092	-1.062	-1.381	0.923	-1.478	-1.426	0.924	-1.471	-1.416
F	-2.264	1.172	4.572	0.594	-3.335	4.175	3.611	-2.254	4.107	3.611	-2.255	4.106
F	-1.686	4.603	1.465	3.262	-4.655	0.584	3.365	-4.632	0.103	3.366	-4.632	0.105
C	0.612	-2.460	1.526	-1.521	0.547	1.604	0.048	1.307	2.580	0.047	1.306	2.566
C	-1.512	-2.611	0.548	-0.059	2.362	1.351	1.328	2.648	1.137	1.333	2.640	1.133
C	0.476	-3.684	2.152	-2.423	1.304	2.328	-0.028	2.313	3.526	-0.026	2.307	3.525
H	1.508	-1.863	1.635	-1.709	-0.490	1.352	-0.450	0.352	2.700	-0.449	0.352	2.698
C	-1.700	-3.857	1.158	-0.932	3.170	2.083	1.288	3.694	2.064	1.288	3.691	2.062
C	-0.707	-4.391	1.959	-2.116	2.639	2.570	0.614	3.520	3.262	0.614	3.520	3.262
H	1.280	-4.067	2.768	-3.344	0.854	2.676	-0.583	2.149	4.442	-0.583	2.149	4.442
H	-2.624	-4.390	0.993	-0.682	4.206	2.248	1.772	4.630	1.830	1.772	4.630	1.830
H	-0.854	-5.358	2.430	-2.800	3.269	3.129	0.579	4.330	3.983	0.579	4.330	3.983
C	-2.020	-0.654	-0.815	1.864	1.799	-0.058	1.711	1.504	-0.991	1.686	1.405	-0.948
C	-2.877	0.079	-1.639	3.092	2.103	-0.648	2.240	1.453	-2.286	2.230	1.469	-2.266
C	-2.458	-1.909	-0.318	1.214	2.770	0.745	1.928	2.666	-0.197	1.906	2.661	-0.206
C	-4.123	-0.431	-1.962	3.649	3.357	-0.454	2.959	2.531	-2.772	2.959	2.526	-2.770
H	-2.594	1.045	-2.040	3.626	1.383	-1.257	2.104	0.586	-2.923	2.104	0.588	-2.922
C	-3.727	-2.372	-0.678	1.823	4.014	0.904	2.667	3.716	-0.741	2.666	3.706	-0.739
C	-4.579	-1.657	-1.497	3.035	4.333	0.317	3.190	3.677	-2.021	3.188	3.677	-2.023
H	-5.556	-2.040	-1.760	3.483	5.307	0.462	3.761	4.508	-2.416	3.761	4.508	-2.415
N	-0.349	-1.934	0.751	-0.371	1.057	1.136	0.728	1.466	1.434	0.719	1.451	1.427
F	-4.934	0.283	-2.755	4.824	3.649	-1.027	3.458	2.480	-4.014	3.458	2.480	-4.013

F	-4.175	-3.560	-0.226	1.248	4.970	1.659	2.905	4.828	-0.020	2.906	4.828	-0.022
C	2.800	-0.496	-0.565	-2.805	0.127	-1.319	-3.561	-0.075	-0.036	-3.557	-0.075	-0.039
C	2.325	0.965	1.234	-3.832	-1.785	-0.594	-5.056	-0.611	1.605	-5.056	-0.611	1.605
C	4.203	-0.436	-0.296	-3.991	0.815	-1.394	-4.551	0.191	-0.948	-4.551	0.191	-0.948
C	3.706	1.126	1.531	-5.121	-1.187	-0.636	-6.172	-0.374	0.756	-6.172	-0.374	0.757
H	4.006	1.776	2.345	-3.743	-2.822	-0.269	-5.238	-0.928	2.633	-5.238	-0.928	2.633
N	1.885	0.200	0.277	-5.201	0.166	-1.053	-5.907	0.045	-0.571	-5.906	0.045	-0.571
O	0.882	-1.153	-1.807	-3.974	1.854	-1.705	-4.273	0.515	-1.945	-4.273	0.515	-1.945
C	2.169	-1.236	-1.718	-2.721	-1.172	-0.917	-3.807	-0.474	1.243	-3.807	-0.473	1.242
O	2.882	-1.849	-2.512	-0.450	0.111	-1.729	-1.252	-0.291	0.408	-1.233	-0.283	0.397
H	1.572	1.478	1.828	-1.516	0.860	-1.643	-2.119	0.086	-0.468	-2.113	0.083	-0.450
C	4.665	0.408	0.781	-1.543	2.071	-1.805	-1.867	0.550	-1.582	-1.858	0.549	-1.580
C	5.161	-1.146	-1.023	-6.301	-1.883	-0.275	-7.512	-0.538	1.187	-7.512	-0.538	1.187
C	6.554	-1.032	-0.720	-6.229	-2.920	0.041	-7.704	-0.860	2.207	-7.704	-0.860	2.207
C	6.988	-0.231	0.295	-6.471	0.797	-1.099	-6.997	0.294	-1.445	-6.997	0.294	-1.445
C	6.030	0.499	1.054	-6.533	1.833	-1.420	-6.794	0.616	-2.462	-6.794	0.616	-2.462
H	4.815	-1.780	-1.830	-7.599	0.103	-0.745	-8.285	0.128	-1.005	-8.285	0.129	-1.005
H	7.261	-1.598	-1.318	-8.569	0.589	-0.782	-9.116	0.320	-1.676	-9.116	0.320	-1.676
H	8.043	-0.139	0.530	-7.516	-1.249	-0.329	-8.547	-0.291	0.323	-8.547	-0.291	0.323
H	6.361	1.146	1.862	-8.422	-1.780	-0.054	-9.574	-0.416	0.651	-9.574	-0.416	0.651

Table S23. Cartesian coordinates for triplet geometry of complex 20.

	T_1			TS			T_1'			MECP		
Atom	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)	x (Å)	y (Å)	z (Å)
Ir	0.218	-0.239	-0.248	-0.442	0.209	-0.115	0.345	0.003	-0.036	0.445	0.008	-0.015
C	1.268	1.480	-2.453	-1.202	1.947	-2.425	0.368	-1.385	-2.702	0.366	-1.382	-2.691
C	0.554	2.652	-0.499	-0.065	3.056	-0.698	1.363	-2.592	-0.950	1.362	-2.587	-0.948
C	1.610	2.668	-3.087	-1.265	3.096	-3.192	0.646	-2.388	-3.614	0.646	-2.384	-3.612
H	1.375	0.516	-2.939	-1.594	0.997	-2.767	-0.187	-0.487	-2.956	-0.187	-0.487	-2.955
C	0.894	3.895	-1.144	-0.107	4.245	-1.429	1.670	-3.630	-1.832	1.670	-3.628	-1.830
C	1.410	3.904	-2.402	-0.714	4.264	-2.675	1.315	-3.522	-3.169	1.315	-3.522	-3.168
H	2.011	2.637	-4.093	-1.730	3.066	-4.169	0.335	-2.275	-4.645	0.335	-2.275	-4.645
H	0.723	4.817	-0.606	0.345	5.136	-1.021	2.174	-4.511	-1.463	2.173	-4.511	-1.463
H	1.661	4.841	-2.886	-0.746	5.187	-3.246	1.552	-4.328	-3.856	1.552	-4.328	-3.856
C	-0.260	1.052	1.161	0.608	1.497	1.070	1.137	-1.427	1.197	1.105	-1.347	1.141
C	0.015	2.455	0.765	0.583	2.838	0.600	1.627	-2.559	0.495	1.611	-2.549	0.502
C	-0.846	0.800	2.400	1.204	1.221	2.304	1.343	-1.325	2.574	1.340	-1.337	2.555
C	-0.302	3.475	1.733	1.168	3.832	1.385	2.303	-3.543	1.217	2.301	-3.535	1.214
C	-1.122	1.842	3.268	1.774	2.249	3.036	2.014	-2.339	3.238	2.013	-2.333	3.236
H	-1.084	-0.213	2.707	1.227	0.218	2.715	0.990	-0.470	3.140	0.990	-0.472	3.140
C	-0.847	3.192	2.944	1.773	3.566	2.601	2.506	-3.459	2.584	2.504	-3.459	2.585
H	-1.073	3.984	3.647	2.217	4.360	3.187	3.035	-4.239	3.116	3.035	-4.239	3.115
N	0.766	1.441	-1.223	-0.641	1.935	-1.207	0.736	-1.479	-1.414	0.729	-1.469	-1.405
F	-1.663	1.595	4.469	2.353	1.973	4.213	2.202	-2.245	4.561	2.202	-2.246	4.561
F	-0.047	4.765	1.431	1.161	5.117	0.981	2.796	-4.634	0.600	2.796	-4.634	0.602
C	0.260	-2.698	1.529	0.993	-2.007	1.312	-0.953	1.338	2.300	-0.951	1.337	2.286
C	-1.798	-2.210	0.521	-1.330	-2.286	1.145	0.640	2.649	1.173	0.641	2.643	1.171
C	-0.245	-3.825	2.149	1.148	-3.234	1.930	-1.211	2.348	3.208	-1.209	2.343	3.208
H	1.292	-2.394	1.652	1.836	-1.372	1.062	-1.488	0.396	2.302	-1.487	0.396	2.301
C	-2.360	-3.341	1.124	-1.228	-3.530	1.772	0.422	3.697	2.071	0.423	3.695	2.070
C	-1.582	-4.148	1.937	0.014	-4.003	2.165	-0.500	3.540	3.094	-0.501	3.540	3.094
H	0.397	-4.430	2.778	2.139	-3.574	2.204	-1.956	2.199	3.980	-1.956	2.199	3.980
H	-3.398	-3.574	0.946	-2.119	-4.118	1.930	0.965	4.622	1.950	0.965	4.622	1.950
H	-2.018	-5.025	2.402	0.095	-4.973	2.644	-0.674	4.352	3.793	-0.674	4.352	3.793
C	-1.689	-0.179	-0.830	-2.378	-0.432	-0.065	1.447	1.492	-0.826	1.407	1.402	-0.781
C	-2.266	0.779	-1.663	-3.500	0.246	-0.548	2.239	1.429	-1.980	2.224	1.443	-1.967
C	-2.480	-1.252	-0.349	-2.552	-1.651	0.642	1.512	2.651	-0.001	1.498	2.643	-0.017
C	-3.601	0.661	-2.011	-4.762	-0.290	-0.347	3.064	2.493	-2.299	3.063	2.488	-2.297
H	-1.694	1.614	-2.050	-3.414	1.189	-1.075	2.224	0.565	-2.634	2.224	0.567	-2.633
C	-3.821	-1.315	-0.736	-3.847	-2.140	0.814	2.371	3.686	-0.373	2.369	3.678	-0.370
C	-4.407	-0.377	-1.563	-4.965	-1.484	0.329	3.153	3.635	-1.513	3.150	3.635	-1.514
H	-5.448	-0.453	-1.846	-5.957	-1.889	0.481	3.810	4.454	-1.775	3.810	4.454	-1.774
N	-0.490	-1.914	0.740	-0.211	-1.543	0.943	-0.034	1.479	1.331	-0.037	1.470	1.319
F	-4.149	1.583	-2.811	-5.833	0.361	-0.819	3.814	2.431	-3.407	3.814	2.432	-3.406

F	-4.608	-2.319	-0.303	-4.063	-3.290	1.481	2.472	4.794	0.386	2.473	4.794	0.385
C	2.861	-1.620	-0.731	2.537	-1.950	-1.703	-3.954	-0.027	-0.915	-3.950	-0.027	-0.918
C	3.254	-0.213	1.080	4.514	-1.273	-0.742	-5.752	-0.391	0.462	-5.752	-0.391	0.462
C	4.144	-2.145	-0.669	3.136	-3.054	-2.306	-4.767	0.162	-2.032	-4.767	0.162	-2.032
C	4.554	-0.707	1.190	5.202	-2.338	-1.330	-6.643	-0.227	-0.602	-6.643	-0.227	-0.602
C	5.005	-1.685	0.314	4.500	-3.239	-2.123	-6.141	0.054	-1.867	-6.140	0.054	-1.866
H	4.413	-2.895	-1.403	2.527	-3.735	-2.887	-4.306	0.389	-2.985	-4.306	0.389	-2.985
H	5.202	-0.312	1.964	6.267	-2.457	-1.159	-7.712	-0.318	-0.434	-7.712	-0.318	-0.434
H	6.015	-2.074	0.397	3.205	-1.084	-0.936	-4.428	-0.294	0.303	-4.428	-0.294	0.302
N	2.417	-0.686	0.133	0.661	-0.494	-1.762	-1.765	-0.272	-0.063	-1.745	-0.269	-0.061
O	0.770	-1.536	-1.874	1.041	-1.738	-1.857	-2.451	0.088	-1.093	-2.441	0.088	-1.085
C	1.921	-2.106	-1.838	0.317	-2.700	-2.060	-1.999	0.504	-2.159	-1.999	0.503	-2.157
O	2.343	-2.959	-2.604	5.011	-4.079	-2.583	-6.812	0.189	-2.709	-6.812	0.189	-2.709
C	2.771	0.864	2.004	5.211	-0.261	0.129	-6.234	-0.682	1.859	-6.234	-0.682	1.859
H	2.491	1.753	1.432	5.416	0.649	-0.443	-5.748	-1.583	2.244	-5.748	-1.583	2.244
H	1.883	0.545	2.555	4.566	0.023	0.964	-5.967	0.142	2.529	-5.967	0.142	2.529
H	3.551	1.139	2.715	6.159	-0.641	0.516	-7.317	-0.821	1.895	-7.317	-0.821	1.895

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