

Supporting Information

Temperature Dependence of Blue Phosphorescent Cyclometallated Ir(III) Complexes

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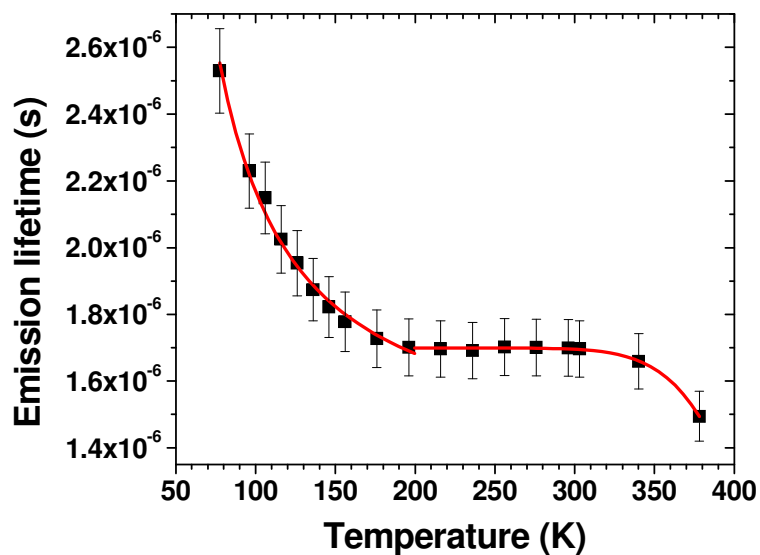


Figure S1. Temperature-dependent luminescent decay of Ir(F₂ppy)₃, **2**. Line is Boltzmann fit to data.

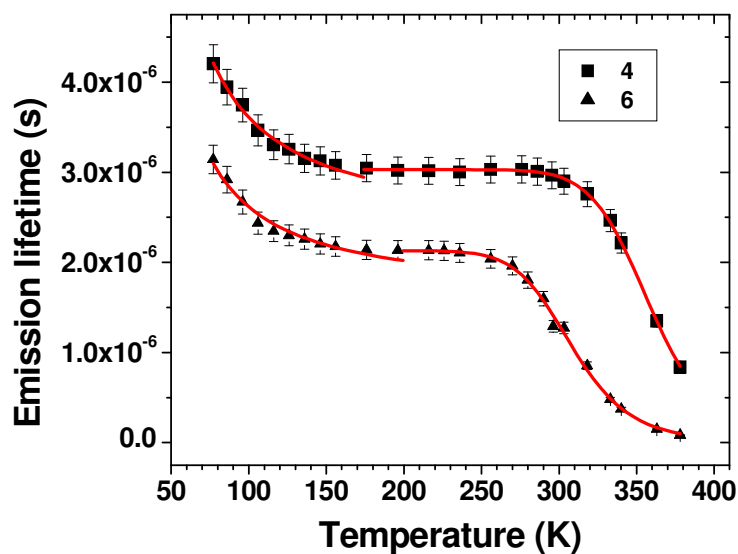


Figure S2. Temperature-dependent luminescent decay of (F₂ppz)₂Ir(ppy), **4** (squares) and (F₂ppz)₂Ir(F₂ppy), **6** (triangles). Lines are Boltzmann fits to data.

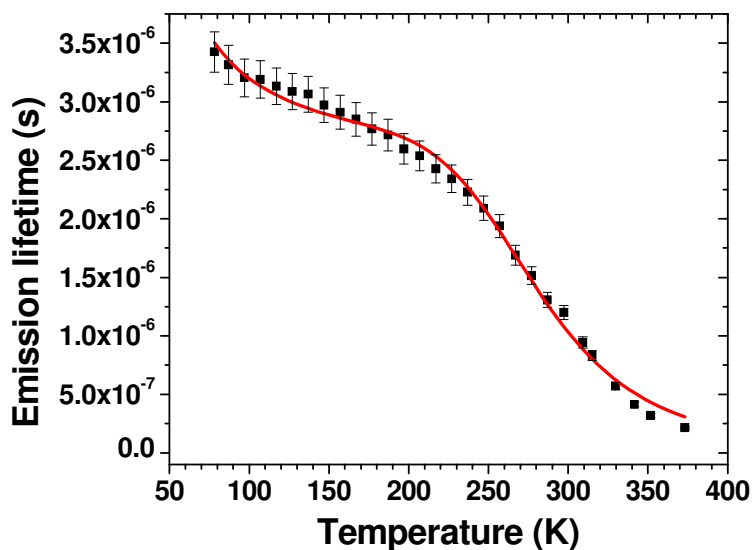


Figure 3. Temperature-dependent luminescent decay of Ir(pmb)₃, **10**. Line is Boltzmann fit to data.

Table S1. Selected structural parameters calculated for the six-coordinate triplet state of **1–10**.

No.	complex	Ir–C (Å) ^a	Ir–C (Å)	Ir–C (Å)	Ir–N (Å) ^a	Ir–N (Å)	Ir–N (Å)	Spin density ^b
1	Ir(ppy) ₃	1.990	2.030	2.052	2.145	2.201	2.193	0.322
2	Ir(F ₂ ppy) ₃	2.000	2.024	2.041	2.136	2.192	2.194	0.243
3	Ir(ppz) ₂ (ppy)	1.984	2.037	2.061	2.146	2.203	2.171	0.275
4	Ir(F ₂ ppz) ₂ (ppy)	1.988	2.038	2.038	2.142	2.193	2.154	0.236
5	Ir(ppz) ₂ (F ₂ ppy)	1.999	2.032	2.065	2.122	2.186	2.172	0.262
6	Ir(F ₂ ppz) ₂ (F ₂ ppy)	2.002	2.035	2.057	2.125	2.177	2.158	0.202
7	Ir(ppz) ₃	1.988	2.040	2.051	2.150	2.182	2.166	0.193
8	Ir(F ₂ ppz) ₃	1.998	2.035	2.044	2.139	2.162	2.159	0.131
9	Ir(flz) ₃ ^c	2.015	2.046	2.049	2.156	2.163	2.157	0.123
10	Ir(pmb) ₃	2.110	2.058	2.143	2.108 ^d	2.068 ^d	2.148 ^d	0.478

(a) ligand with highest spin density (b) density on Ir (c) 9,9'-dihydro analog of flz ligand (d) Ir–C_{carbene}

Table S2. Selected structural parameters calculated for the five-coordinate triplet state of **1–10**.

No	complex	Ir–C _{eq} (Å) ^a	Ir–C _{eq} (Å)	Ir–C _{ax} (Å)	Ir–N _{eq} (Å)	Ir–N _{ax} (Å)	N _{eq} –Ir–C _{eq} (deg)	N _{eq} –Ir–C _{eq} (deg) ^b	C _{eq} –Ir–C _{eq} (deg) ^b	N _{ax} –Ir–C _{ax} (deg)	dihedral (deg) ^c	Spin density ^d
1	Ir(ppy) ₃	2.086	2.051	2.020	2.137	2.184	113.33	129.84	116.72	176.86	-49.14	0.973
2	Ir(F ₂ ppy) ₃	2.090	2.061	2.023	2.144	2.175	111.69	128.75	119.48	177.06	-50.34	1.021
3	Ir(ppz) ₂ (ppy)	2.084	2.062	2.019	2.154	2.178	113.61	123.45	122.80	175.53	-86.09	1.045
4	Ir(F ₂ ppz) ₂ (ppy)	2.084	2.065	2.024	2.163	2.176	114.44	119.71	125.79	175.99	-84.74	1.079
5	Ir(ppz) ₂ (F ₂ ppy)	2.087	2.066	2.017	2.145	2.168	113.37	125.28	121.31	175.40	-68.82	1.043
6	Ir(F ₂ ppz) ₂ (F ₂ ppy)	2.083	2.067	2.021	2.146	2.167	113.84	123.68	122.38	175.80	-79.59	1.063
7	Ir(ppz) ₃	2.090	2.067	2.032	2.161	2.166	112.17	119.50	128.31	175.62	-77.01	1.106
8	Ir(F ₂ ppz) ₃	2.088	2.068	2.033	2.148	2.151	112.59	118.05	129.32	175.85	-81.83	1.111
9	Ir(flz) ₃ ^e	2.092	2.069	2.036	2.158	2.162	109.87	119.63	130.14	175.51	-92.67	1.107
10	Ir(pmb) ₃	2.104	2.067	2.084	2.031 ^f	2.072 ^f	119.73 ^g	129.10 ^g	110.83	174.55 ^h	-56.30	0.808

(a) monodentate phenyl (b) angle to monodentate phenyl (c) dihedral angle between the phenyl and heterocycle in the monodentate ligand (d) density on Ir (e) 9,9'-dihydro analog of flz ligand (f) Ir–C_{carbene} (g) C_{carbene}, eq–Ir–C_{eq} (h) C_{carbene}, ax–Ir–C_{ax}

Table S3. Calculated energies for the triplet state of **1–10**.^a

No.	Complex	<i>E</i> _{oct} (hartree)	<i>ZPE</i> _{oct} (hartree)	<i>E</i> _{TBP} (hartree)	<i>ZPE</i> _{TBP} (hartree)	ΔH (hartree)
1	Ir(ppy) ₃	-1540.953746	0.476823	-1540.945547	0.478269	0.009645
2	Ir(F ₂ ppy) ₃	-2136.344323	0.427676	-2136.338030	0.429376	0.007993
3	Ir(ppz) ₂ (ppy)	-1496.766063	0.441367	-1496.762478	0.442527	0.004745
4	Ir(F ₂ ppz) ₂ (ppy)	-1893.690295	0.408455	-1893.684045	0.409745	0.007540
5	Ir(ppz) ₂ (F ₂ ppy)	-1695.226851	0.424690	-1695.227976	0.426406	0.000591
6	Ir(F ₂ ppz) ₂ (F ₂ ppy)	-2092.150393	0.391839	-2092.148536	0.393469	0.003487
7	Ir(ppz) ₃	-1474.657032	0.422519	-1474.667065	0.424914	-0.007638
8	Ir(F ₂ ppz) ₃	-2070.039291	0.373060	-2070.049853	0.375786	-0.007836
9	Ir(flz) ₃ ^b	-2282.190419	0.684854	-2282.187030	0.686645	0.005180
10	Ir(pmb) ₃	-2053.550945	0.650124	-2053.544413	0.650685	0.007093

(a) ZPE = zero point energy (b) 9,9'-dihydro analog of flz ligand

Table S4. xyz-coordinates for **1**-octahedral.

61

atom	x	y	z
Ir	-0.00777	-0.00048	-0.16906
C	-1.52992	0.75419	0.86745
C	-3.90646	1.66918	2.11973
C	-1.47830	1.58718	1.99992
C	-2.86623	0.37963	0.33621
C	-4.03061	0.86476	1.01189
C	-2.63043	2.04458	2.63109
H	-0.50744	1.86564	2.39698
H	-5.02012	0.59828	0.65396
H	-2.56683	2.67788	3.51102
H	-4.80415	2.02715	2.61946
C	1.46379	1.01211	0.84023
C	3.49599	2.63373	2.00840
C	2.19681	0.58206	1.96034
C	1.79131	2.29677	0.31416
C	2.79608	3.09132	0.89901
C	3.19126	1.37335	2.53605
H	1.97717	-0.38930	2.39409
H	3.03658	4.06930	0.49065
H	3.73388	1.00723	3.40508
H	4.26990	3.24848	2.45896

C	0.08895	-1.75229	0.85288
C	0.35061	-4.31997	2.04602
C	1.01000	-2.71682	0.34993
C	-0.68208	-2.12403	1.97011
C	-0.55455	-3.38193	2.55628
C	1.12966	-3.98566	0.94652
H	-1.38642	-1.41160	2.38734
H	-1.16702	-3.63711	3.41831
H	1.82899	-4.71804	0.55254
H	0.44410	-5.30070	2.50389
C	0.39643	4.29148	-2.61006
C	-0.53453	3.35879	-3.07685
C	-0.63542	2.14779	-2.40756
N	0.12451	1.84699	-1.34241
C	1.03422	2.74121	-0.86259
C	1.17875	3.98279	-1.50664
H	0.50675	5.25358	-3.10249
H	-1.17009	3.56433	-3.93133
H	-1.33986	1.37994	-2.70997
H	1.89790	4.70205	-1.13318
C	3.52029	-2.60597	-2.50192
C	3.25670	-1.31207	-2.96019
C	2.27202	-0.57914	-2.31342
N	1.56658	-1.06503	-1.27974
C	1.81787	-2.31661	-0.80541
C	2.80343	-3.10502	-1.42460
H	4.28131	-3.21636	-2.97969
H	3.79842	-0.88005	-3.79460
H	2.02169	0.43033	-2.62203
H	3.00434	-4.10319	-1.05399
C	-3.97267	-1.70152	-2.59706
C	-2.67687	-2.09551	-3.05902
C	-1.56226	-1.61768	-2.38748
N	-1.62697	-0.79708	-1.32911
C	-2.89732	-0.42234	-0.82214
C	-4.06699	-0.88648	-1.50121
H	-4.86619	-2.04913	-3.10647
H	-2.55419	-2.75483	-3.91109
H	-0.56134	-1.89392	-2.70726
H	-5.04107	-0.58141	-1.13331

Table S5. xyz-coordinates for **1**-TBP.
61

atom	x	y	z
Ir	0.21094	-0.09974	0.03861
N	3.03314	-1.61627	-1.00612
N	0.41582	0.02875	-2.08444
C	0.52204	0.48595	-4.82520
C	0.15985	-0.96836	-2.95972
C	0.73360	1.28298	-2.54628
C	0.78636	1.51186	-3.92910
C	0.20037	-0.78594	-4.32975
H	-0.08201	-1.92875	-2.51908
H	1.03080	2.50316	-4.29346
H	-0.01513	-1.61722	-4.99276
H	0.56099	0.66975	-5.89478
C	-1.71558	0.17499	0.68702
C	-4.39399	0.28015	1.59011
C	-2.33921	1.40562	0.96752
C	-2.47434	-1.01816	0.87751

C	-3.80167	-0.95139	1.32690
C	-3.66030	1.45830	1.41056
H	-1.78187	2.32712	0.83366
H	-4.38198	-1.85788	1.47548
H	-4.12494	2.41996	1.61554
H	-5.42319	0.32236	1.93569
C	1.63420	-0.55800	1.49355
C	3.37349	-1.00792	3.69124
C	3.01232	-0.79713	1.28555
C	1.16252	-0.57191	2.81959
C	2.01278	-0.79128	3.90475
C	3.86079	-1.00826	2.38827
H	0.10666	-0.39767	3.01162
H	1.60716	-0.79467	4.91399
H	4.91586	-1.20396	2.21059
H	4.04484	-1.18696	4.52668
C	-1.59476	-4.69266	0.44017
C	-0.27011	-4.53376	0.02797
C	0.23823	-3.24513	-0.08676
N	-0.50710	-2.15778	0.17537
C	-1.79487	-2.28905	0.59228
C	-2.35747	-3.56706	0.72642
H	-2.02705	-5.68415	0.54257
H	0.36237	-5.38687	-0.19366
H	1.26158	-3.03604	-0.39081
H	-3.38472	-3.67476	1.05505
C	5.38665	-0.23302	-1.60467
C	4.77363	-1.03218	-2.56924
C	3.60115	-1.69580	-2.21542
C	3.62531	-0.84904	-0.06932
C	4.80795	-0.14056	-0.34365
H	6.29579	0.31653	-1.83393
H	5.18674	-1.13714	-3.56775
H	3.08843	-2.32580	-2.94091
H	5.24329	0.49008	0.42408
C	1.56464	4.50076	-0.74096
C	1.39867	4.07304	0.58424
C	1.02404	2.76074	0.86445
C	0.79494	1.82386	-0.16179
C	0.97588	2.27445	-1.50288
C	1.35656	3.60150	-1.77869
H	1.85638	5.52488	-0.95548
H	1.56513	4.77222	1.40093
H	0.90850	2.44931	1.89956
H	1.49093	3.93579	-2.80420

Table S6. xyz-coordinates for **2**-octahedral.

61

atom	x	y	z
Ir	-0.03100	-0.00300	-0.01300
C	-1.53200	0.77500	1.05500
C	-3.86500	1.75500	2.37700
C	-1.42300	1.58300	2.19300
C	-2.88200	0.43500	0.53800
C	-4.00100	0.97400	1.26300
C	-2.55800	2.05200	2.83600
H	-0.45200	1.84200	2.59700
H	-4.73700	2.13600	2.89600
C	1.43000	0.98300	1.01700
C	3.39100	2.57700	2.33500

C	2.12100	0.50100	2.13900
C	1.73600	2.29700	0.53800
C	2.71300	3.04400	1.22000
C	3.06800	1.29500	2.77300
H	1.91400	-0.48400	2.54300
H	4.13000	3.18800	2.83700
C	0.07100	-1.73000	1.03700
C	0.36600	-4.23800	2.35700
C	1.01900	-2.69100	0.56100
C	-0.69800	-2.04800	2.16800
C	-0.53500	-3.27300	2.80100
C	1.12100	-3.91800	1.24000
H	-1.41100	-1.34100	2.57500
H	0.47900	-5.19200	2.85600
C	0.33000	4.35200	-2.35100
C	-0.57500	3.41200	-2.85100
C	-0.65500	2.18200	-2.21100
N	0.10100	1.87300	-1.14400
C	0.99100	2.77500	-0.63400
C	1.11400	4.03800	-1.24600
H	0.42500	5.32800	-2.81700
H	-1.33900	1.40600	-2.53800
C	3.59500	-2.54300	-2.24300
C	3.27800	-1.27600	-2.74200
C	2.24100	-0.57900	-2.13600
N	1.53900	-1.07600	-1.10300
C	1.83800	-2.30600	-0.59200
C	2.87700	-3.06000	-1.17200
H	4.40000	-3.12400	-2.68400
H	1.94700	0.41000	-2.47100
C	-4.06100	-1.69400	-2.34400
C	-2.76900	-2.11900	-2.80000
C	-1.64000	-1.62900	-2.15600
N	-1.68100	-0.77300	-1.12800
C	-2.95700	-0.37600	-0.61000
C	-4.14100	-0.84600	-1.27200
H	-4.96100	-2.04600	-2.83800
H	-0.64700	-1.92600	-2.47900
H	-2.65800	-2.80800	-3.62900
H	-5.10200	-0.51900	-0.90000
H	1.81300	4.75700	-0.84900
H	-1.20600	3.62200	-3.70800
H	3.81800	-0.83500	-3.57300
H	3.11600	-4.03300	-0.77000
F	-1.27400	-3.55000	3.89300
F	1.99400	-4.86800	0.81400
F	-2.44700	2.81900	3.94000
F	-5.26500	0.70500	0.84100
F	3.70200	0.81800	3.86200
F	3.03900	4.29600	0.80400

Table S7. xyz-coordinates for **2**-TBP.
61

atom	x	y	z
Ir	0.20673	-0.09427	0.06924
N	3.02350	-1.64100	-1.01249
N	0.41328	0.04082	-2.06023
C	0.53200	0.46386	-4.79615
C	0.14208	-0.96149	-2.92055
C	0.75102	1.28556	-2.52821

C	0.81344	1.49949	-3.91592
C	0.18702	-0.79609	-4.29342
H	-0.11547	-1.91177	-2.46733
H	1.07744	2.47923	-4.28509
H	-0.04241	-1.63000	-4.94811
H	0.57767	0.63717	-5.86733
C	-1.74865	0.17449	0.66363
C	-4.45656	0.29832	1.47063
C	-2.36251	1.41239	0.90696
C	-2.49821	-1.03317	0.83470
C	-3.83657	-0.91928	1.23445
C	-3.69444	1.44897	1.29999
H	-1.82011	2.34338	0.79109
F	-4.60277	-2.02516	1.40950
F	-4.28522	2.63871	1.52343
H	-5.49410	0.34289	1.77777
C	1.66446	-0.53850	1.49903
C	3.42798	-1.00769	3.67878
C	3.03730	-0.78863	1.25729
C	1.19849	-0.53610	2.82492
C	2.07583	-0.76739	3.87663
C	3.86886	-1.00830	2.36481
H	0.15462	-0.35134	3.05837
F	1.60038	-0.76129	5.13977
F	5.18629	-1.26070	2.16004
H	4.10594	-1.19806	4.50117
C	-1.54441	-4.69952	0.44162
C	-0.21374	-4.51771	0.06540
C	0.27160	-3.21961	-0.03799
N	-0.50142	-2.14676	0.20445
C	-1.80097	-2.30091	0.58294
C	-2.34182	-3.59138	0.70365
H	-1.96151	-5.69823	0.53539
H	0.44171	-5.35771	-0.13832
H	1.29662	-2.99131	-0.32228
H	-3.37236	-3.71318	1.00139
C	5.32354	-0.21661	-1.70435
C	4.69325	-1.03603	-2.64095
C	3.54945	-1.72171	-2.24112
C	3.63102	-0.85156	-0.10670
C	4.78946	-0.12398	-0.42439
H	6.21628	0.34384	-1.96801
H	5.07555	-1.14328	-3.65122
H	3.02594	-2.37160	-2.94060
H	5.25235	0.50340	0.32831
C	1.61090	4.50535	-0.67253
C	1.40659	4.04516	0.62637
C	1.01001	2.74674	0.91265
C	0.79420	1.83114	-0.13014
C	0.99583	2.27057	-1.47829
C	1.40007	3.59819	-1.69556
H	1.92203	5.52138	-0.87839
F	1.60802	4.91087	1.64030
H	0.88255	2.45499	1.94970
F	1.60586	4.05534	-2.95874

Table S8. xyz-coordinates for **3**-octahedral.

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atom	x	y	z
Ir	0.04566	0.03426	-0.15279
C	-1.54462	0.80487	0.86138
C	-3.96159	1.73882	2.05172
C	-1.53812	1.66214	1.97572
C	-2.82349	0.44181	0.38106
C	-4.01687	0.89130	0.94855
C	-2.71934	2.12085	2.56224
H	-0.58484	1.96560	2.39576
H	-4.97878	0.59117	0.54286
H	-2.66993	2.78139	3.42419
H	-4.88172	2.09565	2.50498
C	1.40869	1.01883	0.90099
C	3.28036	2.71551	2.20656
C	2.07641	0.60050	2.06521
C	1.72152	2.37803	0.36778
C	2.67019	3.19077	1.07184
C	2.99667	1.41255	2.72052
H	1.85332	-0.38305	2.46628
H	2.90740	4.18713	0.71244
H	3.49619	1.06901	3.62132
H	3.99628	3.34585	2.72931
C	0.15246	-1.73369	0.90098
C	0.48658	-4.32307	2.05998
C	1.03119	-2.70505	0.37054
C	-0.55310	-2.13070	2.04943
C	-0.39447	-3.39610	2.62110
C	1.21011	-3.97569	0.92100
H	-1.24342	-1.42816	2.50731
H	-0.96268	-3.66074	3.50960
H	1.89798	-4.68999	0.47700
H	0.61217	-5.30761	2.50074
N	-1.65606	-0.80748	-1.27012
C	-1.92324	-1.62741	-2.28905
C	-3.31213	-1.78728	-2.43117
C	-3.86836	-1.01302	-1.42713
N	-2.84756	-0.43417	-0.74411
N	1.52267	-1.07362	-1.29423
C	2.29395	-0.93469	-2.37532
C	3.03973	-2.10505	-2.58928
C	2.67042	-2.96273	-1.56490
N	1.75413	-2.31713	-0.79977
H	-1.11359	-2.05695	-2.86089
H	2.99267	-3.96525	-1.33279
H	3.75325	-2.30010	-3.37519
H	-3.83852	-2.38440	-3.16007
H	-4.89791	-0.84045	-1.15750
H	2.27514	-0.00796	-2.92994
C	0.50855	4.29478	-2.63142
C	-0.39775	3.31341	-3.13596
C	-0.52333	2.11272	-2.44741
N	0.16435	1.81804	-1.34069
C	1.06227	2.77373	-0.80934
C	1.21736	4.02300	-1.49138
H	0.62937	5.24419	-3.14424
H	-0.98658	3.48831	-4.02944
H	-1.20688	1.34237	-2.79433
H	1.90826	4.75776	-1.09174

Table S9. xyz-coordinates for **3**-TBP.

57

atom	x	y	z
Ir	-0.25437	0.13603	0.18983
C	-1.91976	0.93879	1.10386
C	-4.39015	1.85809	2.16102
C	-1.96592	1.82495	2.19639
C	-3.16873	0.53218	0.57210
C	-4.38979	0.97642	1.07993
C	-3.17891	2.27929	2.71772
H	-1.03439	2.16320	2.63887
H	-5.33055	0.64739	0.64772
H	-3.18211	2.96727	3.55928
H	-5.33478	2.21134	2.56410
C	1.18632	1.10616	1.21936
C	3.23528	2.66023	2.43595
C	1.53212	0.93587	2.57295
C	1.91740	2.08417	0.48222
C	2.92847	2.84805	1.09352
C	2.53339	1.69766	3.17323
H	1.00773	0.18859	3.16327
H	3.47930	3.59211	0.52378
H	2.77388	1.54069	4.22237
H	4.01498	3.25198	2.90650
C	0.47340	-1.76444	0.63795
C	1.29353	-4.40448	1.32098
C	1.34714	-2.50334	-0.17538
C	0.02454	-2.39932	1.81167
C	0.42198	-3.69439	2.14873
C	1.75530	-3.80092	0.15511
H	-0.65662	-1.87075	2.47446
H	0.04657	-4.14894	3.06250
H	2.42865	-4.32698	-0.51614
H	1.60554	-5.41262	1.57697
N	-1.88464	-0.76009	-0.94211
C	-2.06910	-1.61601	-1.94944
C	-3.44745	-1.77629	-2.19434
C	-4.08262	-0.97065	-1.26726
N	-3.11621	-0.36868	-0.52307
N	1.18213	-2.03116	-2.56095
C	1.99579	-1.50068	-3.47557
C	3.21568	-1.07462	-2.91178
C	3.09619	-1.38148	-1.56914
N	1.87114	-1.94460	-1.39421
H	-1.20128	-2.06196	-2.42023
H	3.76626	-1.24371	-0.73346
H	4.05755	-0.61292	-3.40597
H	-3.91547	-2.39955	-2.94110
H	-5.13012	-0.78831	-1.08633
H	1.67564	-1.44876	-4.50849
C	1.64871	3.21431	-3.13855
C	0.64771	2.32975	-3.55693
C	0.13739	1.43223	-2.63477
N	0.56743	1.38743	-1.35870
C	1.54787	2.23846	-0.92534
C	2.09569	3.16409	-1.82541
H	2.07299	3.93556	-3.83134
H	0.27243	2.33411	-4.57445
H	-0.63557	0.71812	-2.89453
H	2.86733	3.84570	-1.48743

Table S10. xyz-coordinates for **4**-octahedral.

57

atom	x	y	z
Ir	0.02776	0.03966	-0.13617
C	-1.56937	0.79064	0.88325
C	-3.99950	1.70140	2.08442
C	-1.55806	1.63164	2.00705
C	-2.83982	0.41354	0.37844
C	-4.01471	0.87107	0.97539
C	-2.75047	2.06271	2.57711
H	-0.62213	1.94832	2.45174
F	-5.22142	0.50308	0.47194
F	-2.70523	2.86759	3.65912
H	-4.92042	2.04521	2.53745
C	1.39743	1.02194	0.91797
C	3.33853	2.68525	2.16594
C	2.04764	0.61572	2.09441
C	1.75413	2.35697	0.34779
C	2.74396	3.14957	1.02071
C	3.00040	1.41112	2.72332
H	1.79293	-0.34794	2.52414
H	3.02209	4.12236	0.62797
H	3.48933	1.07558	3.63270
H	4.08427	3.29892	2.66569
C	0.14527	-1.72624	0.91069
C	0.49445	-4.32480	2.05812
C	1.04002	-2.67586	0.35727
C	-0.56354	-2.12242	2.05455
C	-0.38203	-3.38977	2.59724
C	1.19835	-3.93867	0.92823
H	-1.26343	-1.44763	2.53462
F	-1.08285	-3.73940	3.69664
F	2.05958	-4.83442	0.37823
H	0.62573	-5.30862	2.49017
N	-1.65249	-0.80426	-1.26397
C	-1.89448	-1.62200	-2.29056
C	-3.27783	-1.80110	-2.45227
C	-3.86361	-1.04193	-1.45438
N	-2.85906	-0.45034	-0.75136
N	1.50628	-1.02974	-1.28089
C	2.26647	-0.86603	-2.36606
C	3.02251	-2.02400	-2.60388
C	2.67462	-2.90414	-1.59212
N	1.75650	-2.28013	-0.80716
H	-1.07023	-2.03644	-2.85259
H	3.00178	-3.90512	-1.37280
H	3.73049	-2.19943	-3.39924
H	-3.78488	-2.40235	-3.19132
H	-4.89430	-0.87979	-1.19364
H	2.23180	0.06889	-2.90569
C	0.58578	4.24117	-2.68767
C	-0.35674	3.28032	-3.16200
C	-0.52237	2.10186	-2.44169
N	0.15916	1.81302	-1.33101
C	1.09582	2.74855	-0.82928
C	1.29118	3.97441	-1.54438
H	0.73758	5.17141	-3.22636
H	-0.94193	3.45102	-4.05837
H	-1.23129	1.34609	-2.76868
H	2.01002	4.69344	-1.16684

Table S11. xyz-coordinates for **4**-TBP.

57

atom	x	y	z
Ir	-0.32488	0.14020	0.22810
C	-2.00498	0.95505	1.11074
C	-4.48589	1.89461	2.13694
C	-2.04546	1.86699	2.17841
C	-3.24224	0.51598	0.56896
C	-4.44690	0.99027	1.08508
C	-3.26830	2.31437	2.66375
H	-1.13203	2.23478	2.63102
F	-5.62691	0.57254	0.55968
F	-3.29017	3.19514	3.68530
H	-5.43114	2.25242	2.52547
C	1.10543	1.12708	1.26589
C	3.17043	2.65785	2.48104
C	1.41010	0.99346	2.63167
C	1.88009	2.05837	0.51600
C	2.90016	2.81051	1.12605
C	2.42031	1.74436	3.23218
H	0.84961	0.28361	3.23455
H	3.48638	3.51863	0.54745
H	2.62890	1.61698	4.29201
H	3.95820	3.24014	2.94996
C	0.49470	-1.72658	0.66000
C	1.50339	-4.30914	1.34891
C	1.38629	-2.40863	-0.18519
C	0.11598	-2.36356	1.85475
C	0.61548	-3.62152	2.16865
C	1.86953	-3.67308	0.17320
H	-0.57000	-1.89423	2.55284
F	0.23163	-4.20424	3.32336
F	2.73011	-4.29761	-0.65419
H	1.88763	-5.28734	1.60785
N	-1.93738	-0.78860	-0.90039
C	-2.09953	-1.67418	-1.88557
C	-3.47091	-1.86898	-2.13452
C	-4.13256	-1.05423	-1.23544
N	-3.18265	-0.41005	-0.49956
N	1.11037	-2.01559	-2.56757
C	1.89427	-1.54551	-3.53661
C	3.14096	-1.10676	-3.04178
C	3.07048	-1.34087	-1.68317
N	1.84193	-1.86966	-1.43009
H	-1.21946	-2.11102	-2.34190
H	3.77852	-1.17756	-0.88443
H	3.96870	-0.68545	-3.59229
H	-3.91988	-2.52201	-2.86718
H	-5.18028	-0.88385	-1.05959
H	1.53621	-1.54308	-4.55813
C	1.73531	3.07774	-3.14442
C	0.70634	2.22511	-3.55716
C	0.14061	1.37779	-2.61872
N	0.54447	1.35725	-1.33493
C	1.54732	2.18043	-0.90510
C	2.15404	3.05234	-1.82106
H	2.20498	3.75627	-3.85076
H	0.35246	2.21306	-4.58214
H	-0.65468	0.68661	-2.87237
H	2.94888	3.70966	-1.48849

Table S12. xyz-coordinates for **5**-octahedral.

57

atom	x	y	z
Ir	0.02561	0.03853	-0.15269
C	-1.55224	0.80635	0.87155
C	-3.96558	1.74265	2.06480
C	-1.54284	1.66418	1.98593
C	-2.83354	0.44287	0.39347
C	-4.02506	0.89383	0.96236
C	-2.72245	2.12410	2.57397
H	-0.58873	1.96518	2.40568
H	-4.98827	0.59485	0.55908
H	-2.67197	2.78427	3.43594
H	-4.88441	2.10069	2.51948
C	1.41207	1.02165	0.90032
C	3.32807	2.68236	2.21238
C	2.07090	0.57881	2.05022
C	1.73535	2.36750	0.35594
C	2.70390	3.13999	1.08653
C	3.00234	1.38930	2.68299
H	1.85418	-0.39676	2.46946
F	3.02727	4.38863	0.65427
F	3.63320	0.95686	3.79605
H	4.05295	3.29816	2.73122
C	0.14438	-1.73789	0.89252
C	0.50280	-4.32926	2.03866
C	1.04357	-2.69234	0.36637
C	-0.56889	-2.15230	2.02992
C	-0.39769	-3.41897	2.59560
C	1.23421	-3.96395	0.91047
H	-1.27417	-1.46270	2.48470
H	-0.97115	-3.69698	3.47638
H	1.93761	-4.66492	0.46987
H	0.63838	-5.31430	2.47481
N	-1.66346	-0.80584	-1.25469
C	-1.92805	-1.62191	-2.27715
C	-3.31693	-1.77665	-2.42655
C	-3.87619	-1.00346	-1.42372
N	-2.85719	-0.43005	-0.73319
N	1.53348	-1.04367	-1.28181
C	2.31879	-0.88638	-2.34984
C	3.08382	-2.04500	-2.56036
C	2.71146	-2.91353	-1.54698
N	1.77529	-2.28619	-0.79181
H	-1.11684	-2.05271	-2.84572
H	3.04548	-3.91239	-1.31599
H	3.81121	-2.22510	-3.33701
H	-3.84114	-2.37015	-3.15987
H	-4.90665	-0.82736	-1.15985
H	2.29515	0.04319	-2.89956
C	0.52965	4.25094	-2.67946
C	-0.39097	3.26079	-3.15717
C	-0.52356	2.07710	-2.44477
N	0.16449	1.79651	-1.33373
C	1.08502	2.76693	-0.82194
C	1.24218	4.00280	-1.54052
H	0.65526	5.18591	-3.21597
H	-0.98563	3.42111	-4.04960
H	-1.21582	1.30707	-2.77373
H	1.94231	4.73241	-1.16052

Table S13. xyz-coordinates for **5**-TBP.

57

atom	x	y	z
Ir	-0.22510	0.14934	0.12571
C	-1.87706	0.94106	1.08171
C	-4.33519	1.82991	2.19051
C	-1.91122	1.81379	2.18500
C	-3.13162	0.53281	0.56549
C	-4.34710	0.96176	1.09893
C	-3.11838	2.25316	2.73218
H	-0.97550	2.15255	2.61778
H	-5.29274	0.63092	0.67919
H	-3.11227	2.93004	3.58249
H	-5.27532	2.17081	2.61426
C	1.21509	1.10785	1.16301
C	3.24755	2.64834	2.42949
C	1.54405	0.89917	2.51286
C	1.93095	2.10967	0.43056
C	2.92434	2.84381	1.09778
C	2.53620	1.66273	3.11036
H	1.04048	0.14065	3.10234
F	3.62559	3.80545	0.44239
F	2.83535	1.45314	4.40974
H	4.01860	3.23454	2.91269
C	0.49791	-1.74941	0.60316
C	1.35339	-4.33982	1.42227
C	1.40536	-2.50459	-0.15815
C	0.02352	-2.34936	1.78462
C	0.43944	-3.61870	2.19132
C	1.83017	-3.77804	0.24154
H	-0.68653	-1.80883	2.40639
H	0.04718	-4.04119	3.11315
H	2.52637	-4.32229	-0.39130
H	1.68226	-5.32793	1.72982
N	-1.86480	-0.73295	-0.98563
C	-2.06083	-1.57894	-1.99853
C	-3.44177	-1.74739	-2.22037
C	-4.06624	-0.95665	-1.27375
N	-3.09152	-0.35515	-0.54066
N	1.19806	-1.81709	-2.48880
C	2.05563	-1.42711	-3.43349
C	3.37731	-1.35560	-2.94858
C	3.27395	-1.73218	-1.62293
N	1.96093	-1.99399	-1.38019
H	-1.19543	-2.00850	-2.48627
H	4.01037	-1.82132	-0.83830
H	4.27194	-1.06789	-3.48039
H	-3.91848	-2.36592	-2.96539
H	-5.11172	-0.78415	-1.07245
H	1.69140	-1.21616	-4.43052
C	1.59741	3.28957	-3.17419
C	0.59875	2.40054	-3.58515
C	0.11821	1.48642	-2.66398
N	0.57333	1.43248	-1.39678
C	1.55258	2.29043	-0.96953
C	2.07405	3.23300	-1.87127
H	2.00181	4.02362	-3.86545
H	0.20236	2.41316	-4.59473
H	-0.65058	0.76549	-2.91573
H	2.84352	3.91237	-1.53734

Table S14. xyz-coordinates for **6**-octahedral.

57

atom	x	y	z
Ir	0.01106	0.04113	-0.13842
C	-1.57583	0.79388	0.88900
C	-4.00407	1.71441	2.08567
C	-1.56296	1.63846	2.00995
C	-2.84779	0.41722	0.38576
C	-4.02178	0.87956	0.97972
C	-2.75448	2.07490	2.57800
H	-0.62687	1.95423	2.45473
F	-5.22872	0.51330	0.47653
F	-2.70797	2.88360	3.65649
H	-4.92424	2.06254	2.53716
C	1.39976	1.02261	0.91727
C	3.37346	2.65742	2.18507
C	2.03811	0.59432	2.08133
C	1.76261	2.34927	0.34158
C	2.76719	3.10510	1.04773
C	2.99667	1.39084	2.69440
H	1.79352	-0.36283	2.52698
F	3.13810	4.32394	0.57495
F	3.60979	0.96829	3.81808
H	4.12316	3.25820	2.68603
C	0.13596	-1.72919	0.90238
C	0.50672	-4.32190	2.05367
C	1.04723	-2.66730	0.35677
C	-0.57804	-2.13312	2.03977
C	-0.38596	-3.39797	2.58499
C	1.21617	-3.92758	0.93013
H	-1.28971	-1.46638	2.51374
F	-1.09236	-3.75514	3.67773
F	2.09356	-4.81223	0.38867
H	0.64760	-5.30351	2.48775
N	-1.65765	-0.80256	-1.25249
C	-1.89765	-1.61942	-2.28040
C	-3.28081	-1.79761	-2.44508
C	-3.86883	-1.03894	-1.44814
N	-2.86587	-0.44826	-0.74219
N	1.51369	-1.01361	-1.27284
C	2.28429	-0.83984	-2.34890
C	3.05304	-1.99063	-2.58283
C	2.70250	-2.87674	-1.57785
N	1.77052	-2.26281	-0.80043
H	-1.07229	-2.03437	-2.84034
H	3.03605	-3.87542	-1.35779
H	3.76996	-2.15733	-3.37204
H	-3.78627	-2.39856	-3.18542
H	-4.89999	-0.87623	-1.18930
H	2.24657	0.09546	-2.88780
C	0.58070	4.22128	-2.70874
C	-0.37842	3.25722	-3.15573
C	-0.54003	2.08696	-2.42017
N	0.15379	1.80298	-1.31788
C	1.11170	2.74965	-0.83286
C	1.30089	3.96843	-1.57522
H	0.73105	5.14185	-3.26317
H	-0.97866	3.42056	-4.04368
H	-1.25865	1.33338	-2.73013
H	2.02994	4.68027	-1.21688

Table S15. xyz-coordinates for **6**-TBP.

57

atom	x	y	z
Ir	-0.18931	0.17971	0.20317
C	-1.95482	0.89193	1.00701
C	-4.53415	1.67092	1.90742
C	-2.10434	1.75162	2.10745
C	-3.13144	0.42301	0.36610
C	-4.38690	0.81960	0.82208
C	-3.37498	2.12017	2.53203
H	-1.24020	2.13708	2.63572
F	-5.50920	0.37416	0.20389
F	-3.50391	2.94847	3.58784
H	-5.51831	1.96704	2.24890
C	1.12852	1.19361	1.35226
C	3.02192	2.78561	2.76049
C	1.35409	1.00198	2.72360
C	1.87625	2.20594	0.66933
C	2.79940	2.96529	1.40570
C	2.28051	1.79096	3.39228
H	0.82245	0.23692	3.27927
F	3.53100	3.93446	0.79813
F	2.48074	1.59435	4.71029
H	3.74112	3.39106	3.29695
C	0.58828	-1.68840	0.69827
C	1.48538	-4.29762	1.42745
C	1.57859	-2.34943	-0.04619
C	0.05340	-2.35654	1.81292
C	0.50303	-3.62832	2.14851
C	2.00403	-3.62917	0.32927
H	-0.71809	-1.90453	2.42825
F	-0.03151	-4.24427	3.22264
F	2.95835	-4.23697	-0.40167
H	1.82599	-5.28812	1.70077
N	-1.67727	-0.76959	-1.05447
C	-1.73252	-1.62153	-2.08054
C	-3.07386	-1.85670	-2.43548
C	-3.82991	-1.10286	-1.55743
N	-2.96133	-0.45380	-0.73101
N	1.55511	-1.77585	-2.40804
C	2.44144	-1.25306	-3.25432
C	3.65000	-0.91184	-2.61083
C	3.44604	-1.26498	-1.29231
N	2.18436	-1.76657	-1.20190
H	-0.80426	-2.00635	-2.48461
H	4.08132	-1.20246	-0.42137
H	4.53860	-0.47576	-3.04193
H	-3.44365	-2.49563	-3.22281
H	-4.89348	-0.97732	-1.45263
H	2.18050	-1.14344	-4.29906
C	1.80085	3.35891	-2.95810
C	0.86347	2.44174	-3.44249
C	0.33431	1.51916	-2.55667
N	0.68790	1.48517	-1.25754
C	1.60645	2.36970	-0.75826
C	2.17341	3.32212	-1.62102
H	2.23939	4.10042	-3.61943
H	0.55046	2.43816	-4.48079
H	-0.39282	0.77729	-2.86427
H	2.89499	4.02397	-1.23147

Table S16. xyz-coordinates for 7-octahedral.

55

atom	x	y	z
Ir	-0.00769	-0.04448	-0.29126
C	-1.50020	0.78305	0.84556
C	-3.81886	1.78607	2.17925
C	-1.40568	1.64377	1.95254
C	-2.81765	0.45551	0.44950
C	-3.96384	0.93364	1.08675
C	-2.53702	2.13796	2.60835
H	-0.42087	1.92993	2.30937
H	-4.95601	0.65029	0.74623
H	-2.41759	2.80214	3.46093
H	-4.69961	2.16803	2.68678
C	1.50495	1.04390	0.53798
C	3.56745	2.79609	1.44654
C	2.29544	0.73982	1.65999
C	1.80335	2.27088	-0.09761
C	2.80728	3.14062	0.33162
C	3.30658	1.59373	2.10726
H	2.10702	-0.18503	2.19606
H	2.99820	4.07514	-0.18839
H	3.89493	1.31821	2.97894
H	4.35198	3.46205	1.79297
C	0.24490	-1.64537	0.86040
C	0.95769	-4.07556	2.22213
C	1.24248	-2.62093	0.31988
C	-0.34730	-1.99591	2.07686
C	-0.02379	-3.17332	2.75978
C	1.58762	-3.82225	1.03785
H	-1.07593	-1.31802	2.50978
H	-0.50348	-3.41129	3.70371
H	2.32885	-4.50732	0.64094
H	1.20333	-4.97970	2.77373
N	0.03479	1.71502	-1.58082
C	0.00548	3.44244	-3.01593
C	1.00778	3.65316	-2.08430
N	1.00276	2.59643	-1.23194
N	-1.77741	-0.84562	-1.24883
C	-2.11808	-1.63669	-2.26885
C	-3.51670	-1.72890	-2.35928
C	-3.99905	-0.94158	-1.32584
N	-2.92997	-0.42070	-0.67312
N	1.37565	-1.15501	-1.50636
C	2.10310	-1.07382	-2.64663
C	2.95421	-2.17820	-2.77578
C	2.75288	-2.97431	-1.65783
N	1.78645	-2.32521	-0.87165
H	-1.34584	-2.09540	-2.86917
H	3.19931	-3.90135	-1.34275
H	3.63650	-2.37728	-3.58908
H	-0.26630	4.08771	-3.83719
H	1.70896	4.46441	-1.97325
H	-4.09769	-2.29351	-3.07243
H	-5.00925	-0.72307	-1.01873
C	-0.57569	2.21451	-2.65716
H	-1.39124	1.67222	-3.11288
H	1.96572	-0.23034	-3.30707

Table S17. xyz-coordinates for **7**-TBP.

55

atom	x	y	z
Ir	0.09839	-0.27386	0.03550
C	-1.40144	0.51007	1.15965
C	-3.70922	1.55830	2.46929
C	-1.35897	0.95368	2.49393
C	-2.65808	0.62682	0.52163
C	-3.79811	1.13852	1.14367
C	-2.48638	1.46487	3.14048
H	-0.41717	0.90367	3.03350
H	-4.74255	1.21301	0.61187
H	-2.41167	1.79739	4.17288
H	-4.58622	1.95871	2.96893
C	1.28192	1.43217	0.27243
C	2.95110	3.68293	0.78488
C	2.09371	1.50836	1.42060
C	1.34887	2.52234	-0.61090
C	2.16524	3.63255	-0.36291
C	2.91496	2.60823	1.67537
H	2.07983	0.68939	2.13636
H	2.17962	4.44576	-1.08406
H	3.52462	2.62608	2.57578
H	3.58508	4.54363	0.97679
C	0.28283	-2.10310	0.98077
C	0.81511	-4.66275	2.08973
C	1.24816	-2.98023	0.42887
C	-0.39880	-2.56602	2.12028
C	-0.14278	-3.82483	2.66690
C	1.52033	-4.24028	0.96262
H	-1.14553	-1.92670	2.58102
H	-0.69272	-4.15520	3.54431
H	2.26753	-4.88967	0.51570
H	1.01797	-5.64172	2.51366
N	0.90000	1.83837	-2.90891
C	-0.90024	3.15263	-3.35974
C	-0.51273	3.36502	-2.05007
N	0.55785	2.56035	-1.81218
N	-1.53430	-0.24821	-1.37942
C	-1.81127	-0.63435	-2.63198
C	-3.17573	-0.45594	-2.89724
C	-3.71067	0.06430	-1.72773
N	-2.70187	0.17978	-0.82975
N	1.62023	-1.25587	-1.15201
C	2.38028	-1.01052	-2.22009
C	3.20489	-2.12167	-2.48572
C	2.89810	-3.05156	-1.50948
N	1.93745	-2.50384	-0.71621
H	-1.01907	-1.00680	-3.26309
H	3.28412	-4.04156	-1.32515
H	3.92867	-2.22900	-3.27923
H	-1.72011	3.61912	-3.88517
H	-0.90518	4.00720	-1.27546
H	-3.70465	-0.67048	-3.81333
H	-4.72072	0.34915	-1.47929
C	0.01425	2.19330	-3.84075
H	0.07158	1.75094	-4.82729
H	2.27801	-0.05577	-2.72030

Table S18. xyz-coordinates for **8**-octahedral.

55

atom	x	y	z
Ir	0.01112	-0.02514	-0.29680
C	-1.48164	0.79709	0.83164
C	-3.80003	1.76139	2.19654
C	-1.37416	1.66479	1.92888
C	-2.79188	0.42537	0.43649
C	-3.91244	0.90356	1.11419
C	-2.51374	2.12441	2.57953
H	-0.40383	1.98543	2.28995
F	-5.15863	0.53182	0.72098
F	-2.37792	2.95929	3.63116
H	-4.67878	2.12474	2.71404
C	1.51568	1.06015	0.54041
C	3.57953	2.81521	1.45952
C	2.30144	0.74179	1.65903
C	1.79377	2.29191	-0.10477
C	2.80398	3.13536	0.35648
C	3.30074	1.60732	2.08968
H	2.13669	-0.17740	2.20876
F	3.05203	4.30951	-0.27952
F	4.03893	1.26972	3.16775
H	4.35996	3.48023	1.80620
C	0.24076	-1.63206	0.86895
C	0.86056	-4.11094	2.22697
C	1.20257	-2.63649	0.30654
C	-0.35382	-1.94903	2.08332
C	-0.06073	-3.14464	2.74071
C	1.47116	-3.85441	1.04510
H	-1.05413	-1.26388	2.54687
F	-0.65346	-3.43464	3.91597
F	2.35011	-4.75062	0.53432
H	1.06582	-5.02445	2.77218
N	0.04216	1.71496	-1.57960
C	-0.04795	3.45456	-2.99651
C	0.95854	3.68825	-2.07541
N	0.99123	2.62161	-1.23051
N	-1.73876	-0.86270	-1.24525
C	-2.06210	-1.66376	-2.26236
C	-3.45788	-1.78354	-2.35642
C	-3.96328	-1.00324	-1.32974
N	-2.90337	-0.45781	-0.67377
N	1.38058	-1.15382	-1.49024
C	2.11249	-1.06607	-2.62529
C	2.93655	-2.19129	-2.77785
C	2.71785	-3.00820	-1.68544
N	1.76124	-2.35257	-0.87741
H	-1.27988	-2.10840	-2.86009
H	3.13375	-3.95164	-1.38613
H	3.61425	-2.38857	-3.59530
H	-0.34713	4.10042	-3.80771
H	1.63876	4.51254	-1.95427
H	-4.02519	-2.36199	-3.06947
H	-4.97271	-0.79797	-1.01991
C	-0.59212	2.20863	-2.64443
H	-1.39889	1.64941	-3.09511
H	1.99585	-0.20560	-3.26714

Table S19. xyz-coordinates for **8**-TBP.

55

atom	x	y	z
Ir	0.13169	-0.27219	0.10543
C	-1.33706	0.56582	1.23410
C	-3.60003	1.73168	2.53516
C	-1.26483	1.00533	2.56638
C	-2.58023	0.72889	0.57126
C	-3.67360	1.30351	1.21864
C	-2.37729	1.56740	3.18285
H	-0.34078	0.92896	3.13013
F	-4.85023	1.45644	0.55846
F	-2.27778	1.97806	4.46430
H	-4.45625	2.17558	3.02731
C	1.34958	1.41328	0.29233
C	3.09435	3.64010	0.66289
C	2.19588	1.49566	1.41151
C	1.39284	2.46286	-0.64036
C	2.25715	3.54648	-0.43759
C	3.04074	2.58831	1.57039
H	2.21085	0.71842	2.16913
F	2.27550	4.54340	-1.34419
F	3.84061	2.64136	2.65420
H	3.75489	4.48664	0.80125
C	0.27165	-2.10257	1.05841
C	0.72472	-4.68390	2.16037
C	1.20072	-3.00109	0.47293
C	-0.41391	-2.52662	2.20752
C	-0.18061	-3.79309	2.72945
C	1.40738	-4.26206	1.02818
H	-1.13238	-1.88024	2.69844
F	-0.85502	-4.18798	3.82786
F	2.29329	-5.11875	0.46139
H	0.89816	-5.66771	2.57790
N	0.95116	1.79840	-2.93464
C	-0.87880	3.07924	-3.36525
C	-0.50433	3.27364	-2.05003
N	0.58254	2.48417	-1.81975
N	-1.48537	-0.19842	-1.30602
C	-1.75914	-0.57792	-2.56117
C	-3.10785	-0.33994	-2.84847
C	-3.64207	0.21028	-1.69261
N	-2.64340	0.28477	-0.77585
N	1.59886	-1.28791	-1.09615
C	2.33786	-1.05655	-2.18303
C	3.11666	-2.19040	-2.48060
C	2.80809	-3.12253	-1.50716
N	1.88627	-2.55290	-0.67983
H	-0.97334	-0.98653	-3.17789
H	3.16125	-4.12469	-1.33573
H	3.81479	-2.31229	-3.29459
H	-1.70461	3.53913	-3.88603
H	-0.91014	3.89924	-1.26970
H	-3.62987	-0.53281	-3.77284
H	-4.63617	0.54776	-1.45709
C	0.06203	2.15277	-3.86233
H	0.13380	1.73384	-4.85751
H	2.25188	-0.09527	-2.67541

Table S20. xyz-coordinates for **9**-octahedral.

88

atom	x	y	z
Ir	0.03919	-0.01646	-0.21100
C	-1.39999	0.94272	0.88758
C	-3.67308	2.08027	2.17981
C	-1.24985	1.80270	1.98772
C	-2.73575	0.68900	0.48262
C	-3.86785	1.23561	1.09838
C	-2.36464	2.35980	2.62486
H	-0.25044	2.02502	2.34851
H	-4.87063	1.00291	0.74892
C	1.63775	0.95821	0.61522
C	3.87016	2.54236	1.41479
C	2.42219	0.59430	1.72271
C	2.02766	2.14988	-0.04965
C	3.11747	2.94434	0.32384
C	3.52139	1.36810	2.11300
H	2.16493	-0.30397	2.27566
H	3.37438	3.84606	-0.22619
C	0.10584	-1.63893	0.98142
C	0.44635	-4.19083	2.28206
C	0.98286	-2.72410	0.46516
C	-0.57049	-1.90367	2.15022
C	-0.44135	-3.15806	2.81895
C	1.14965	-3.98873	1.13962
H	-1.22200	-1.14520	2.57000
H	1.80542	-4.75342	0.73425
N	0.21802	1.69823	-1.51785
C	0.28288	3.42314	-2.95502
C	1.30029	3.57603	-2.02860
N	1.23747	2.52192	-1.17439
N	-1.76174	-0.72184	-1.16491
C	-2.14386	-1.50849	-2.17363
C	-3.54380	-1.49820	-2.28967
C	-3.98422	-0.65397	-1.28367
N	-2.88962	-0.19992	-0.62122
N	1.37378	-1.27392	-1.34573
C	2.11535	-1.27320	-2.46527
C	2.83192	-2.47332	-2.58621
C	2.50426	-3.22988	-1.47242
N	1.61488	-2.47943	-0.71953
H	-1.40007	-2.03685	-2.75208
H	2.82380	-4.20763	-1.15418
H	3.50528	-2.75478	-3.38189
H	0.04416	4.08441	-3.77395
H	2.04611	4.34692	-1.92037
H	-4.15267	-2.03373	-3.00208
H	-4.98034	-0.35293	-1.00163
C	-0.36787	2.23185	-2.59179
H	-1.21906	1.74033	-3.03981
H	2.09186	-0.41421	-3.11978
C	-2.02306	-5.11397	6.18797
C	-2.47525	-3.80522	5.94685
C	-2.01103	-3.07237	4.86406
C	-1.06269	-3.66415	3.98910
C	-0.60734	-4.99784	4.24568
C	-1.07999	-5.71131	5.32702
H	-2.40212	-5.66847	7.04150
H	-3.20279	-3.36167	6.62191
H	-2.36711	-2.06206	4.68460
H	-0.73500	-6.72448	5.51923

C	-3.18371	4.91345	5.90521
C	-1.83368	4.64833	5.65004
C	-1.46125	3.82016	4.58922
C	-2.45746	3.25911	3.78530
C	-3.81796	3.52826	4.04506
C	-4.18404	4.35332	5.10196
H	-3.45869	5.55887	6.73523
H	-1.06923	5.08948	6.28393
H	-0.41249	3.61381	4.39490
H	-5.23158	4.56267	5.30746
C	6.57128	1.27981	5.05256
C	5.64296	0.23408	5.09088
C	4.59775	0.17438	4.16744
C	4.49242	1.17821	3.20123
C	5.42949	2.23288	3.16479
C	6.46805	2.28718	4.08660
H	7.37970	1.30937	5.77827
H	5.73779	-0.54041	5.84750
H	3.87924	-0.64037	4.20058
H	7.19392	3.09696	4.06008
C	0.39513	-5.41056	3.18152
H	0.07695	-6.30894	2.63530
H	1.38002	-5.64382	3.60934
C	-4.69197	2.80109	3.03976
H	-5.30998	3.49743	2.45609
H	-5.38820	2.10652	3.52961
C	5.09973	3.18149	2.02790
H	4.90323	4.20044	2.38871
H	5.92695	3.26065	1.30906

Table S21. xyz-coordinates for **9**-TBP.

88

atom	x	y	z
Ir	0.17478	-0.25204	0.25444
C	-1.24305	0.85459	1.20884
C	-3.44093	2.36723	2.20817
C	-1.21219	1.40434	2.50359
C	-2.42264	1.10312	0.45825
C	-3.51244	1.84658	0.92564
C	-2.29182	2.14475	2.99709
H	-0.32828	1.25725	3.11901
H	-4.38858	2.01695	0.30526
C	1.66815	1.20810	0.37907
C	3.88497	2.97942	0.51446
C	2.52727	1.20159	1.49362
C	1.95147	2.13721	-0.63883
C	3.04152	3.01941	-0.58303
C	3.62354	2.06597	1.55580
H	2.34875	0.49961	2.30472
H	3.21038	3.70514	-1.40979
C	-0.02960	-2.04090	1.27307
C	-0.09616	-4.63163	2.41754
C	0.78232	-3.10654	0.80264
C	-0.87526	-2.31843	2.36022
C	-0.91531	-3.59785	2.91927
C	0.76429	-4.39155	1.35513
H	-1.51006	-1.52937	2.75241
H	1.39587	-5.18429	0.96268
N	1.44388	1.50993	-2.93256
C	-0.31167	2.89596	-3.34295

C	0.08714	3.06382	-2.03044
N	1.12912	2.21702	-1.81710
N	-1.33695	-0.10389	-1.27797
C	-1.60005	-0.56659	-2.50697
C	-2.90474	-0.21633	-2.87990
C	-3.41751	0.48753	-1.80046
N	-2.45311	0.54117	-0.84891
N	1.55948	-1.54053	-0.79345
C	2.40595	-1.48045	-1.82272
C	3.03168	-2.73032	-1.99896
C	2.51177	-3.54785	-1.01241
N	1.62277	-2.80438	-0.29819
H	-0.83979	-1.10988	-3.04718
H	2.70552	-4.58084	-0.77056
H	3.76646	-2.99841	-2.74277
H	-1.11646	3.40378	-3.85343
H	-0.27724	3.70302	-1.23987
H	-3.40936	-0.43900	-3.80768
H	-4.38570	0.93731	-1.64778
C	0.56640	1.91639	-3.85113
H	0.60231	1.49323	-4.84709
H	2.49926	-0.55216	-2.37269
C	-3.00817	-5.65614	5.97486
C	-3.32657	-4.30383	5.80733
C	-2.69037	-3.53594	4.82998
C	-1.72706	-4.13993	4.01778
C	-1.40544	-5.50355	4.18824
C	-2.04254	-6.26311	5.16318
H	-3.51447	-6.23900	6.73938
H	-4.07857	-3.84651	6.44492
H	-2.94387	-2.48655	4.70487
H	-1.79887	-7.31474	5.29594
C	-3.35786	4.22367	6.53130
C	-2.10462	3.60218	6.53212
C	-1.66055	2.89219	5.41525
C	-2.48978	2.81120	4.29357
C	-3.75392	3.43834	4.29459
C	-4.19044	4.14457	5.40933
H	-3.68723	4.77293	7.40930
H	-1.47056	3.67411	7.41190
H	-0.68525	2.41280	5.42075
H	-5.16348	4.63049	5.41431
C	6.87111	2.87674	4.15013
C	5.97803	1.88467	4.56847
C	4.87258	1.54671	3.78606
C	4.67199	2.21634	2.57680
C	5.57239	3.21777	2.15588
C	6.67204	3.54937	2.93929
H	7.72777	3.12586	4.77075
H	6.14826	1.37132	5.51127
H	4.18312	0.77287	4.11366
H	7.37142	4.31832	2.61932
C	-0.34006	-5.91481	3.18780
H	-0.68283	-6.72863	2.53371
H	0.57065	-6.27840	3.68383
C	-4.45158	3.20335	2.96792
H	-4.67877	4.14703	2.45313
H	-5.41011	2.68199	3.09612
C	5.13593	3.78122	0.81610
H	4.93548	4.85986	0.87207
H	5.90785	3.64896	0.04537

Table S22. xyz-coordinates for **10**-octahedral.

82

atom	x	y	z
Ir	1.34439	1.85160	-4.51263
C	1.41873	1.87016	-6.65402
C	1.83370	1.91589	-9.46101
C	0.46430	2.41194	-7.52735
C	2.57908	1.34200	-7.24826
C	2.81323	1.37989	-8.62534
C	0.65470	2.41932	-8.91244
H	-0.45312	2.82727	-7.12008
H	3.74575	1.03502	-9.05272
H	-0.11481	2.83080	-9.56166
H	2.00151	1.94498	-10.53412
C	-0.58993	2.53753	-4.35961
C	-3.12236	3.79060	-4.03195
C	-1.77803	1.78993	-4.24066
C	-0.74259	3.95177	-4.34077
C	-1.97481	4.57791	-4.15931
C	-3.02319	2.39920	-4.08083
H	-1.71749	0.70705	-4.27788
H	-2.06316	5.65421	-4.09761
H	-3.91773	1.78842	-3.98963
H	-4.08708	4.27118	-3.89592
C	0.75390	-0.16685	-4.33715
C	-0.01613	-2.82198	-3.67976
C	0.55435	-0.58347	-2.99580
C	0.54980	-1.13339	-5.32987
C	0.15461	-2.43945	-5.01338
C	0.19370	-1.89629	-2.65841
H	0.68363	-0.85821	-6.37306
H	-0.01480	-3.16171	-5.80879
H	0.11484	-2.20149	-1.62031
H	-0.29817	-3.84180	-3.43173
C	1.62519	3.89900	-4.58417
C	2.16976	6.08503	-4.85542
C	0.77435	6.02260	-4.67911
N	0.48039	4.66414	-4.50325
C	3.26592	1.01318	-4.97856
N	4.28687	0.40034	-4.31540
C	5.15562	-0.22318	-5.20935
C	4.65650	0.01770	-6.50035
N	3.51581	0.80665	-6.31513
C	1.57016	1.56127	-2.43670
N	1.39000	2.46372	-1.34982
C	0.50413	1.96955	-0.42622
C	0.09946	0.67403	-0.85778
N	0.78062	0.41645	-2.03185
N	2.64556	4.77636	-4.78771
C	2.84589	7.28398	-5.06437
C	2.08394	8.45181	-5.09758
C	0.69295	8.40165	-4.93367
C	0.01787	7.19722	-4.72563
H	3.92180	7.30704	-5.20375
H	2.57304	9.40725	-5.25999
H	0.11823	9.32212	-4.97405
H	-1.05799	7.19778	-4.62183
C	-0.91113	1.77119	1.49462
C	0.00189	2.53131	0.74977
C	-0.84427	-0.05417	-0.12656
C	-1.33191	0.51020	1.06028
H	-1.30610	2.17706	2.42196

H	0.30217	3.52325	1.07100
H	-1.19808	-1.01869	-0.46648
H	-2.05464	-0.04570	1.65045
C	5.29058	-0.54429	-7.61285
C	6.43829	-1.30452	-7.38921
C	6.94595	-1.51287	-6.09845
C	6.30468	-0.97748	-4.98280
H	4.90611	-0.42900	-8.61633
H	6.94436	-1.75198	-8.23952
H	7.84281	-2.11026	-5.96472
H	6.67766	-1.15011	-3.97870
C	4.04221	4.42326	-4.96546
H	4.66407	4.98528	-4.26123
H	4.15182	3.35676	-4.77848
H	4.36884	4.64687	-5.98639
C	4.47993	0.35202	-2.87422
H	5.40987	0.86321	-2.60076
H	3.61966	0.84206	-2.40670
H	4.53392	-0.68945	-2.54203
C	2.03339	3.74836	-1.23744
H	2.43703	3.88569	-0.22670
H	2.85722	3.79307	-1.95106
H	1.34202	4.57598	-1.44808

Table S23. xyz-coordinates for **10**-TBP.

82

atom	x	y	z
Ir	1.02148	1.34609	-4.36556
C	1.02992	1.68611	-6.42211
C	1.35896	2.11659	-9.21369
C	-0.06767	1.89360	-7.27002
C	2.30104	1.71190	-7.03713
C	2.48130	1.92317	-8.40511
C	0.08562	2.10306	-8.64508
H	-1.06821	1.89220	-6.84316
H	3.46374	1.94401	-8.85757
H	-0.79004	2.25732	-9.27153
H	1.48876	2.28083	-10.27986
C	-0.25963	2.98730	-4.06570
C	-2.18025	5.05768	-3.72378
C	-1.57288	2.72006	-3.62836
C	0.06129	4.33586	-4.30518
C	-0.88233	5.35580	-4.12741
C	-2.52412	3.72975	-3.47348
H	-1.86495	1.69357	-3.42602
H	-0.58406	6.38635	-4.29985
H	-3.53108	3.47551	-3.15077
H	-2.90692	5.85451	-3.59259
C	-0.04753	-0.42299	-4.40644
C	-1.26387	-2.96761	-4.14441
C	-0.30132	-1.00663	-3.13627
C	-0.44347	-1.16143	-5.53524
C	-1.05155	-2.41319	-5.40780
C	-0.88202	-2.26586	-2.99690
H	-0.26847	-0.74801	-6.52296
H	-1.35034	-2.96218	-6.29728
H	-1.01688	-2.72090	-2.02374
H	-1.71804	-3.94912	-4.04224
C	2.51306	4.43065	-4.01433
C	3.03523	5.70817	-5.85534

C	1.64689	5.51101	-5.85603
N	1.37661	4.73146	-4.72257
C	3.00856	1.33202	-4.78468
N	4.18086	1.11705	-4.10282
C	5.26359	1.17732	-4.96578
C	4.75330	1.42111	-6.25979
N	3.36956	1.50366	-6.11353
C	0.83481	0.92773	-2.34457
N	1.06977	1.55838	-1.16208
C	0.49286	0.85508	-0.10569
C	-0.13341	-0.27974	-0.65674
N	0.11619	-0.20919	-2.03261
N	3.51157	5.03713	-4.72853
C	3.67100	6.44820	-6.85131
C	2.86732	6.98109	-7.85904
C	1.47876	6.77184	-7.86921
C	0.84493	6.03325	-6.87063
H	4.74585	6.59998	-6.84816
H	3.32480	7.56341	-8.65376
H	0.88414	7.19136	-8.67572
H	-0.22546	5.86268	-6.88364
C	-0.23583	0.24417	2.07626
C	0.45771	1.13508	1.25768
C	-0.84025	-1.15849	0.16813
C	-0.87659	-0.87901	1.53549
H	-0.28772	0.42905	3.14505
H	0.94352	2.01612	1.66395
H	-1.36467	-2.02003	-0.22184
H	-1.42208	-1.54904	2.19337
C	5.63290	1.52932	-7.34200
C	6.99992	1.39638	-7.09078
C	7.49458	1.16072	-5.80072
C	6.62811	1.04690	-4.71391
H	5.28796	1.71102	-8.34988
H	7.69512	1.48056	-7.92064
H	8.56509	1.06680	-5.64383
H	7.00114	0.86802	-3.71070
C	4.90845	5.00414	-4.34080
H	5.29837	6.01968	-4.20421
H	4.97867	4.46407	-3.39670
H	5.51567	4.49204	-5.09520
C	4.31520	0.89708	-2.67694
H	4.75339	1.77311	-2.18745
H	3.33017	0.70855	-2.26010
H	4.95534	0.02944	-2.49341
C	1.74605	2.83927	-1.00627
H	2.61669	2.72384	-0.35045
H	2.06144	3.21736	-1.98472
H	1.05995	3.56173	-0.55268