Electronic Supplementary Information

En route to phosphonato iridium(I) complexes: the decisive effect of an intramolecular hydrogen bond

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1. Selected NMR data of IrCl(SiNP)(tfbb) (1)

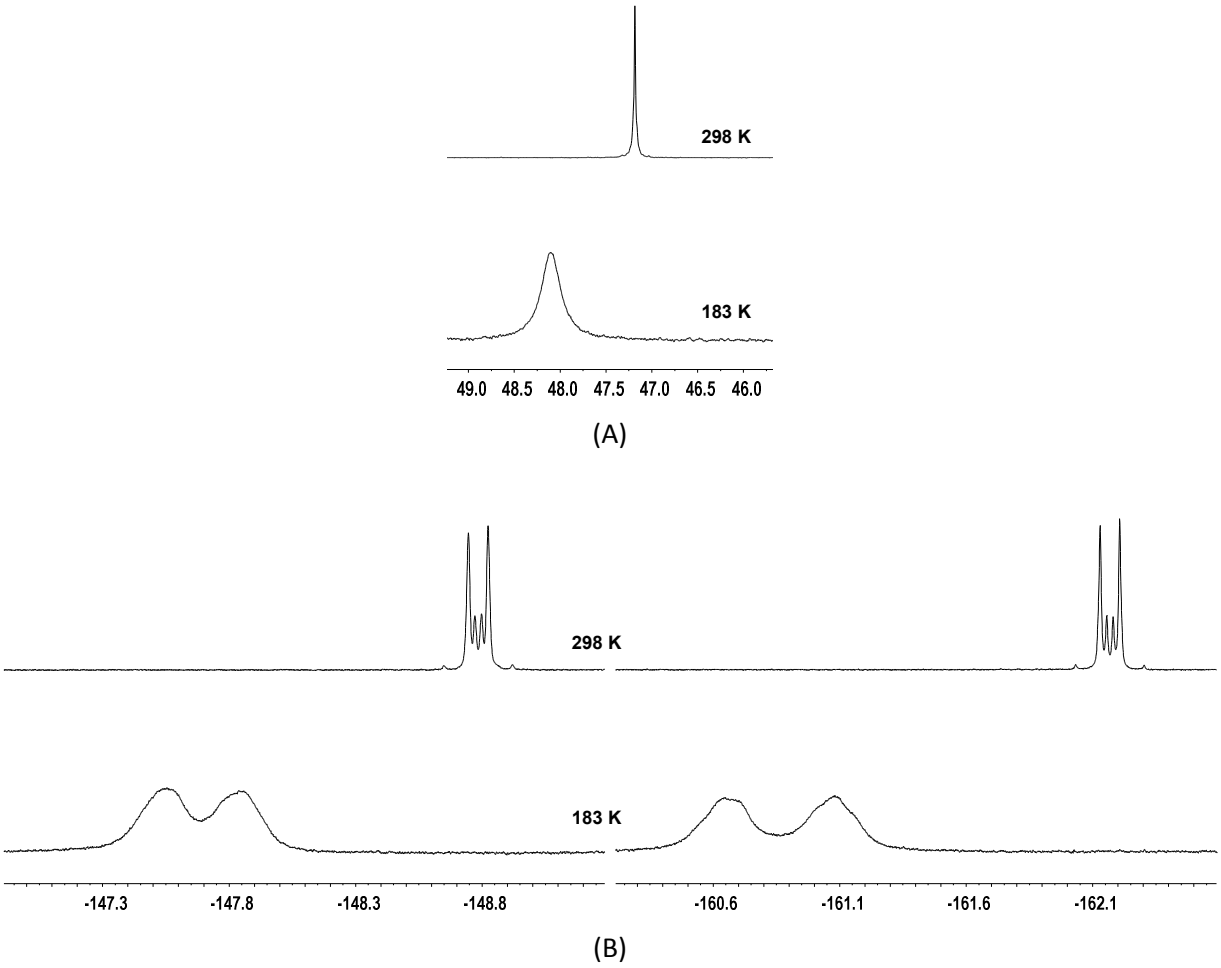


Figure S1. Selected regions of the NMR spectra of IrCl(SiNP)(tfbb) (**1**) (A, $^{31}P\{^{1}H\}$; B, ^{19}F) at 183 K and 298 K.

2. Selected NMR and kinetic data of $[Ir(SiNP)\{P(OMe)_3\}(tfbb)]^+$ (3^+)

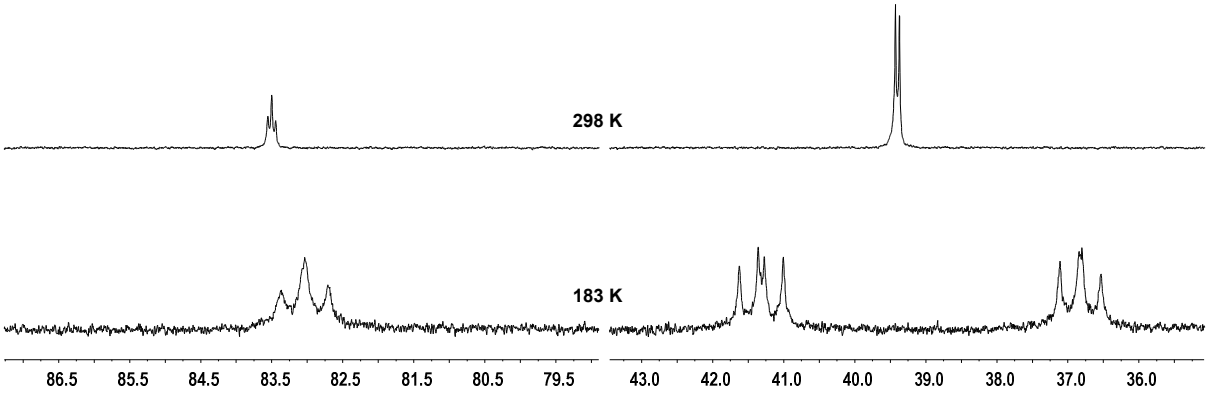
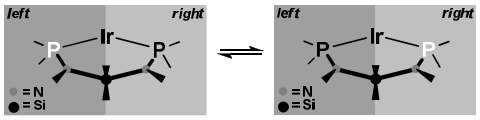


Figure S2. Selected regions of the $^{31}P\{^1H\}$ NMR spectrum (CD_2Cl_2) of $[Ir(SiNP)\{P(OMe)_3\}(tfbb)]Cl$ ([**3**]Cl) at 183 K and 298 K.

Table S1. Kinetic constants and activation parameters for the observed dynamics of [**3**]Cl (in CD_2Cl_2).



ΔH_{act} = 48.1±0.5 kJ·mol^{-1}

ΔS_{act} = 48.0±2.5 J·mol^{-1}·K^{-1}

T (K)	k (sec^{-1})
183	$3.00\cdot10^{1}$
193	$1.00\cdot10^{2}$
203	$4.50\cdot10^{2}$
213	$2.50\cdot10^{3}$
223	$8.00\cdot10^{3}$
233	$2.90\cdot10^{4}$

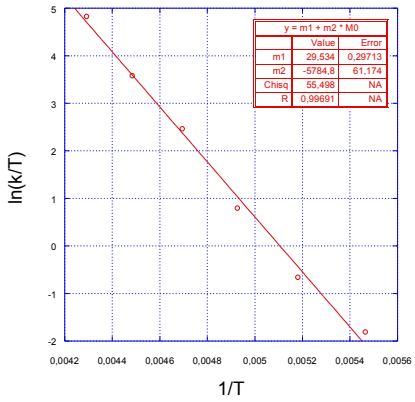


Figure S3. Eyring plot for the left-right exchange at the SiNP ligand in [**3**]Cl (CD_2Cl_2).

3. Selected bond lengths and angles of the calculated structure of IrCl(SiNP)(tfbb) (1)

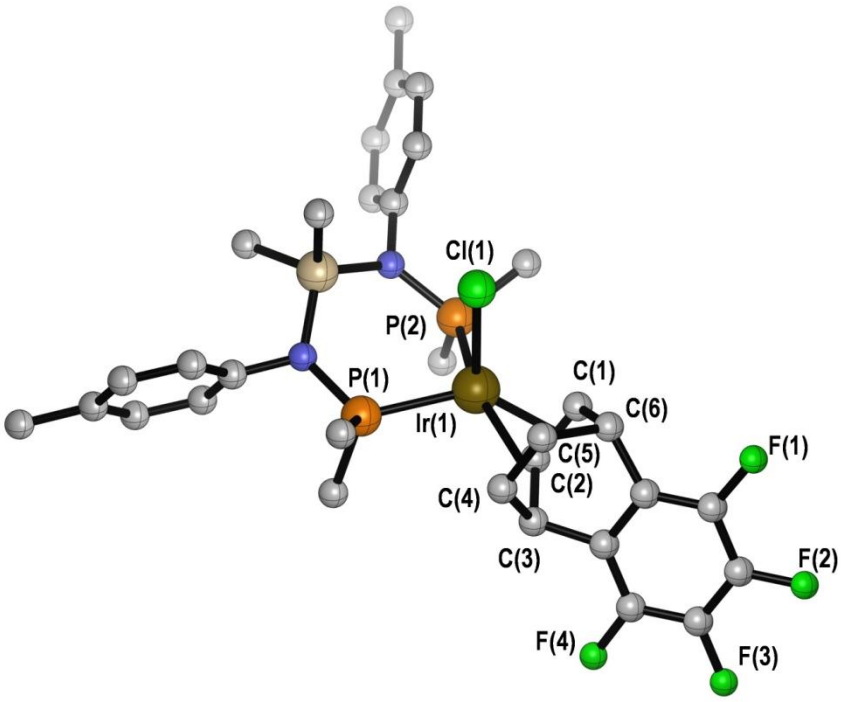


Figure S4. View of the DFT–B3LYP calculated structure of IrCl(SiNP)(tfbb) (**1**) (CH_2Cl_2, 298 K) with the numbering scheme adopted. Most hydrogen atoms are omitted and only *ipso* carbon atoms are shown for clarity.

Table S2. Selected bond lengths (Å) and angles (°) of the DFT-B3LYP calculated structure of IrCl(SiNP)(tfbb) (**1**).*

Ir(1)–C(1)	2.127	P(1)–Ir(1)–P(2)	95.48
Ir(1)–C(2)	2.118	P(1)–Ir(1)–Cl(1)	94.24
Ir(1)–ct[1–2]	1.993	P(2)–Ir(1)–Cl(1)	90.13
Ir(1)–C(4)	2.297	ct[1–2]–Ir(1)–P(1)	138.45
Ir(1)–C(5)	2.280	ct[4–5]–Ir(1)–P(1)	99.00
Ir(1)–ct[4–5]	2.181	ct[1–2]–Ir(1)–P(2)	96.98
C(1)–C(2)	1.458	ct[4–5]–Ir(1)–P(2)	163.75
C(4)–C(5)	1.387	ct[1–2]–Ir(1)–Cl(1)	125.13
Ir(1)–P(1)	2.373	ct[4–5]–Ir(1)–Cl(1)	96.09
Ir(1)–P(2)	2.315	ct[1–2]–Ir(1)–ct[4–5]	67.20
Ir(1)–Cl(1)	2.576		

* ct[X–Y]: centroid of the C(X)–C(Y) bond.

4. Selected bond lengths and angles of the calculated structure of $IrCl(HNP)_2(tfbb)$ (2)

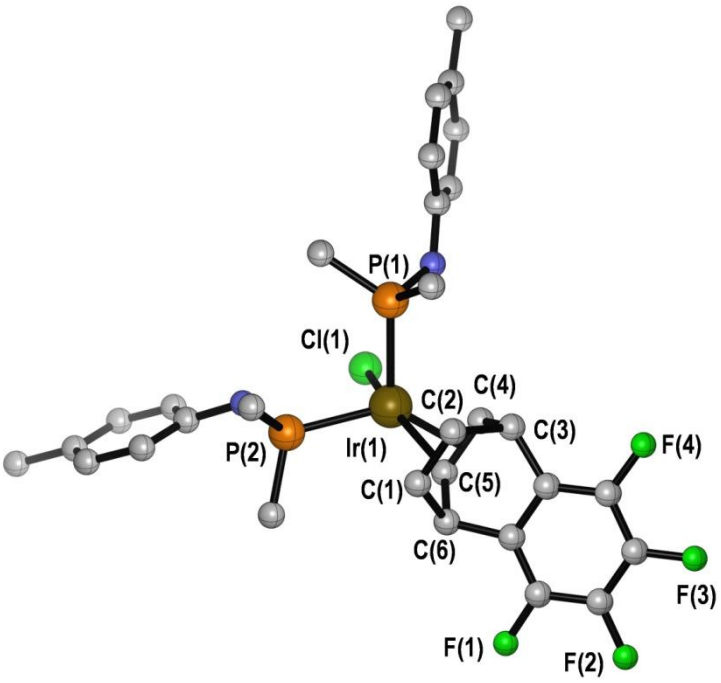


Figure S5. View of the DFT–B3LYP calculated structure of $IrCl(HNP)_2(tfbb)$ (**2**) (CH_2Cl_2, 298 K) with the numbering scheme adopted. Most hydrogen atoms are omitted and only *ipso* carbon atoms are shown for clarity.

Table S3. Selected bond lengths (Å) and angles (°) of the DFT-B3LYP calculated structure of $IrCl(HNP)_2(tfbb)$ (**2**).*

Ir(1)–C(1)	2.191	P(1)–Ir(1)–P(2)	99.99
Ir(1)–C(2)	2.176	P(1)–Ir(1)–Cl(1)	87.33
Ir(1)–ct[1–2]	2.066	P(2)–Ir(1)–Cl(1)	91.33
Ir(1)–C(4)	2.121	ct[1–2]–Ir(1)–P(1)	107.49
Ir(1)–C(5)	2.128	ct[4–5]–Ir(1)–P(1)	123.41
Ir(1)–ct[4–5]	1.997	ct[1–2]–Ir(1)–P(2)	101.39
C(1)–C(2)	1.413	ct[4–5]–Ir(1)–P(2)	136.58
C(4)–C(5)	1.451	ct[1–2]–Ir(1)–Cl(1)	158.20
Ir(1)–P(1)	2.462	ct[4–5]–Ir(1)–Cl(1)	89.92
Ir(1)–P(2)	2.404	ct[1–2]–Ir(1)–ct[4–5]	68.66
Ir(1)–Cl(1)	2.466		

* ct[X–Y]: centroid of the C(X)–C(Y) bond.

5. Selected bond lengths and angles of the calculated structure of $[Ir(SiNP)\{P(OMe)_3\}(tfbb)]^+$ (3^+)

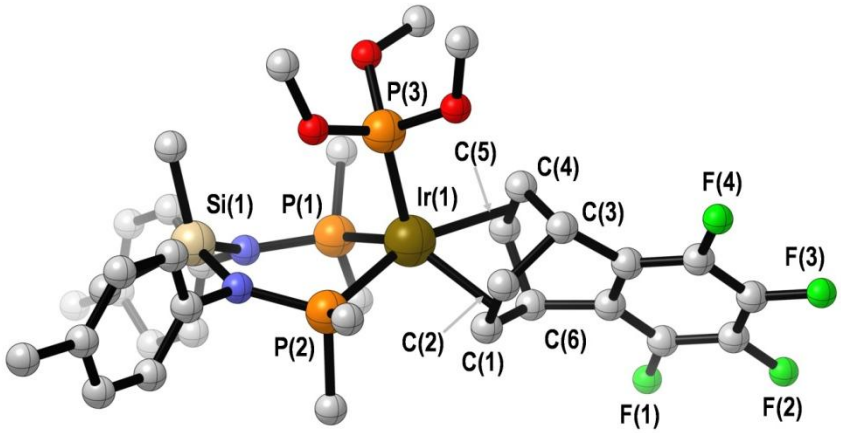


Figure S6. View of the DFT–B3LYP calculated structure of $[Ir(SiNP)\{P(OMe)_3\}(tfbb)]^+$ ($\mathbf{3}^+$) (CH_2Cl_2, 298 K) with the numbering scheme adopted. Most hydrogen atoms are omitted and only *ipso* carbon atoms are shown for clarity.

Table S4. Selected bond lengths (Å) and angles (°) of the DFT-B3LYP calculated structure of $[Ir(SiNP)\{P(OMe)_3\}(tfbb)]^+$ ($\mathbf{3}^+$).*

Ir(1)–C(1)	2.165	P(1)–Ir(1)–P(2)	94.59
Ir(1)–C(2)	2.148	P(1)–Ir(1)–P(3)	102.96
Ir(1)–ct[1-2]	2.031	P(2)–Ir(1)–P(3)	95.72
Ir(1)–C(4)	2.340	ct[1-2]–Ir(1)–P(1)	129.67
Ir(1)–C(5)	2.348	ct[4-5]–Ir(1)–P(1)	98.62
Ir(1)–ct[4-5]	2.239	ct[1-2]–Ir(1)–P(2)	93.28
C(1)–C(2)	1.448	ct[4-5]–Ir(1)–P(2)	158.62
C(5)–C(4)	1.387	ct[1-2]–Ir(1)–P(3)	125.54
Ir(1)–P(1)	2.436	ct[4-5]–Ir(1)–P(3)	97.60
Ir(1)–P(2)	2.355	ct[4-5]–Ir(1)–ct[1-2]	65.36
Ir(1)–P(3)	2.339		

* ct[X–Y]: centroid of the C(X)–C(Y) bond.

6. Selected bond lengths and angles of the calculated structure of Ir{PO(OMe)$_2$}(SiNP)(tfbb) (4)

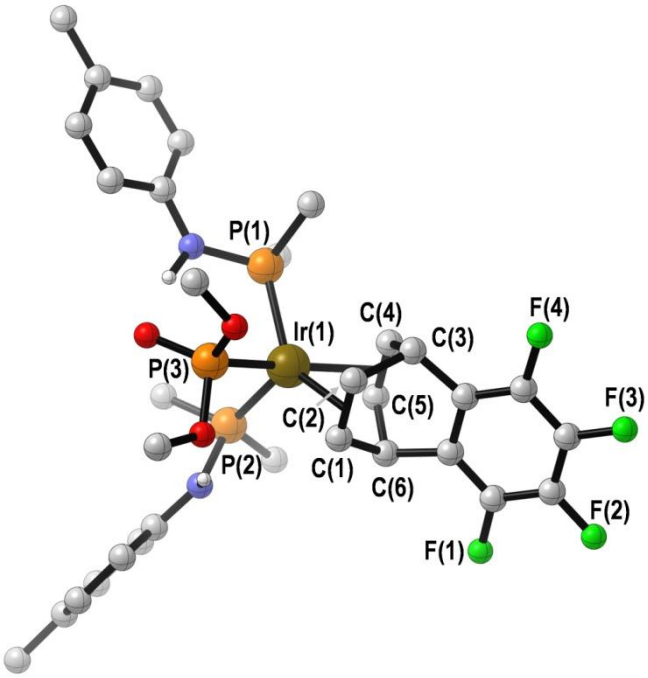


Figure S7. View of the DFT–B3LYP calculated structure of Ir{PO(OMe)$_2$}(SiNP)(tfbb) (**4**) (CH_2Cl_2, 298 K) with the numbering scheme adopted. Most hydrogen atoms are omitted and only *ipso* carbon atoms are shown for clarity.

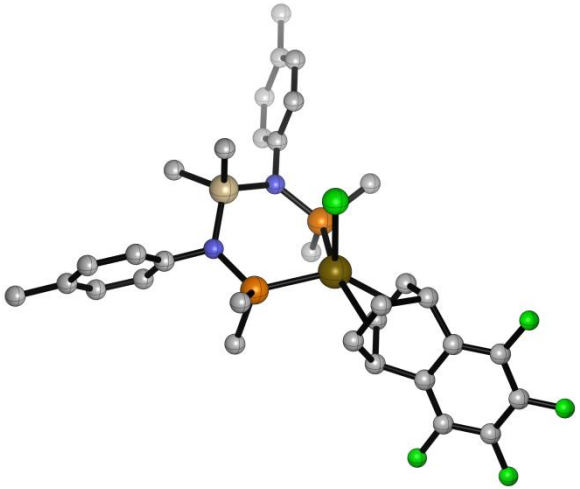
Table S5. Selected bond lengths (Å) and angles (°) of the DFT-B3LYP calculated structure of Ir{PO(OMe)$_2$}(SiNP)(tfbb) (**4**).*

Ir(1)–C(1)	2.143	P(1)–Ir(1)–P(2)	100.46
Ir(1)–C(2)	2.160	P(1)–Ir(1)–P(3)	91.56
Ir(1)–ct[1–2]	2.027	P(2)–Ir(1)–P(3)	93.49
Ir(1)–C(4)	2.317	ct[1–2]–Ir(1)–P(1)	139.62
Ir(1)–C(5)	2.305	ct[4–5]–Ir(1)–P(1)	97.78
Ir(1)–ct[4–5]	2.204	ct[1–2]–Ir(1)–P(2)	119.38
C(1)–C(2)	1.446	ct[4–5]–Ir(1)–P(2)	106.82
C(4)–C(5)	1.391	ct[1–2]–Ir(1)–P(3)	92.29
Ir(1)–P(1)	2.397	ct[4–5]–Ir(1)–P(3)	155.57
Ir(1)–P(2)	2.436	ct[1–2]–Ir(1)–ct[4–5]	66.14
Ir(1)–P(3)	2.313		

* ct[X–Y]: centroid of the C(X)–C(Y) bond.

7. Atomic coordinates of the calculated structures

IrCl(SiNP)(tfbb) (1)



Ir	-0.80391	0.15105	-0.51781
P	0.62901	-1.73156	-0.33469
P	0.71429	1.66903	0.34878
Si	3.18486	0.06504	-0.82208
N	2.34912	1.50425	-0.16406
N	2.34405	-1.43332	-0.33595
C	3.896	3.10078	0.94725
H	3.81023	2.53073	1.86576
C	4.11769	4.5713	-1.40179
H	4.18985	5.14333	-2.32367
C	3.23977	-2.54121	-0.07159
C	3.18361	2.69109	-0.1864
C	3.3016	3.44235	-1.36376
H	2.73244	3.14309	-2.23769
C	4.8373	4.98785	-0.27332
C	3.68946	-3.38018	-1.09919
H	3.33891	-3.21854	-2.11187
C	3.70637	-2.77388	1.23043
H	3.35787	-2.13433	2.03455
C	4.58015	-4.42088	-0.82694
H	4.91825	-5.05574	-1.64234
C	3.44366	0.17577	-2.67928
H	2.49913	0.32083	-3.20856
H	3.92804	-0.73882	-3.04094
H	4.10775	1.0131	-2.91885
C	0.78344	1.61135	2.20127
C	1.78143	0.8668	2.84664
H	2.55699	0.39253	2.25544
C	-0.21741	2.20954	2.98693
H	-0.99322	2.80579	2.51743
C	1.78837	0.72984	4.23592
H	2.57398	0.15287	4.71564
C	4.90228	0.02285	-0.03713
H	5.44838	0.93209	-0.30429
H	5.47297	-0.83148	-0.41237
H	4.87925	-0.0466	1.05431
C	-2.51383	1.36419	-0.16073
C	-2.33229	0.40946	0.92554
C	-2.56207	-1.32527	-0.58945
C	5.74074	6.19707	-0.33067
H	5.92331	6.60865	0.66629
H	5.30992	6.98948	-0.95082
H	6.71674	5.94338	-0.76331
C	-2.71282	-0.41807	-1.62808
C	5.05084	-4.65628	0.46997
C	-0.21214	2.07044	4.37614
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C	4.70674	4.23532	0.90045
H	5.24935	4.53802	1.79292
C	-4.63805	-0.46913	0.48321
C	-4.8015	0.44236	-0.57741
C	-3.19469	-0.85669	0.72863
C	4.59848	-3.81012	1.49285
H	4.94929	-3.96575	2.51035
C	0.79108	1.33056	5.00537
H	0.79674	1.22679	6.08656
C	-6.0687	0.90072	-0.89978
C	-7.18343	0.46426	-0.17938
C	-7.02132	-0.43728	0.86993
C	0.33925	-2.96478	-1.69407
C	0.83671	-2.67023	-2.97565
H	1.42921	-1.77719	-3.13024
C	0.3814	-2.736	1.20754
C	-0.3449	3.76879	-1.19828
H	-0.59594	2.9808	-1.90101
C	-0.48215	-4.09489	-1.54454
H	-0.89426	-4.34623	-0.57335
C	0.29636	3.43968	0.00716
C	-0.21795	-2.10999	2.31087
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C	5.99779	-5.79533	0.76608
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C	-0.25169	-4.62835	-3.89446
H	-0.47549	-5.27053	-4.74152
C	-5.7445	-0.89975	1.19715
C	-3.49526	0.84174	-1.23183
Cl	-0.03884	0.74067	-2.90617
F	-8.09265	-0.857	1.558
F	-5.61814	-1.76993	2.2189
F	-6.25772	1.77306	-1.90839
F	-8.4098	0.90542	-0.49243
H	-2.13068	0.7353	1.94229
H	-3.62212	1.53122	-2.06487
H	-3.07892	-1.58302	1.53181
H	-2.44603	2.43574	-0.00182
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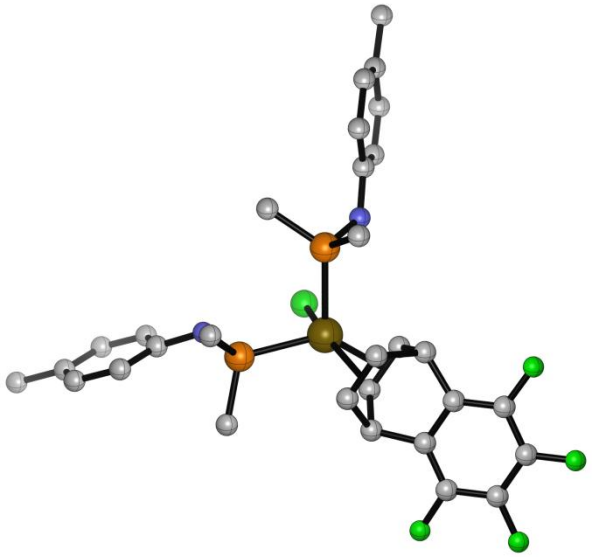
$IrCl(HNP)_2(tfbb)$ (2)



Ir	0.50028	-0.16778	-0.54292
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P	-1.16283	-1.69441	0.28644
C	2.08751	-1.0098	-1.68319
C	2.00497	-1.30061	0.57469
C	2.30516	0.41183	-1.49392
C	3.16882	0.70048	-0.24621
C	2.20495	0.08215	0.78643
C	4.25629	-1.47354	-0.49321
C	6.84392	-0.4537	-0.25648
C	5.74378	0.40321	-0.1752
C	4.45581	-0.09446	-0.29221
N	-2.53975	-1.67112	-0.71823
N	-0.20595	3.03897	-1.08701
F	5.96631	1.71759	0.01886
F	8.08918	0.02781	-0.14212
F	5.18844	-3.64615	-0.76325
F	7.70295	-2.63911	-0.53206
C	-0.62356	-3.46953	0.29975
C	-0.68129	-4.32171	1.41051
C	5.34887	-2.32231	-0.57254
C	-0.13449	-3.97805	-0.91641
C	-0.24442	-5.64616	1.31321
C	0.24024	-6.13938	0.10289
C	6.64636	-1.81833	-0.45575
C	0.28719	-5.30247	-1.01574
C	-1.80133	-1.40474	1.99532
C	-0.93557	-1.48719	3.10096
C	-3.1286	-1.00824	2.21151
C	-3.55801	-2.62527	-0.92775
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C	-4.2155	-2.63352	-2.1714
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C	-5.25249	-3.52463	-2.42144
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C	-2.72355	-0.83035	4.59322
C	-5.00955	-4.43703	-0.22486
C	-6.78695	-5.42902	-1.74516
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C	-0.94502	4.66892	-2.71882
C	-2.71602	2.71857	1.86915
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C	0.35228	2.18601	2.92653
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C	1.35322	3.79284	1.42321
C	-1.21631	5.18936	-0.3818
C	-1.75942	6.42457	-0.73723
C	-4.54596	1.97206	-0.0988
C	-1.47862	5.90839	-3.05507
C	-4.08676	2.86017	2.09668
C	-5.00528	2.48663	1.11598
C	1.10658	2.70282	3.98058
C	2.1118	4.3031	2.47989
C	1.98812	3.76433	3.76077
C	-2.45638	8.16977	-2.44511
H	-6.49684	-6.15505	-2.51471
H	-7.06431	-5.99279	-0.84971
H	-7.68637	-4.91947	-2.10973
H	-5.74191	-3.5031	-3.39267
H	-5.30941	-5.13906	0.54975
H	-3.4991	-3.55953	1.0209
H	-3.9041	-1.93317	-2.94257
H	-2.83167	1.43379	-1.27801
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H	-6.07103	2.60242	1.29215
H	-4.43275	3.27293	3.04033
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H	-1.12205	4.93234	0.66601
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H	1.00935	2.27087	4.9727
H	-0.31158	1.34596	3.10995
H	0.10309	-1.77378	2.96425
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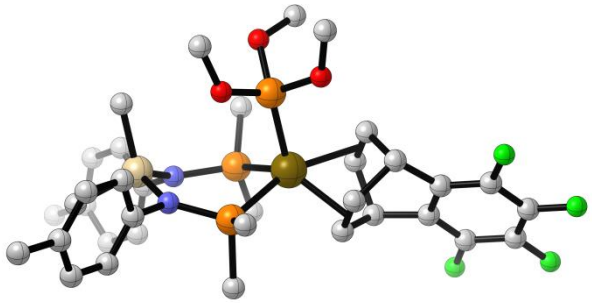
H	-0.71421	-1.29407	5.23254
H	-4.61515	-0.41542	3.64609
H	-3.80147	-0.91089	1.36739
H	-0.00685	2.49637	-1.92192
H	-2.35421	-1.08361	-1.53018
H	-0.08741	-3.32935	-1.78653
H	0.57659	-7.16941	0.02788
H	-0.29244	-6.29197	2.18553
H	-1.07308	-3.96184	2.35572
H	0.65551	-5.68094	-1.965
Cl	-0.76126	0.15902	-2.63724

[Ir(SiNP){P(OMe)$_3$}(tfbb)]$^+$ (3^+)



C	-3.61602	-0.15731	2.28879
H	-4.20544	-1.07033	2.42299
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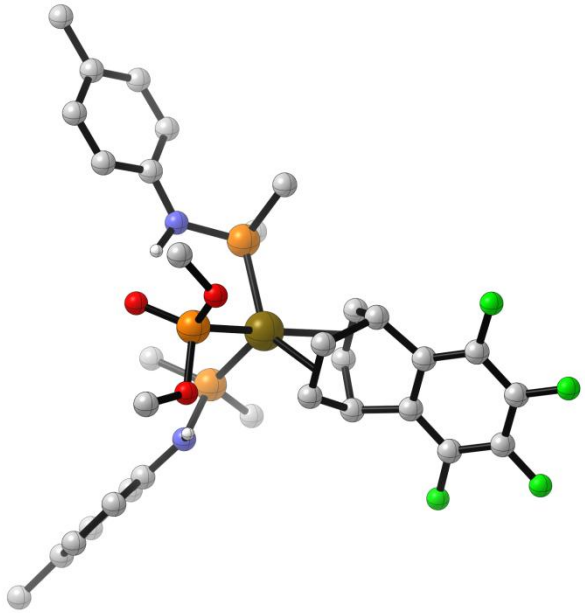
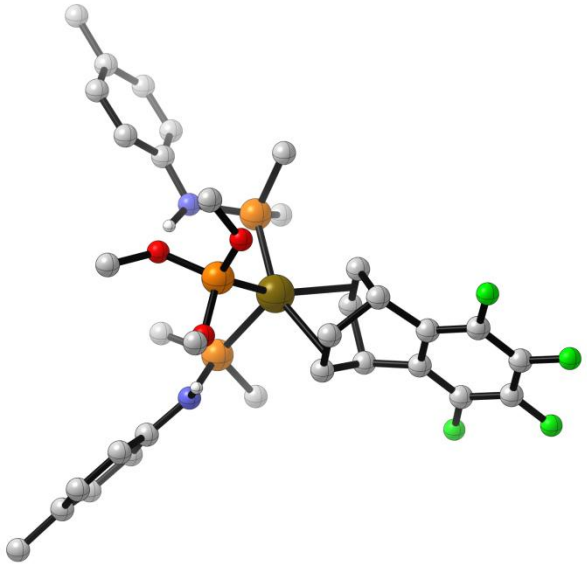
H	-2.725	-0.23469	2.9123
C	-4.91049	0.29801	-0.39284
H	-4.83005	0.44514	-1.47302
H	-5.43902	1.16206	0.01924
H	-5.52821	-0.58723	-0.21902
C	-0.42253	2.87046	1.90163
C	-1.28345	2.66646	2.99071
H	-2.07338	1.9301	2.91923
C	-1.14481	3.40286	4.16814
H	-1.83656	3.23646	4.98896
C	-0.12551	4.34846	4.29123
H	-0.01891	4.92477	5.20522
C	0.75179	4.55208	3.22524
H	1.54394	5.29095	3.30262
C	0.60254	3.82422	2.04202
H	1.26787	4.04187	1.21333
C	-0.17731	3.00476	-0.97804
C	0.28033	2.49593	-2.20331
H	0.42317	1.42895	-2.31482
C	0.53616	3.34429	-3.28204
H	0.88858	2.92829	-4.2212
C	0.34128	4.71993	-3.15108
H	0.54905	5.38307	-3.98554
C	-0.13077	5.23817	-1.94418
H	-0.30214	6.30518	-1.83834
C	-0.39822	4.38922	-0.86994
H	-0.79337	4.81155	0.04616
C	-0.44344	-3.3519	-0.65232
C	0.37236	-3.92072	0.337
H	0.84691	-3.29396	1.07866
C	0.60797	-5.29673	0.3661
H	1.25154	-5.71353	1.13534
C	0.03131	-6.13023	-0.59127
H	0.21733	-7.19988	-0.56954
C	-0.77918	-5.57804	-1.58435
H	-1.23102	-6.21491	-2.33869
C	-1.01073	-4.20414	-1.61867
H	-1.64007	-3.80166	-2.40235
C	-0.7605	-1.22509	-2.53905
C	0.18718	-1.8465	-3.37202
H	0.88621	-2.56772	-2.9615
C	0.22112	-1.57242	-4.74065
H	0.95492	-2.06868	-5.36868
C	-0.69276	-0.67838	-5.3018
H	-0.67219	-0.47446	-6.36802
C	-1.63911	-0.0571	-4.48555
H	-2.35911	0.63393	-4.91403
C	-1.66822	-0.32478	-3.11554
H	-2.40746	0.16372	-2.4919
C	-3.11988	2.73813	-0.17834
C	-3.74202	3.51776	0.80432
H	-3.58504	3.29315	1.85231
C	-4.56558	4.58665	0.44603
H	-5.03737	5.17612	1.22793
C	-4.79776	4.90999	-0.89619
C	-4.16558	4.12739	-1.87319
H	-4.31947	4.35775	-2.92427
C	-3.34235	3.05994	-1.5241
H	-2.85321	2.47686	-2.29673
C	-5.71688	6.04443	-1.27995
H	-6.74126	5.68444	-1.43619
H	-5.3967	6.52276	-2.21012
H	-5.75671	6.80958	-0.49969
C	-3.34102	-2.44037	-0.45868
C	-4.03307	-2.59593	-1.66692
H	-3.86626	-1.89327	-2.47566
C	-4.92914	-3.65092	-1.83438
H	-5.45486	-3.75515	-2.78011
C	-5.16861	-4.57508	-0.80723
C	-4.4679	-4.41151	0.39499
H	-4.62471	-5.11944	1.20482
C	-3.56701	-3.3618	0.56988
H	-3.00989	-3.25806	1.49344
C	-6.16701	-5.69349	-0.98348
H	-5.92721	-6.54931	-0.34626
H	-6.20232	-6.03997	-2.0204
H	-7.17848	-5.36232	-0.71785
C	2.6032	1.28338	0.50264
H	2.32822	2.27118	0.84464
C	2.88258	0.23939	1.37175
H	2.86579	0.34541	2.44762
C	3.57355	-0.95187	0.69645
H	3.78177	-1.7591	1.39477
C	2.45955	-1.29945	-0.31015
H	2.34691	-2.33287	-0.61903
C	2.17625	-0.20129	-1.21077
H	1.83893	-0.374	-2.22565
C	3.06784	1.0225	-0.93171
H	2.86682	1.85909	-1.59706
C	4.52397	0.60817	-0.92064
C	5.54225	1.15041	-1.6881
C	6.84147	0.64418	-1.59181
C	7.11332	-0.41033	-0.7209
C	6.08574	-0.95766	0.05258
C	4.79777	-0.45591	-0.04322
C	-1.50465	-2.6072	3.90788
H	-1.32654	-1.94559	4.75647
H	-1.05971	-3.58901	4.08682
H	-2.57909	-2.72034	3.75744
C	1.04185	0.69372	4.47708
H	1.96234	0.14482	4.70162
H	0.62144	1.0827	5.40478
H	1.25589	1.53265	3.81085
C	1.73385	-2.70758	4.25625
H	1.21314	-2.20538	5.0755
H	2.79794	-2.77471	4.49069
H	1.33156	-3.71619	4.12697
O	-0.97377	-2.04722	2.68735
O	0.04752	-0.1754	3.91377
O	1.62327	-1.97296	3.02228
F	5.30414	2.16664	-2.53519
F	7.82555	1.16658	-2.32759
F	8.35585	-0.89021	-0.6291
F	6.37247	-1.97437	0.88421
Si	-3.24664	0.09477	0.46049
P	-0.59811	1.81507	0.37924
P	-0.78169	-1.52898	-0.70888
P	0.32154	-1.07551	2.56053
Ir	0.77919	-0.19362	0.44251
N	-2.30112	1.5828	0.16955
N	-2.42217	-1.32992	-0.24787

Ir{PO(OMe)$_2$}(HNP)$_2$(tfbb) (4)



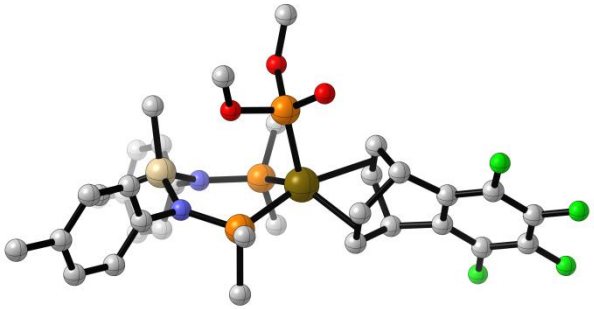
Ir	0.4646	-0.2704	-0.4152
C	2.63293	-2.23169	-0.47297
P	-0.13384	1.94328	0.40929
P	-1.35537	-1.56524	0.45366
P	-0.62793	0.02996	-2.43129
C	2.07772	-1.22288	-1.49098
C	1.8773	-1.6941	0.74513
C	2.42738	0.14403	-1.17229
C	3.24704	0.2288	0.13463
C	2.2083	-0.38798	1.08928
O	-2.11128	0.35904	-2.5168
O	-0.34696	-1.26581	-3.44123
O	0.24816	1.20491	-3.23003
C	4.11922	-2.01623	-0.28268
C	6.78833	-1.29382	0.08829
C	5.77896	-0.33747	0.22683
C	4.4511	-0.68785	0.04473
N	-2.85123	-1.16193	-0.24914
N	0.29864	3.05089	-0.82884
F	6.1292	0.92469	0.54095
F	8.07262	-0.95611	0.26768
F	4.83202	-4.24126	-0.73396
F	7.42897	-3.5233	-0.36667
C	-1.16387	-3.39802	0.22572
C	-1.57119	-4.3647	1.15744
C	5.12071	-2.96326	-0.42071
C	-0.62447	-3.83006	-0.9991
C	-1.43121	-5.72653	0.87866
C	-0.89557	-6.14284	-0.3396
C	6.45915	-2.60777	-0.23614
C	-0.49701	-5.19021	-1.28028
C	-0.13485	1.54693	-4.57013
C	-1.4187	-1.81294	-4.22124
C	-1.63342	-1.36535	2.27512
C	-0.8008	-1.96891	3.234
C	-2.64064	-0.49366	2.71945
C	-4.08084	-1.85267	-0.27991
C	-4.54822	-2.66492	0.7617
C	-6.61624	-3.1271	-0.45434
C	-4.9036	-1.67843	-1.40952
C	-2.81106	-0.2372	4.08145
C	-6.14482	-2.29934	-1.4848
C	-0.97213	-1.71156	4.59515
C	-1.97811	-0.84274	5.02366
C	-5.79243	-3.29105	0.66264
C	-7.95562	-3.81824	-0.55944
C	-1.85827	2.45731	0.88274
C	0.87471	2.47456	1.86564
C	-0.03235	4.41208	-1.00961
C	-0.0072	4.93445	-2.31591
C	-2.19666	3.02558	2.12066
C	-2.86992	2.28506	-0.07816
C	0.66512	1.88437	3.12599
C	-0.61006	7.15361	-1.51124
C	1.92765	3.38833	1.71735
C	-0.34976	5.28371	0.04131
C	-0.63676	6.62509	-0.21774
C	-4.18407	2.65909	0.20433
C	-0.28569	6.27493	-2.55521
C	-3.51434	3.39398	2.4002
C	-4.51365	3.20834	1.44486
C	1.47272	2.22426	4.21187
C	2.73982	3.72036	2.80537
C	2.51305	3.14421	4.05507
C	-0.90594	8.61047	-1.78007
H	-7.93936	-4.61874	-1.30988
H	-8.24697	-4.2693	0.39377
H	-8.74767	-3.12044	-0.85406
H	-6.75958	-2.14192	-2.36857
H	-6.13016	-3.91632	1.48614
H	-3.95928	-2.79265	1.66109
H	-4.55319	-1.04638	-2.22103
H	-2.64066	1.85092	-1.04679
H	-4.95201	2.51482	-0.55019
H	-5.53877	3.49523	1.66216
H	-3.75367	3.83506	3.36409
H	-1.4361	3.19441	2.8736
H	-0.37715	4.92592	1.06218
H	-0.88537	7.27495	0.61812
H	-0.25704	6.64425	-3.57808
H	0.23225	4.27537	-3.14597
H	-1.66127	8.72998	-2.56526
H	-1.27781	9.11282	-0.88232
H	-0.01063	9.15071	-2.11247
H	0.07395	0.71433	-5.24975
H	-1.19706	1.80584	-4.61731
H	0.46806	2.40847	-4.8665
H	-0.95902	-2.50776	-4.92887
H	-2.12894	-2.35653	-3.58972
H	-1.96409	-1.03883	-4.76707
H	3.5111	1.24859	0.40938
H	2.37244	-3.26257	-0.70678
H	1.98721	0.04824	2.05341
H	1.34651	-2.3682	1.40297
H	2.57983	0.88483	-1.94897
H	1.88858	-1.54871	-2.5068
H	2.1076	3.84161	0.74858
H	3.5495	4.43216	2.67196
H	3.14407	3.40429	4.89996
H	1.29168	1.76346	5.17884
H	-0.12545	1.15141	3.26242
H	-0.02663	-2.66567	2.92983
H	-2.11425	-0.64493	6.08307
H	-0.32336	-2.19655	5.31915
H	-3.59789	0.43962	4.4011
H	-3.29178	-0.01915	1.99384
H	0.48864	2.56428	-1.70199
H	-2.72179	-0.53523	-1.05472
H	-0.30075	-3.09332	-1.72861
H	-0.78843	-7.20207	-0.55544
H	-1.74728	-6.45998	1.61513
H	-1.9922	-4.06358	2.10988
H	-0.08006	-5.50577	-2.23263

$[Ir(HNP)_2\{P(OMe)_3\}(tfbb)]^+$ (5^+)



Ir	0.48863	-0.2634	-0.45816
C	2.98181	-1.49254	-1.3224
P	-0.2522	1.88495	0.48212
P	-1.13675	-1.71	0.47032
P	-0.55298	-0.04076	-2.50186
C	2.43592	-0.10618	-1.68168
C	1.9836	-1.80655	-0.19525
C	2.51508	0.81943	-0.64201
C	3.12568	0.22419	0.63662
C	2.05691	-0.85916	0.89455
O	-2.19078	0.12751	-2.5246
O	-0.2652	-1.20998	-3.61106
O	-0.01257	1.31379	-3.27613
C	4.37652	-1.35008	-0.7552
C	6.80826	-0.89721	0.52954
C	5.66371	-0.20575	0.93718
C	4.45201	-0.42613	0.30182
N	-2.72411	-1.11652	0.25585
N	-0.09723	3.06781	-0.74457
F	5.76501	0.67057	1.95076
F	7.9769	-0.68414	1.13845
F	5.45882	-2.92281	-2.16895
F	7.82779	-2.46856	-0.90809
C	-1.11483	-3.44403	-0.1632
C	-1.74088	-4.47842	0.55601
C	5.51031	-2.03591	-1.16018
C	-0.55885	-3.73524	-1.41882
C	-1.80777	-5.76761	0.02721
C	-1.24884	-6.04603	-1.22093
C	6.73208	-1.81252	-0.5197
C	-0.62358	-5.02751	-1.94165
C	0.2012	1.44175	-4.69841
C	-1.20077	-1.72604	-4.57835
C	-0.94172	-1.92055	2.28707
C	-0.03256	-2.85483	2.8111
C	-1.64521	-1.08494	3.16883
C	-3.95047	-1.84777	0.33614
C	-4.37754	-2.46568	1.51763
C	-6.45335	-3.17888	0.44722
C	-4.78749	-1.90022	-0.78754
C	-1.45018	-1.19127	4.54747
C	-6.02094	-2.54369	-0.72498
C	0.16497	-2.95203	4.18984
C	-0.54363	-2.1219	5.06051
C	-5.60564	-3.1261	1.56019
C	-7.77435	-3.90833	0.49983
C	-1.9547	2.18053	1.1465
C	0.87086	2.44105	1.83577
C	-0.58596	4.39862	-0.83097
C	-0.70081	4.97602	-2.10628
C	-2.23554	2.37625	2.5063
C	-3.01399	2.23698	0.22597
C	0.97521	1.68216	3.01505
C	-1.50273	7.06883	-1.15073
C	1.7013	3.56011	1.67397
C	-0.93941	5.17023	0.28304
C	-1.39292	6.47908	0.11297
C	-4.3205	2.46282	0.65369
C	-1.14588	6.28568	-2.25733
C	-3.54719	2.59857	2.9342
C	-4.59262	2.6377	2.01232
C	1.87081	2.05254	4.01839
C	2.60545	3.92028	2.67662
C	2.69024	3.17188	3.85101
C	-1.96179	8.49764	-1.31842
H	-7.6788	-4.93124	0.11495
H	-8.15105	-3.9801	1.524
H	-8.5348	-3.4055	-0.10525
H	-6.65546	-2.56061	-1.60769
H	-5.9176	-3.59464	2.49016
H	-3.76716	-2.41256	2.41114
H	-4.46397	-1.433	-1.71379
H	-2.81185	2.12447	-0.83392
H	-5.12641	2.51144	-0.07258
H	-5.61005	2.81525	2.34685
H	-3.7459	2.75469	3.99045
H	-1.43617	2.3774	3.23784
H	-0.86733	4.76149	1.28316
H	-1.66422	7.05424	0.9945
H	-1.22011	6.7057	-3.25749
H	-0.4333	4.39228	-2.98438
H	-2.60484	8.61242	-2.19678
H	-2.52127	8.84267	-0.44448
H	-1.11072	9.17706	-1.45075
H	0.71369	0.56116	-5.09121
H	-0.74631	1.587	-5.22525
H	0.82707	2.32413	-4.83778
H	-0.77708	-2.66169	-4.9445
H	-2.16995	-1.92175	-4.11453
H	-1.31913	-1.03424	-5.41844
H	3.19909	0.94865	1.44312
H	2.92108	-2.19511	-2.15236
H	1.82278	-1.13908	1.91518
H	1.67352	-2.83506	-0.04932
H	2.42859	1.88849	-0.79272
H	2.27315	0.18443	-2.71175
H	1.64429	4.1514	0.76706
H	3.24244	4.78839	2.53638
H	3.39375	3.45382	4.62831
H	1.93617	1.45935	4.92568
H	0.36813	0.79266	3.15087
H	0.50733	-3.52469	2.14958
H	-0.39627	-2.20579	6.13298
H	0.86444	-3.68413	4.58189
H	-2.01218	-0.55009	5.22017
H	-2.35407	-0.36601	2.77275
H	0.12672	2.66941	-1.64923
H	-2.73829	-0.43753	-0.49769
H	-0.06732	-2.94953	-1.97992
H	-1.29584	-7.0522	-1.62653
H	-2.29428	-6.55475	0.5951
H	-2.17298	-4.28642	1.53072
H	-0.17734	-5.24051	-2.90882
C	-2.93702	0.95492	-3.4421
H	-2.92334	0.53796	-4.45284
H	-3.96476	0.96616	-3.0768
H	-2.54019	1.97287	-3.45103

Ir{PO(OMe)$_2$}(SiNP)(tfbb) (3–Me)



C	3.31795	-0.07951	-2.53353
H	3.88226	-0.98715	-2.77116
H	3.89283	0.77405	-2.91392
H	2.36294	-0.13598	-3.0547
C	4.90017	0.28115	-0.00271
H	4.94217	0.39641	1.08381
H	5.38752	1.15273	-0.44908
H	5.48476	-0.6038	-0.2698
C	0.21637	3.00569	-1.67501
C	0.85668	2.81144	-2.90875
H	1.55911	1.99722	-3.0261
C	0.58523	3.63976	-3.99741
H	1.10295	3.47408	-4.93814
C	-0.35246	4.66821	-3.88526
H	-0.56675	5.31011	-4.735
C	-1.01335	4.86226	-2.67309
H	-1.74533	5.65836	-2.5696
C	-0.72903	4.04156	-1.57852
H	-1.23663	4.23287	-0.63904
C	0.23152	2.88262	1.2055
C	-0.31122	2.30368	2.36117
H	-0.57832	1.25463	2.34314
C	-0.51127	3.05767	3.52004
H	-0.93133	2.58343	4.40238
C	-0.17643	4.41136	3.54004
H	-0.33985	5.00292	4.43664
C	0.37164	5.00207	2.3997
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H	3.14862	2.3597	2.1646
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C	3.55884	-3.28665	-0.78301
H	2.97117	-3.13998	-1.68144
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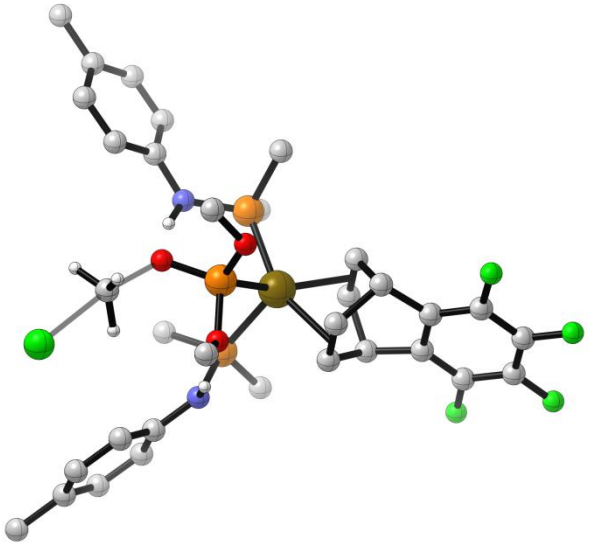

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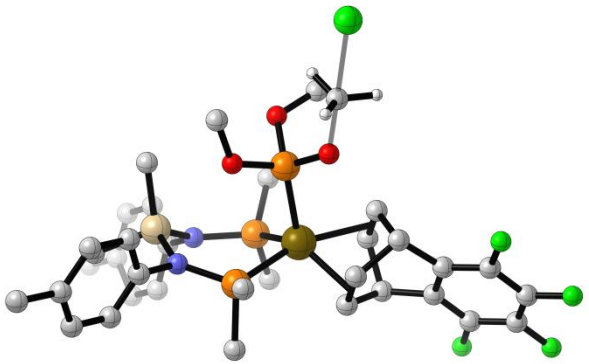

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