

SUPPORTING INFORMATION TO ACCOMPANY:

Synthesis, Structure, and Reactivity of Iridium Perfluorocarbene Complexes: Regio- and Stereo-specific Addition of HCl Across a Metal Carbon Double Bond.

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DFT Calculation Details.

All calculations were carried out using the hybrid B3LYP-D3 functional¹ with the zero-damping, two-body only D3 correction of Grimme et al.,² and the 6-311G**++ basis,³ as implemented in the Jaguar⁴ suite of programs. Computed structures were confirmed as energy minima by calculating the vibrational frequencies using second derivative analytic methods, and confirming the absence of imaginary frequencies. Thermodynamic quantities were calculated assuming an ideal gas, and are zero point energy corrected.

Material Relevant to all DFT output

Jaguar version 7.9, release 23

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Jaguar, version 7.9, Schrodinger, LLC, New York, NY, 2011.

Non-default options chosen:

SCF calculation type: DFT(b3lyp-d3)

DFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)

Vibrational frequencies and related properties will be computed from analytic second derivatives

Molecular symmetry not used

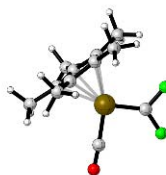
Energy convergence criterion: 1.00E-05 hartrees

RMS density matrix convergence criterion: 1.00E-06

Highest accuracy cutoffs used in SCF

Coordinates.

Compound 17

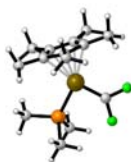


31

Ir_CPSTAR_CO_CF2_D3

C	-0.10870	0.55180	-0.00500
Ir	-1.97350	0.78080	0.04560
F	0.78740	1.55740	-0.05350
F	0.62280	-0.56380	0.00230
C	-4.12840	1.59570	-0.13810
C	-3.34230	2.19800	-1.17650
C	-2.30470	2.96490	-0.53950
C	-2.48610	2.87150	0.88870
C	-3.61220	2.02630	1.13900
O	-2.47300	-2.18910	0.17940
C	-2.24340	-1.06020	0.12990
C	-1.29980	3.83320	-1.23650
H	-0.36310	3.87940	-0.68120
H	-1.07260	3.45260	-2.23290
H	-1.68380	4.85360	-1.34310
C	-3.61910	2.13890	-2.64770
H	-2.69820	2.19570	-3.22870
H	-4.12570	1.21270	-2.92090
H	-4.26100	2.97440	-2.95160
C	-1.68430	3.60670	1.91930
H	-1.67220	3.07080	2.86900
H	-0.65060	3.73830	1.59780
H	-2.11020	4.60060	2.09730
C	-5.36540	0.77090	-0.34260
H	-5.51070	0.05890	0.47090
H	-6.25050	1.41500	-0.38520
H	-5.31830	0.20480	-1.27350
C	-4.21970	1.73670	2.47810
H	-3.46190	1.71520	3.26220
H	-4.95600	2.50500	2.74160
H	-4.72920	0.77250	2.48480

Compound 18



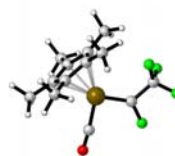
41

Ir_CPSTAR_PMe3_CF2_D3

C	-0.62310	2.05340	-0.64530
C	0.30950	1.92860	0.42740
C	-1.85500	1.40930	-0.24560
Ir	-0.16480	-0.21610	-0.27570

F	1.26540	-2.78700	-0.20640
C	0.85670	-1.62230	0.38440
C	-0.32900	1.18390	1.48680
C	-1.68050	0.88990	1.07130
P	-0.33700	-1.27840	-2.27710
F	1.38790	-1.70880	1.63120
C	-1.30460	-0.39640	-3.57200
H	-1.32280	-0.98200	-4.49460
H	-2.32650	-0.24330	-3.22490
H	-0.84930	0.57370	-3.77260
C	1.23720	-1.63020	-3.17020
H	1.05260	-2.15140	-4.11390
H	1.74990	-0.68690	-3.36480
H	1.87090	-2.24260	-2.52930
C	-1.15090	-2.93310	-2.27410
H	-1.17940	-3.36570	-3.27830
H	-0.59750	-3.59170	-1.60510
H	-2.16680	-2.82530	-1.89080
C	-2.74080	0.25720	1.92020
H	-2.31230	-0.46280	2.61840
H	-3.27250	1.01720	2.50660
H	-3.47600	-0.27000	1.31060
C	0.24110	0.93640	2.85220
H	-0.16960	0.02780	3.29340
H	1.32340	0.81300	2.81280
H	0.01580	1.77350	3.52290
C	-3.15320	1.44350	-0.99640
H	-3.71680	0.51730	-0.86720
H	-3.78230	2.26710	-0.63850
C	-0.41370	2.86810	-1.88700
H	-1.07910	2.55560	-2.69250
H	-0.61570	3.92840	-1.69300
H	0.61250	2.78750	-2.25020
C	1.67110	2.55090	0.49290
H	2.34680	1.96010	1.11240
H	2.11810	2.63380	-0.49870
H	1.61550	3.55840	0.92340

Compound 12a



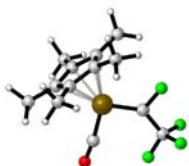
34

Ir_CPSTAR_CO_CFCF3_SYN_D3

C	-0.12550	0.44190	-0.03170
Ir	-1.97140	0.80950	0.04410
C	1.03210	1.43500	-0.08940
F	2.16050	0.96170	0.47020
F	1.33120	1.76950	-1.37300
F	0.72740	2.58910	0.54840
F	0.43420	-0.79740	-0.13200
C	-4.13980	1.60350	-0.13690
C	-3.34130	2.19050	-1.17150
C	-2.32890	3.00470	-0.53610

C	-2.51580	2.91340	0.88410
C	-3.62290	2.03130	1.13330
O	-2.67280	-2.12000	0.09660
C	-2.34910	-1.01640	0.08120
C	-1.39760	3.92670	-1.26470
H	-0.55620	4.22350	-0.64280
H	-0.99520	3.45720	-2.16310
H	-1.93400	4.83240	-1.56810
C	-3.59310	2.11120	-2.64580
H	-2.66140	2.16930	-3.20920
H	-4.08820	1.17830	-2.91650
H	-4.23510	2.93930	-2.96890
C	-1.79030	3.68990	1.93940
H	-1.58300	3.07210	2.81420
H	-0.84280	4.07890	1.57430
H	-2.40540	4.53650	2.26440
C	-5.35370	0.74680	-0.34510
H	-5.49390	0.04340	0.47660
H	-6.25160	1.37040	-0.40850
H	-5.28230	0.16910	-1.26730
C	-4.21350	1.73950	2.47910
H	-3.44200	1.69640	3.24860
H	-4.92830	2.52110	2.76200
H	-4.74290	0.78620	2.48550

Compound 12b

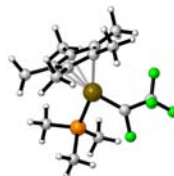


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Ir_CPSTAR_CO_CFCF3_ANTI_D3_REDONE			
C	-0.18310	0.50410	0.19270
Ir	-2.04040	0.73570	0.01660
C	0.76310	-0.68380	0.19570
F	1.66730	-0.58880	-0.81030
F	1.46790	-0.74490	1.35200
F	0.12610	-1.85690	0.05230
F	0.63630	1.60050	0.35800
C	-4.18280	1.59860	-0.15470
C	-3.37450	2.16120	-1.20120
C	-2.31540	2.91730	-0.57700
C	-2.47170	2.81280	0.84650
C	-3.62860	1.99180	1.11150
O	-2.80800	-2.16610	-0.27370
C	-2.42890	-1.08650	-0.15540
C	-1.27470	3.73060	-1.28490
H	-0.33280	3.72340	-0.73640
H	-1.07910	3.33870	-2.28330
H	-1.60550	4.76980	-1.38620
C	-3.64790	2.08760	-2.67210
H	-2.72200	2.10520	-3.24780
H	-4.18140	1.17290	-2.93210
H	-4.26150	2.93750	-2.99180
C	-1.62020	3.49740	1.87210
H	-1.63480	2.95900	2.82010

H	-0.58310	3.55780	1.54190
H	-1.98300	4.51490	2.05290
C	-5.43260	0.79230	-0.35140
H	-5.58850	0.09110	0.46930
H	-6.30710	1.44920	-0.40250
H	-5.39350	0.21490	-1.27580
C	-4.21130	1.71120	2.46250
H	-3.43170	1.63170	3.22070
H	-4.89330	2.51560	2.76110
H	-4.77320	0.77680	2.46710

Compound 13a

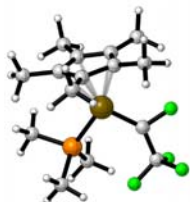


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Ir_CPSTAR_PMe3_CFCF3_TRANS_D3			
C	-0.62840	2.06620	-0.59470
C	0.26390	1.93470	0.52480
C	-1.84730	1.38100	-0.26620
Ir	-0.10080	-0.18850	-0.29900
F	1.40560	-2.69540	-0.51610
C	1.16580	-1.48940	0.15490
C	-0.39060	1.14440	1.52850
C	-1.69890	0.78910	1.02360
P	-0.48490	-1.31230	-2.24840
C	2.11500	-1.51430	1.34210
F	3.25080	-2.20870	1.11330
F	2.49540	-0.26400	1.70190
F	1.54050	-2.07160	2.44860
C	-1.63410	-0.50400	-3.43790
H	-1.67500	-1.08470	-4.36270
H	-2.63460	-0.44440	-3.01270
H	-1.28310	0.50330	-3.66300
C	0.98610	-1.59180	-3.32060
H	0.71350	-2.15370	-4.21820
H	1.39670	-0.62220	-3.60670
H	1.73980	-2.13850	-2.75690
C	-1.22630	-2.99200	-2.10720
H	-1.36320	-3.44890	-3.09130
H	-0.56860	-3.61130	-1.49860
H	-2.19110	-2.90810	-1.60420
C	-2.76700	0.08840	1.80660
H	-2.33830	-0.65650	2.47830
H	-3.33190	0.80530	2.41590
H	-3.47300	-0.42190	1.14940
C	0.05570	0.91950	2.94300
H	-0.13100	-0.10670	3.26360
H	1.11870	1.11220	3.06750
H	-0.49320	1.58980	3.61400
C	-3.12970	1.42010	-1.04280
H	-3.65450	0.46300	-1.00950
H	-3.79900	2.17540	-0.61590
C	-0.38140	2.92780	-1.79660
H	-0.99730	2.62400	-2.64450
H	-0.61650	3.97680	-1.58000

H	0.66250	2.87940	-2.11060
C	1.59020	2.61860	0.65680
H	2.23820	2.09730	1.35860
H	2.10800	2.66330	-0.30240
H	1.45250	3.64610	1.01410

Compound 13b

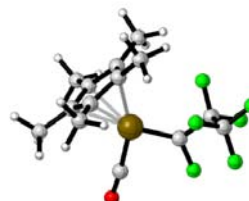


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Ir_CPSTAR_PMe3_CFCF3_CIS_D3			
C	7.38980	2.26190	-0.29310
C	8.24260	2.03900	0.84710
C	6.13360	1.61660	-0.03010
Ir	7.85300	-0.01290	-0.04000
C	9.25110	-1.11870	0.52990
C	7.51780	1.24150	1.79590
F	10.04550	-0.68570	1.60220
C	6.21160	0.96570	1.23910
P	7.42530	-1.11930	-2.00620
C	9.87590	-2.44870	0.16860
F	11.03810	-2.30470	-0.53540
F	10.17870	-3.19190	1.25610
F	9.06590	-3.21590	-0.60280
C	6.41440	-0.13670	-3.19770
H	6.34260	-0.67320	-4.14730
H	5.41140	0.01610	-2.80460
H	6.88300	0.83260	-3.36850
C	6.43210	-2.67390	-1.96820
H	6.29000	-3.07110	-2.97740
H	6.92090	-3.41840	-1.34510
H	5.45920	-2.44100	-1.53060
C	5.08470	0.28300	1.95180
H	5.45320	-0.50200	2.61300
H	4.52100	0.99960	2.56230
H	4.38920	-0.17630	1.24800
C	7.96350	0.87880	3.18010
H	7.54930	-0.08250	3.48680
H	9.04740	0.80030	3.23880
H	7.62900	1.63730	3.89700
C	9.61450	2.60550	1.04950
H	10.23620	1.91740	1.62280
H	10.11150	2.78560	0.09540
H	9.56430	3.55720	1.59100
C	7.71070	3.15860	-1.45060
H	7.10070	2.92330	-2.32380
H	7.52510	4.20850	-1.19420
H	8.75800	3.06770	-1.74290
C	4.87550	1.75380	-0.83370
H	4.30890	0.82090	-0.86620
H	4.22790	2.51160	-0.37850
H	5.07430	2.06840	-1.85730
C	8.85320	-1.51720	-3.10460
H	8.50470	-2.00820	-4.01740

H	9.34510	-0.57770	-3.36320
H	9.57600	-2.15550	-2.60520

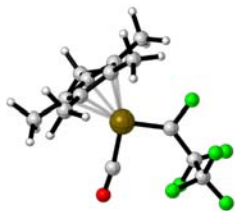
Compound 14a



37

Ir_CPSTAR_CO_CFCF2CF3_TRANS_D3			
C	-0.05260	0.42610	-0.09280
Ir	-1.88860	0.84050	-0.19490
C	1.11480	1.33580	0.25890
F	2.22190	1.05880	-0.48520
F	0.79070	2.64220	0.02980
F	0.48540	-0.81960	-0.25740
C	-4.06910	1.58560	-0.03580
C	-3.45950	2.23300	-1.16440
C	-2.39220	3.06220	-0.67110
C	-2.33350	2.91280	0.75340
C	-3.36830	1.98590	1.14810
O	-2.59200	-2.01350	-0.84790
C	-2.26610	-0.93920	-0.59940
C	-1.58410	4.00890	-1.50410
H	-0.66670	4.30290	-0.99860
H	-1.30900	3.56010	-2.45940
H	-2.16640	4.91350	-1.71240
C	-3.92980	2.17840	-2.58570
H	-3.09540	2.27500	-3.28130
H	-4.43650	1.23770	-2.80340
H	-4.63390	2.99370	-2.78810
C	-1.53070	3.74580	1.70490
H	-1.27530	3.19130	2.60590
H	-0.60430	4.09810	1.25740
H	-2.11830	4.62140	2.00270
C	-5.27520	0.69440	-0.07940
H	-5.25410	-0.04550	0.72160
H	-6.18880	1.28700	0.03510
H	-5.34320	0.15630	-1.02560
C	-3.72730	1.63960	2.56040
H	-2.83870	1.58190	3.18990
H	-4.39280	2.40070	2.98430
H	-4.23840	0.67830	2.61770
C	1.53020	1.24130	1.75620
F	2.52650	2.09720	2.03250
F	0.48170	1.55440	2.54100
F	1.93330	0.00400	2.06280

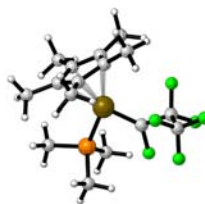
Compound 14b



37

Ir_CPSTAR_CO_CFCF2CF3_CIS_D3			
C	-0.11430	0.53280	0.02360
Ir	-1.98180	0.74040	-0.05250
C	0.80560	-0.67120	0.14550
F	0.23980	-1.78190	-0.39380
F	1.99300	-0.46010	-0.49500
F	0.69540	1.64150	0.13110
C	-4.13580	1.58360	-0.09600
C	-3.39680	2.16830	-1.17770
C	-2.30690	2.92340	-0.60690
C	-2.37920	2.80290	0.82160
C	-3.50920	1.96350	1.14310
O	-2.71320	-2.18220	-0.20700
C	-2.35030	-1.09200	-0.15380
C	-1.31780	3.75690	-1.36220
H	-0.34740	3.75750	-0.86650
H	-1.17230	3.37700	-2.37300
H	-1.66700	4.79230	-1.43490
C	-3.74970	2.11210	-2.63090
H	-2.85710	2.14280	-3.25540
H	-4.29120	1.19760	-2.87300
H	-4.38440	2.96190	-2.90570
C	-1.47000	3.47780	1.80360
H	-1.42400	2.92560	2.74290
H	-0.45520	3.54890	1.41200
H	-1.82630	4.49060	2.02110
C	-5.38390	0.76150	-0.22550
H	-5.47400	0.04360	0.59120
H	-6.27030	1.40390	-0.20680
H	-5.39610	0.20040	-1.16040
C	-3.99780	1.65580	2.52620
H	-3.16750	1.57170	3.22870
H	-4.66580	2.44820	2.88340
H	-4.54890	0.71490	2.55300
C	1.14590	-1.01900	1.62760
F	2.05180	-2.00380	1.69420
F	1.64100	0.05560	2.26160
F	0.04100	-1.41930	2.27670

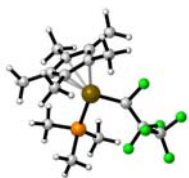
Compound 15a



48

Ir_CPSTAR_PMe3_CFCF2CF3_TRANS_D3			
C	-0.64230	2.09910	-0.65270
C	0.27560	2.02440	0.44990
C	-1.84600	1.41310	-0.26670
Ir	-0.07680	-0.12320	-0.27960
F	1.45620	-2.60660	-0.55990
C	1.15950	-1.45160	0.18440
C	-0.35720	1.29440	1.51200
C	-1.66290	0.89140	1.04930
P	-0.42670	-1.23500	-2.24580
C	2.01070	-1.61030	1.42970
F	3.24260	-2.14410	1.15930
F	2.22860	-0.40570	2.03330
C	-1.60410	-0.45550	-3.42600
H	-1.63620	-1.04080	-4.34820
H	-2.60270	-0.42210	-2.99330
H	-1.28180	0.55920	-3.65920
C	1.04940	-1.45310	-3.32470
H	0.79310	-2.01750	-4.22570
H	1.42170	-0.46640	-3.60530
H	1.82530	-1.97550	-2.76880
C	-1.12630	-2.93310	-2.11920
H	-1.25010	-3.38090	-3.10920
H	-0.46040	-3.54690	-1.51560
H	-2.09520	-2.87300	-1.62060
C	-2.69770	0.20350	1.88500
H	-2.23810	-0.51820	2.56100
H	-3.24850	0.93230	2.49270
H	-3.41980	-0.33050	1.26590
C	0.08420	1.23780	2.94320
H	-0.11970	0.26900	3.39580
H	1.14750	1.43880	3.05050
H	-0.46220	1.99780	3.51420
C	-3.14720	1.39790	-1.01170
H	-3.63890	0.42480	-0.95140
H	-3.83060	2.13730	-0.57920
H	-3.02010	1.65060	-2.06350
C	-0.42970	2.90990	-1.89580
H	-1.08410	2.58770	-2.70650
H	-0.64010	3.96960	-1.70870
H	0.60020	2.83290	-2.24840
C	1.61270	2.69570	0.52460
H	2.28920	2.14670	1.17910
H	2.07870	2.75680	-0.45960
H	1.50950	3.71570	0.91360
C	1.36750	-2.53330	2.50670
F	2.14910	-2.63120	3.59620
F	0.17680	-2.04300	2.90380
F	1.16690	-3.76580	2.02000

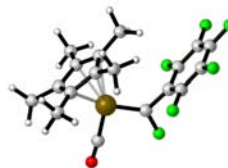
Compound 15b



48

Ir_CPSTAR_PMe3_CFCF2CF3_CIS_D3			
C	7.36130	2.28380	-0.28920
C	8.23320	2.06360	0.83900
C	6.13270	1.58980	-0.03060
Ir	7.89140	0.01470	-0.08140
C	9.31840	-1.06280	0.46810
C	7.54360	1.22560	1.77840
F	10.13340	-0.59070	1.51870
C	6.24460	0.91230	1.22490
P	7.44050	-1.11470	-2.02960
C	9.86440	-2.44770	0.23130
F	11.11200	-2.43240	-0.35590
F	9.05930	-3.16640	-0.60770
C	6.43580	-0.13440	-3.22820
H	6.36330	-0.67430	-4.17580
H	5.43240	0.02420	-2.83820
H	6.90900	0.83240	-3.40060
C	6.43130	-2.65800	-1.96720
H	6.26600	-3.05670	-2.97220
H	6.92270	-3.40670	-1.35120
H	5.46930	-2.41290	-1.51250
C	5.14970	0.17160	1.92990
H	5.55350	-0.61190	2.57190
H	4.56160	0.85240	2.55800
H	4.46910	-0.30090	1.22020
C	8.01560	0.84110	3.14790
H	7.64330	-0.14530	3.42800
H	9.10210	0.80470	3.19660
H	7.65660	1.56390	3.88900
C	9.58760	2.67060	1.04060
H	10.23310	1.99670	1.60400
H	10.07380	2.87490	0.08590
H	9.50970	3.61510	1.59130
C	7.64100	3.21240	-1.43150
H	7.03720	2.96630	-2.30620
H	7.41430	4.24950	-1.15660
H	8.68980	3.16860	-1.72920
C	4.86310	1.69420	-0.82060
H	4.33360	0.74030	-0.86710
H	4.19030	2.41590	-0.34400
H	5.04030	2.03720	-1.83920
C	8.86450	-1.53750	-3.12200
H	8.51580	-2.05290	-4.02130
H	9.35340	-0.60370	-3.40540
H	9.58800	-2.16060	-2.60430
C	9.99900	-3.31850	1.52730
F	10.13780	-4.61680	1.19690
F	11.05540	-2.97320	2.26840
F	8.88870	-3.20140	2.27830

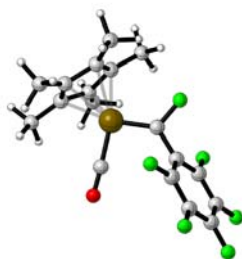
Compound 16a



41

Ir_CPSTAR_CO_CFC6F5_TRANS_D3			
C	-0.09180	0.51990	-0.00790
Ir	-1.94470	0.80140	0.04980
F	0.55560	-0.68530	-0.00920
C	-4.11610	1.62380	-0.12770
C	-3.31580	2.21440	-1.15920
C	-2.29110	3.00370	-0.51780
C	-2.46950	2.89600	0.90370
C	-3.59110	2.03300	1.14730
O	-2.53310	-2.14990	0.15670
C	-2.26360	-1.03130	0.11850
C	-1.33970	3.92020	-1.22540
H	-0.47890	4.16610	-0.60390
H	-0.97150	3.47680	-2.15140
H	-1.84160	4.85930	-1.48120
C	-3.56380	2.14930	-2.63520
H	-2.62800	2.19000	-3.19400
H	-4.07480	1.22700	-2.91250
H	-4.18800	2.99070	-2.95840
C	-1.70020	3.63900	1.95250
H	-1.56560	3.03620	2.85050
H	-0.71180	3.92870	1.59650
H	-2.23130	4.55530	2.23290
C	-5.33820	0.78010	-0.33990
H	-5.47800	0.06730	0.47380
H	-6.23310	1.40940	-0.39060
H	-5.27460	0.21310	-1.26940
C	-4.17880	1.72930	2.49180
H	-3.40480	1.67440	3.25820
H	-4.89060	2.50920	2.78620
H	-4.71020	0.77700	2.48950
C	2.71800	3.76870	-0.17740
C	2.27810	3.29200	1.05310
C	1.39790	2.21790	1.09650
C	0.92900	1.60630	-0.06480
C	1.39080	2.10120	-1.28250
C	2.27270	3.17180	-1.35150
F	3.55750	4.80510	-0.23100
F	2.69830	3.87430	2.18170
F	0.97910	1.79250	2.29530
F	0.94310	1.57750	-2.43150
F	2.67200	3.65040	-2.53500

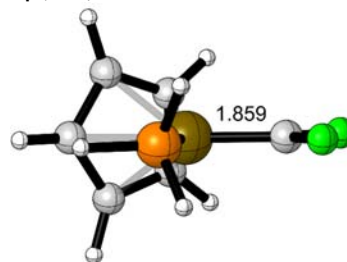
Compound 16b



41
Ir_CPSTAR_CO_CFC6F5_CIS_D3

C	-0.15800	0.46880	0.09390
Ir	-2.01490	0.75900	0.11850
F	0.72090	1.52990	0.00050
C	-4.16020	1.62900	-0.11410
C	-3.34110	2.11410	-1.18720
C	-2.27530	2.89550	-0.60500
C	-2.45140	2.89540	0.82200
C	-3.61240	2.10350	1.12860
O	-2.60270	-2.18890	0.37870
C	-2.34680	-1.06870	0.28060
C	-1.23620	3.66410	-1.36480
H	-0.30570	3.73160	-0.80190
H	-1.00820	3.18180	-2.31580
H	-1.58820	4.68000	-1.57410
C	-3.60460	1.94950	-2.65270
H	-2.67510	1.92880	-3.22230
H	-4.13970	1.02200	-2.85910
H	-4.21310	2.78000	-3.02920
C	-1.60950	3.64710	1.80700
H	-1.61630	3.16270	2.78380
H	-0.57340	3.70880	1.47250
H	-1.98770	4.66780	1.93110
C	-5.41310	0.81800	-0.26830
H	-5.58160	0.17390	0.59550
H	-6.28410	1.47400	-0.37150
H	-5.36830	0.18130	-1.15280
C	-4.20520	1.90540	2.49040
H	-3.43140	1.87550	3.25810
H	-4.89410	2.72210	2.73480
H	-4.76320	0.97020	2.54820
C	2.01510	-3.22520	-0.06620
C	1.90880	-2.41980	-1.19570
C	1.22510	-1.21600	-1.10870
C	0.63290	-0.78840	0.07990
C	0.76040	-1.61040	1.19700
C	1.43990	-2.82160	1.13270
F	2.67080	-4.38630	-0.13480
F	2.45520	-2.81690	-2.35070
F	1.10290	-0.46500	-2.21200
F	0.22720	-1.24830	2.37040
F	1.55070	-3.59860	2.21580

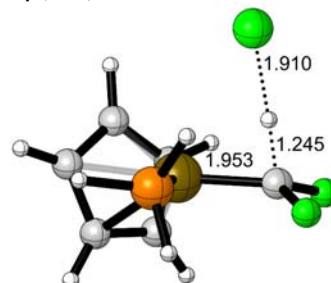
Cp(PH₃)Ir=CF₂



18
IrCp_PH3_CF2_D3

H	-0.01090	0.84840	-2.60290
C	0.04930	1.12470	-1.56290
H	2.25210	1.24060	-1.18480
H	-2.09430	1.26260	-0.94340
C	1.24370	1.32720	-0.81100
C	-1.05080	1.34480	-0.67800
Ir	0.18220	-0.44090	0.17700
F	1.32850	-2.91760	1.20700
C	1.45170	-1.61170	0.86600
C	0.87410	1.71050	0.52350
F	2.73720	-1.31900	1.14010
C	-0.54940	1.74550	0.59850
H	1.55870	1.95990	1.31930
H	-1.13650	2.01520	1.46130
P	-1.36410	-2.07590	0.21530
H	-1.73450	-2.69130	1.43630
H	-1.18240	-3.26010	-0.54070
H	-2.65430	-1.72680	-0.24540

Cp(PH₃)Ir=CF₂ + HCl: C---H Transition State

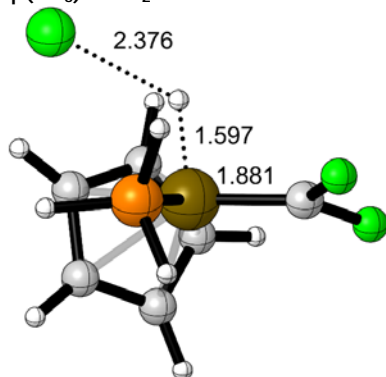


20
IrCp_PH3_CF2_HCl_TS_SEARCH_1_D3

H	-0.89400	0.81260	-2.04660
C	-0.67970	1.17830	-1.05410
H	1.57420	1.17770	-1.00170
H	-2.71740	1.70710	-0.24120
C	0.63950	1.40460	-0.51310
C	-1.64620	1.71010	-0.11560
Ir	-0.41480	-0.12870	0.67720
F	0.92170	-2.69810	1.27990
C	0.87940	-1.35060	1.48070
C	0.47170	1.93270	0.79590
F	2.15820	-0.96460	1.71780
C	-0.94760	2.13410	1.02170
H	1.26060	2.18630	1.48720
H	-1.38520	2.49080	1.94160
P	-1.84150	-1.91330	0.36390
H	-2.12040	-2.63380	1.54180
H	-1.46900	-2.93420	-0.53540

H	-3.12920	-1.60410	-0.11950
H	0.16510	-1.16330	2.48330
Cl	-1.13500	-1.25080	3.88040

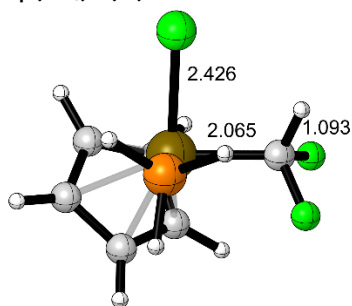
Cp(PH₃)Ir=CF₂ + HCl: Ir---H Transition State



20
IrCp_PH3_CF2_HCl_TS_SEARCH_4_D3

H	-0.84220	0.61720	-2.22730
C	-0.30370	0.96910	-1.36020
H	1.82900	0.86390	-2.02790
H	-1.94680	1.37490	0.12640
C	1.10920	1.10330	-1.26080
C	-0.89750	1.39280	-0.12850
Ir	0.36530	-0.45970	0.38190
F	1.66420	-2.80720	1.49020
C	1.74020	-1.56280	1.03860
C	1.40390	1.57440	0.05750
F	3.01710	-1.21830	1.15390
C	0.16220	1.77950	0.74510
H	2.38750	1.78580	0.44830
H	0.04500	2.15350	1.74990
P	-0.99410	-2.26680	-0.10080
H	-1.37450	-3.07950	0.97060
H	-0.39200	-3.20020	-0.98560
H	-2.18620	-1.96560	-0.76680
H	-0.50740	-0.68250	1.70090
Cl	-2.87810	-0.80130	1.80590

Cp(PH₃)Ir(Cl)CHF₂

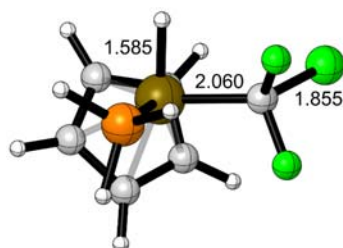


20
IrCp_PH3_Cl_CHF2_D3

H	-1.70410	1.45380	-1.05560
C	-0.67800	1.21210	-0.82340
H	0.00500	0.16060	-2.65560
H	-0.44880	2.02550	1.26770
C	0.20960	0.51060	-1.65610
C	-0.03020	1.47660	0.43980

Ir	-0.12070	-0.76010	0.29860
F	1.57790	-2.13280	2.22540
C	0.39090	-1.38420	2.19940
C	1.43280	0.29120	-0.90510
F	0.64570	-0.30410	3.03500
C	1.29650	0.94330	0.35880
H	2.32920	-0.18370	-1.27350
H	2.04430	0.98380	1.13590
P	0.05690	-2.94350	-0.35790
H	-0.08860	-3.92590	0.64220
H	1.26240	-3.37340	-0.95390
H	-0.87480	-3.41870	-1.30540
Cl	-2.40810	-1.30980	0.89120
H	-0.36870	-1.99010	2.69970

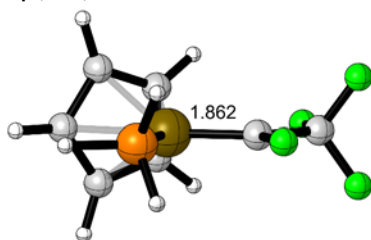
Cp(PH₃)Ir(H)CCIF₂



20
IrCp_PH3_H_CF2Cl

H	-1.82990	1.28550	-1.15250
C	-0.80110	1.17080	-0.84980
H	0.13360	0.19270	-2.61990
H	-0.76720	2.05930	1.21900
C	0.23460	0.58530	-1.61970
C	-0.24710	1.56220	0.41650
Ir	-0.08920	-0.68460	0.31330
F	-0.25540	-2.42000	2.68120
C	0.39620	-1.30330	2.21770
C	1.45980	0.65430	-0.85810
F	1.73450	-1.62510	2.34670
C	1.15810	1.25620	0.38400
H	2.43070	0.31250	-1.18050
H	1.85240	1.42640	1.19250
P	0.17300	-2.81420	-0.40100
H	0.15320	-3.84300	0.56330
H	1.36350	-3.15270	-1.08690
H	-0.75720	-3.34340	-1.32570
H	-1.53640	-1.15340	0.75760
Cl	0.11000	-0.02360	3.52920

Cp(PH₃)Ir=CFCF₃

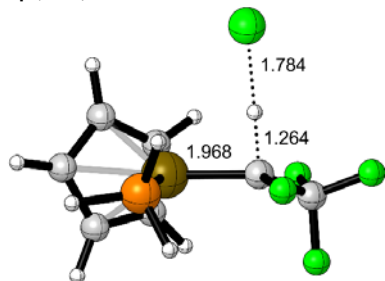


21
IrCp_PH3_CFCF3_D3

H	-0.37500	3.09320	-1.59230
C	-0.54390	2.50610	-0.70430

H	1.32370	2.83780	0.49610
H	-2.56730	1.62740	-1.04790
C	0.35530	2.37260	0.40240
C	-1.70870	1.74210	-0.40360
Ir	0.13620	0.29180	-0.47740
F	2.10530	-1.77500	-1.00920
C	1.72610	-0.65820	-0.28390
C	-0.26560	1.53260	1.37990
C	-1.55090	1.14490	0.88050
H	0.15600	1.25880	2.33390
H	-2.27190	0.52890	1.39300
P	-0.49310	-1.13720	-2.11130
H	-0.63470	-2.51550	-1.82930
H	0.28140	-1.25040	-3.28910
H	-1.75650	-0.89610	-2.69600
C	2.88850	-0.41320	0.66810
F	4.04470	-0.18660	-0.00050
F	2.67970	0.65590	1.46670
F	3.10470	-1.47610	1.47960

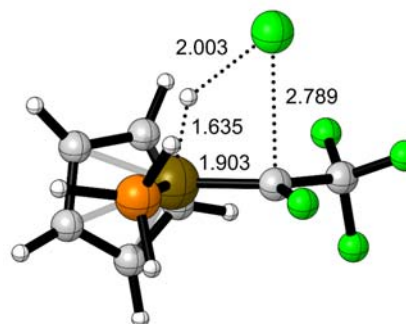
Cp(PH₃)Ir=CFCF₃ + HCl: C---H Transition State



23
IrCp_PH3_CF3CF3_HCl_TS_SEARCH_CH_D3

H	-0.87150	2.14460	-1.01490
C	-1.21070	1.60460	-0.14460
H	0.59200	1.65990	1.21410
H	-3.36360	1.15800	-0.61480
C	-0.43820	1.37900	1.05950
C	-2.54730	1.12480	0.08990
Ir	-0.95370	-0.56560	0.13230
F	0.85040	-2.84090	-0.37420
C	0.44350	-1.88310	0.56090
C	-1.26440	0.66980	1.96780
C	-2.57150	0.51310	1.35850
H	-0.97900	0.28630	2.93480
H	-3.39500	-0.02510	1.80150
P	-1.32460	-1.64700	-1.85900
H	-1.80890	-2.96920	-1.78770
H	-0.23530	-1.82490	-2.73470
H	-2.26950	-1.06360	-2.72840
C	1.66190	-1.58290	1.41730
F	2.61160	-0.91770	0.70740
F	1.33350	-0.79410	2.46700
F	2.24160	-2.69010	1.90480
H	-0.42690	-2.41420	1.30850
Cl	-1.64760	-3.05290	2.44230

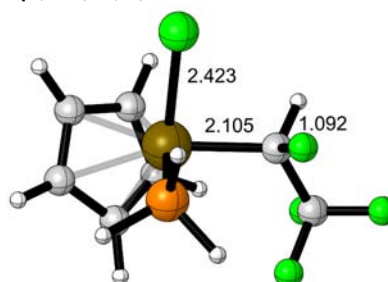
Cp(PH₃)Ir=CFCF₃ + HCl: Ir---H Transition State



23
IrCp_PH3_CF3CF3_HCl_TS_SEARCH_CCl_D3

H	-0.30030	2.28470	-0.65140
C	-0.87200	1.75150	0.09150
H	0.59160	1.48310	1.77180
H	-2.85460	1.47950	-0.88660
C	-0.39370	1.30980	1.36900
C	-2.21850	1.32190	-0.02850
Ir	-0.88710	-0.63880	0.26710
F	1.17080	-2.51220	-0.52540
C	0.75240	-1.60150	0.35630
C	-1.47120	0.66530	2.05510
C	-2.60110	0.66050	1.17990
H	-1.43000	0.25050	3.04980
H	-3.57590	0.25770	1.40410
P	-1.59080	-2.02400	-1.40020
H	-1.49260	-3.39980	-1.11730
H	-0.98150	-1.96300	-2.67360
H	-2.94530	-1.90510	-1.77560
C	1.92910	-1.29610	1.30790
F	2.66100	-0.29750	0.72700
F	1.51000	-0.83460	2.49130
F	2.74610	-2.32600	1.50190
H	-1.25300	-1.96160	1.15620
Cl	-0.39400	-3.59520	1.93470

Cp(PH₃)Ir(Cl)CHFCF₃

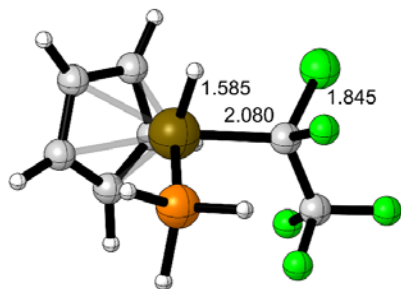


23
IrCp_PH3_Cl_CFHCF3

H	-1.78100	1.82590	-1.30960
C	-1.59670	1.51340	-0.29320
H	0.61730	1.89830	-0.01680
H	-3.59120	0.79900	0.37230
C	-0.30990	1.51200	0.37600
C	-2.55410	0.99350	0.59680
Ir	-0.96100	-0.62670	0.26690
F	0.50170	-3.18990	0.22550
C	0.30650	-2.08710	1.09820
C	-0.52620	1.04950	1.71210

C	-1.89560	0.68410	1.84750
H	0.23080	0.95810	2.47240
H	-2.37080	0.28980	2.73160
P	-0.22560	-1.37270	-1.77030
H	-0.84260	-2.53680	-2.26810
H	1.13860	-1.68090	-1.93120
H	-0.40940	-0.48600	-2.85430
C	1.72190	-1.65310	1.45880
F	2.37890	-1.06680	0.42720
F	1.70950	-0.75930	2.48300
F	2.48820	-2.68720	1.86450
H	-0.14830	-2.49650	2.00250
Cl	-2.62020	-2.39170	0.29290

Cp(PH₃)Ir(H)CClCF₃

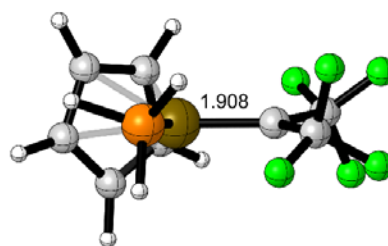


23

IrCp_PH3_H_CFClCF3

H	-1.81170	1.85270	-1.24290
C	-1.67220	1.48640	-0.23700
H	0.45180	2.07820	0.23350
H	-3.67400	0.62680	0.25290
C	-0.46900	1.61110	0.54400
C	-2.66010	0.83970	0.55190
Ir	-0.96410	-0.67340	0.25100
F	0.28780	-3.31300	0.64950
C	0.28380	-2.03560	1.20780
C	-0.72020	1.01040	1.80290
C	-2.06640	0.51680	1.82100
H	-0.00770	0.90770	2.60590
H	-2.55520	0.04340	2.65690
P	-0.22400	-1.38760	-1.76430
H	-1.16490	-1.47150	-2.81680
H	0.33640	-2.67750	-1.84210
H	0.77580	-0.64280	-2.43130
C	1.78860	-1.65250	1.23410
F	2.26090	-1.55450	-0.03770
F	1.99240	-0.45850	1.82470
F	2.56520	-2.55280	1.85740
Cl	-0.18550	-2.28470	2.97460
H	-1.89300	-1.95610	0.18130

Cp(PH₃)Ir=C(CF₃)₂

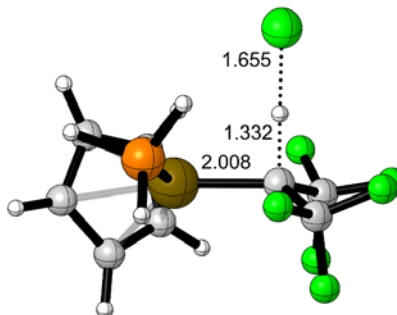


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IrCp_PH3_bisCF3_D3

H	0.24610	1.78210	-3.28240
C	-0.08330	1.94470	-2.26870
H	1.81720	2.47880	-1.18490
H	-2.28620	1.61640	-2.39480
C	0.75220	2.31640	-1.15480
C	-1.42500	1.87670	-1.79850
Ir	-0.11850	0.29310	-0.71090
C	1.30120	-0.75160	0.01860
C	-0.08490	2.45580	-0.00860
C	-1.43200	2.17120	-0.40180
H	0.24550	2.71450	0.98450
H	-2.29710	2.20070	0.24110
P	-1.58650	-1.42960	-0.96800
H	-1.74320	-2.42200	0.02070
H	-1.54170	-2.25510	-2.11270
H	-2.92640	-0.98910	-1.06480
C	2.56060	-0.11220	0.58260
F	3.01100	-0.72760	1.70580
F	3.58770	-0.12710	-0.31090
F	2.39630	1.19200	0.92810
C	1.38750	-2.25920	0.14530
F	2.64320	-2.74610	0.02490
F	0.90710	-2.70590	1.33980
F	0.65770	-2.91640	-0.80480

Cp(PH₃)Ir=C(CF₃)₂ + HCl: C---H Transition State



26

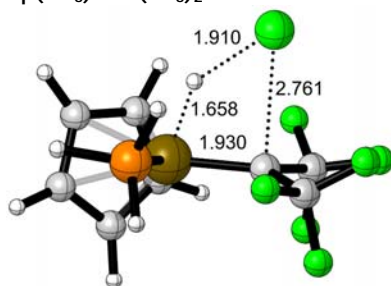
IrCp_PH3_bis_CF3_HCl_TS_SEARCH_3_D3_RES

TART

H	0.34280	1.19740	-2.48230
C	-0.15530	1.51490	-1.57940
H	1.55380	2.05650	-0.21130
H	-2.32600	1.36730	-2.12450
C	0.49130	1.99430	-0.37970
C	-1.57570	1.63540	-1.39690
Ir	-0.64640	0.12150	0.03770
C	0.57380	-0.97780	1.19350
C	-0.53050	2.30420	0.55400
C	-1.81210	2.08300	-0.07540

H	-0.37900	2.62100	1.57400
H	-2.77190	2.23230	0.39330
P	-2.19590	-1.56740	-0.28970
H	-2.56910	-2.30160	0.84930
H	-1.96740	-2.57320	-1.24790
H	-3.43990	-1.07130	-0.73530
C	1.77970	-0.23290	1.74930
F	2.46850	-0.89610	2.69380
F	2.68640	0.09360	0.77710
F	1.40200	0.94780	2.31070
C	0.90040	-2.43900	0.95060
F	1.88190	-2.58270	0.02070
F	1.30320	-3.10780	2.04370
F	-0.17320	-3.13710	0.47130
H	-0.32260	-1.02060	2.17810
Cl	-1.46140	-1.20750	3.36440

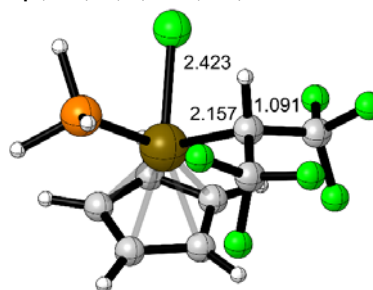
Cp(PH₃)Ir=C(CF₃)₂ + HCl: Ir---H TransitionState



26
IrCp_PH3_bis_CF3_HCl_TS_SEARCH_Ir_H_D3

H	0.03880	1.39280	-2.12140
C	-0.54210	1.62300	-1.24200
H	1.01760	2.19020	0.26500
H	-2.63320	1.23610	-1.90090
C	-0.02110	2.02390	0.03240
C	-1.95120	1.53420	-1.11880
Ir	-1.02830	-0.00780	0.43170
C	0.37280	-1.02280	1.28700
C	-1.12140	2.23930	0.91820
C	-2.31990	1.91690	0.21120
H	-1.05190	2.56830	1.94280
H	-3.32420	1.98940	0.59740
P	-2.44760	-1.74350	0.00540
H	-2.89510	-2.50320	1.10000
H	-2.13050	-2.75080	-0.92770
H	-3.67630	-1.29940	-0.53200
C	1.60720	-0.25440	1.80940
F	2.41090	-0.93790	2.63110
F	2.37080	0.11110	0.73560
F	1.26460	0.88170	2.44330
C	0.62260	-2.53560	1.27440
F	1.54870	-2.75190	0.29430
F	1.09470	-3.08800	2.38810
F	-0.47360	-3.25030	0.92520
H	-1.55330	-0.30270	1.97680
Cl	-1.09920	-1.16810	3.61830

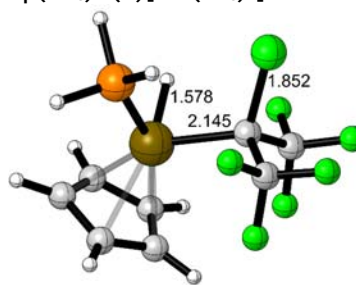
Cp(PH₃)Ir(Cl)[CH(CF₃)₂]



26
IrCp_PH3_Cl_CH_bisCF3

H	-0.50910	0.21590	-2.35660
C	-0.63500	0.82830	-1.47730
H	1.42640	0.87900	-0.61780
H	-2.81550	1.42800	-1.54250
C	0.40040	1.20310	-0.57170
C	-1.85490	1.48740	-1.05540
Ir	-1.12310	0.01790	0.54080
C	0.32540	-1.11860	1.66410
C	-0.16970	2.04990	0.43750
C	-1.55930	2.21920	0.11880
H	0.35230	2.49450	1.26800
H	-2.27460	2.75890	0.72040
P	-2.38640	-1.80510	-0.05430
H	-1.84290	-3.09350	-0.21700
H	-3.04360	-1.67450	-1.29790
H	-3.48160	-2.08190	0.78990
C	1.26260	-0.22690	2.47790
F	1.95050	-0.91860	3.41790
F	2.19770	0.39020	1.69460
F	0.61520	0.75060	3.13980
C	1.13010	-2.10030	0.82190
F	1.60460	-1.56540	-0.33320
F	2.20320	-2.63180	1.45110
F	0.35630	-3.16180	0.45900
H	-0.20560	-1.71620	2.40700
Cl	-2.42410	0.04310	2.58430

Cp(PH₃)Ir(H)[CCl(CF₃)₂]



26
IrCp_PH3_H_CClbisCF3

H	-0.34880	0.26580	-2.46130
C	-0.52660	0.87490	-1.58950
H	1.48860	1.04870	-0.67340
H	-2.74360	1.26750	-1.66410
C	0.44190	1.30140	-0.65690
C	-1.80030	1.39780	-1.15560
Ir	-1.09810	0.04040	0.54600
C	0.28340	-1.17350	1.64940
C	-0.20010	2.10100	0.35270

C	-1.59070	2.18360	0.01190	F	1.92540	0.56310	1.83930
H	0.29260	2.60460	1.16770	F	0.43890	0.43700	3.42060
H	-2.34660	2.73300	0.55040	C	1.17490	-2.04460	0.72820
P	-2.49340	-1.71600	0.18260	F	1.88130	-1.28060	-0.13840
H	-2.02220	-3.04280	0.23150	F	2.07390	-2.80980	1.37750
H	-3.11630	-1.73020	-1.08700	F	0.42880	-2.88850	-0.02280
H	-3.64270	-1.84870	0.99180	Cl	-0.52000	-2.38040	2.80100
C	1.17470	-0.30220	2.57110	H	-1.77740	0.12000	1.96850
F	2.04540	-1.00500	3.32440				

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