SUPPORTING INFORMATION TO ACCOMPANY:

A (Pentafluoroethyl)(trifluoromethyl)carbene Complex of Iridium and Reductive Activation of its sp^3 α, β, and γ Carbon-Fluorine Bonds to Give Perfluoro-2-butyne, Perfluoro-1,2,3-butatriene and Perfluoro-1-irida-2-methyl-2-cyclobutene) Complexes.

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DFT Calculation Details.

Full-molecule calculations were carried out using the hybrid B3LYP-D3 functional[1] with the zero-damping, two-body only D3 correction of Grimme et al.,[2] and the 6-311G**++ basis,[3] as implemented in the Jaguar[4] 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 7.

Ir_CPSTAR_CO_bis_CF3_CARBENE

C	-0.07340	0.30880	0.00520
Ir	-1.93670	0.76270	0.07750
C	0.55840	-1.06140	-0.10430
F	1.51290	-1.10130	-1.07380
F	1.16420	-1.43770	1.05420
F	-0.31280	-2.04910	-0.40540
C	0.98930	1.38830	-0.00150
F	2.19690	1.00240	0.46540
F	0.62780	2.45780	0.76030
F	1.20310	1.88260	-1.25590
C	-4.06790	1.61630	-0.12010
C	-3.22860	2.16930	-1.14020
C	-2.21170	2.98030	-0.49090
C	-2.41670	2.88970	0.91800
C	-3.53860	2.01090	1.15340
O	-3.12000	-1.99440	0.20040
C	-2.54730	-1.00000	0.14770
C	-1.25820	3.87960	-1.21600
H	-0.43140	4.18560	-0.57960
H	-0.83280	3.38410	-2.08830
H	-1.78480	4.77780	-1.55630
C	-3.45180	2.08780	-2.61810
H	-2.50670	2.11200	-3.16100
H	-3.97220	1.17010	-2.89280
H	-4.05860	2.93540	-2.95690
C	-1.70660	3.64590	1.99620
H	-1.37630	2.98190	2.79620
H	-0.83310	4.16880	1.61520
H	-2.38960	4.38350	2.43130
C	-5.29920	0.79040	-0.34450
H	-5.46860	0.09030	0.47420
H	-6.17830	1.43860	-0.41890
H	-5.23090	0.21150	-1.26600
C	-4.13260	1.71960	2.49690
H	-3.35810	1.64800	3.26120
H	-4.82400	2.51800	2.79010
H	-4.68740	0.78110	2.49410

Compound 10a

Ir_CPSTAR_CO_C_CF3_C2F5_CARBENE

C	-0.06260	0.38770	-0.02410
Ir	-1.94000	0.80540	0.04580
C	0.98780	1.47940	-0.06840
F	2.17650	1.16670	0.49250
F	1.25630	1.85970	-1.35210
F	0.57960	2.60900	0.57280
C	0.53620	-1.00200	-0.10080
F	1.73990	-1.02290	-0.75360
F	-0.26690	-1.87610	-0.78800
C	0.76600	-1.67520	1.29380
F	-0.41380	-1.97230	1.86810
F	1.46200	-2.81410	1.16580
F	1.43550	-0.86180	2.12260
C	-4.09120	1.60320	-0.12700
C	-3.27890	2.17660	-1.15860
C	-2.27620	3.01560	-0.52420
C	-2.45700	2.91810	0.88720
C	-3.55420	2.01050	1.13890
O	-3.06930	-1.97620	0.12930
C	-2.51880	-0.96960	0.09240
C	-1.36030	3.93700	-1.27020
H	-0.57690	4.33320	-0.62950
H	-0.87590	3.42590	-2.10280
H	-1.93540	4.77650	-1.67500
C	-3.51340	2.08480	-2.63400
H	-2.57400	2.13780	-3.18460
H	-4.00640	1.15030	-2.90200
H	-4.14980	2.91200	-2.96900
C	-1.74900	3.68670	1.95800
H	-1.40700	3.02880	2.75820
H	-0.88380	4.21860	1.57130
H	-2.43820	4.41710	2.39550
C	-5.30250	0.74420	-0.33550
H	-5.44380	0.04170	0.48640
H	-6.19900	1.36870	-0.40170
H	-5.22850	0.16470	-1.25630
C	-4.11950	1.70140	2.49080
H	-3.33180	1.64940	3.24310
H	-4.82820	2.47960	2.79600
H	-4.64740	0.74750	2.49460

Compound 10b

Ir_CPSTAR_CO_C_CF3_C2F5_CARBENE_ISOMER

C	-0.04050	0.39900	0.02970
Ir	-1.91790	0.83840	0.05380
C	0.45740	-1.03750	-0.03930
F	1.79810	-1.19060	-0.06960
F	0.02150	-1.76670	1.02520
F	-0.01240	-1.67910	-1.14710
C	1.05010	1.44160	0.03570
F	2.09290	1.14200	0.87050
F	0.57060	2.65300	0.47860
C	1.67120	1.76010	-1.36440
F	0.71000	2.18230	-2.21050
F	2.58660	2.73770	-1.26550
F	2.25520	0.68850	-1.90710
C	-4.08690	1.60090	-0.05710
C	-3.31820	2.21840	-1.09700
C	-2.32880	3.07540	-0.47050
C	-2.45410	2.92880	0.94030
C	-3.52320	1.98860	1.20250
O	-2.97810	-1.96930	-0.03890
C	-2.46510	-0.94310	-0.00350
C	-1.49830	4.08200	-1.20210

H	-0.60870	4.36070	-0.64300
H	-1.17840	3.70680	-2.17230
H	-2.09600	4.98520	-1.36920
C	-3.59070	2.15260	-2.56750
H	-2.66480	2.20470	-3.14090
H	-4.09890	1.22690	-2.83750
H	-4.22740	2.99030	-2.87450
C	-1.73250	3.69700	2.00240
H	-1.40190	3.04260	2.81000
H	-0.85790	4.20770	1.60780
H	-2.40680	4.44600	2.43230
C	-5.28740	0.72410	-0.25360
H	-5.39910	0.00540	0.55870
H	-6.19480	1.33540	-0.28820
H	-5.22620	0.16250	-1.18630
C	-4.04670	1.64020	2.56130
H	-3.23750	1.57710	3.28950
H	-4.75250	2.40490	2.90520
H	-4.56650	0.68190	2.55620

Compound 11

Ir_CPSTAR_CO_CF3CCCF3_ALKYNE

Ir	-1.88980	0.84750	-0.36430
C	-3.99830	1.55730	0.03240
C	-3.40610	2.46650	-0.94240
C	-2.32120	3.13900	-0.30870
C	-2.20360	2.62800	1.03440
C	-3.27480	1.68470	1.25900
O	-2.28670	-1.47690	-2.23800
C	-2.11210	-0.59100	-1.52310
C	-1.47300	4.21540	-0.91260
H	-0.45760	4.19250	-0.51880
H	-1.40870	4.11060	-1.99580
H	-1.90140	5.19920	-0.69150
C	-3.94030	2.73790	-2.31620
H	-3.15080	3.07350	-2.98900
H	-4.38830	1.84410	-2.75140
H	-4.71030	3.51650	-2.28180
C	-1.20910	3.08240	2.06010
H	-0.98890	2.28780	2.77360
H	-0.26770	3.37710	1.59390
H	-1.59220	3.94360	2.61730
C	-5.24280	0.74920	-0.18260
H	-5.26080	-0.12790	0.46450
H	-6.13120	1.35140	0.03530
H	-5.31780	0.40290	-1.21390
C	-3.59800	1.02300	2.56360
H	-2.69350	0.79790	3.12820
H	-4.22790	1.67810	3.17580
H	-4.13350	0.08590	2.41090
C	-0.22960	0.00300	0.57430
C	0.19950	0.71030	-0.39900
C	1.36420	1.21030	-1.13860
F	2.53250	0.68690	-0.70910
F	1.25340	0.93750	-2.45800
F	1.46630	2.56450	-1.02140
C	0.08650	-0.85620	1.72070
F	-0.39670	-0.31370	2.87610
F	-0.49140	-2.07100	1.58710
F	1.41040	-1.04860	1.89820

Compound 13

Ir_CPSTAR_CO_CF3CCFCF2_METALLACYCYLOBUTENE

C	7.82000	-16.18900	2.47700
Ir	7.25730	-14.21870	2.96320
C	9.34280	-14.56280	2.70920
C	9.13540	-16.01200	2.41940
F	10.00420	-13.88290	1.71550
F	10.10670	-14.35660	3.84830
F	10.13050	-16.87690	2.16290
C	7.04380	-17.43800	2.29090
F	7.65860	-18.34110	1.49710
F	6.81410	-18.06350	3.48560
F	5.82300	-17.19880	1.75070
C	6.27550	-12.45410	4.05020
C	7.32820	-12.95840	4.87330
C	7.01860	-14.33050	5.20500
C	5.71600	-14.63360	4.64450
C	5.26860	-13.49640	3.91800
O	6.89370	-13.43380	0.06900
C	7.06190	-13.75530	1.15720
C	8.50920	-12.18460	5.36940
H	9.37430	-12.83000	5.50650
H	8.79020	-11.39470	4.67270
H	8.26770	-11.72070	6.33190
C	7.81590	-15.21910	6.11170
H	7.65010	-16.27030	5.87310
H	8.88280	-15.02360	6.00550
H	7.53800	-15.05970	7.15880
C	4.94030	-15.89440	4.86280
H	4.32820	-16.14370	3.99600
H	5.59540	-16.74030	5.05830
H	4.27640	-15.77080	5.72530
C	3.94540	-13.34790	3.23060
H	3.57330	-14.30880	2.87480
H	3.20240	-12.93200	3.92000
H	4.01370	-12.67790	2.37280
C	6.14220	-11.05130	3.53980
H	5.60450	-11.02170	2.59150
H	5.58750	-10.43780	4.25800
H	7.11750	-10.59010	3.38470

Compound 17

Ir_CPSTAR_CO_CF2CCCF2_BUTATRIENE

C	6.47310	1.49020	-1.21310
O	4.64840	-2.28180	0.93150
C	7.81750	1.53790	-0.68590
C	5.48680	-1.54990	0.63660
C	5.57810	1.58620	-0.09650

Ir	6.79120	-0.30810	0.15510
C	7.74040	1.72750	0.74090
C	6.36530	1.74830	1.11680
C	8.36500	-1.57750	0.59360
C	8.01630	-1.71070	-0.74140
C	9.21350	-1.88300	1.54480
F	9.17060	-1.39180	2.78840
F	10.25420	-2.71540	1.43560
C	8.31780	-2.22070	-1.91060
F	9.32450	-3.06140	-2.16960
F	7.65690	-1.96190	-3.04540
C	9.08010	1.49300	-1.49200
H	9.87810	0.98720	-0.94640
H	8.92960	0.95390	-2.42730
H	9.42240	2.50490	-1.73180
C	6.10040	1.44050	-2.66320
H	6.13090	2.44400	-3.10250
H	6.78310	0.80190	-3.22430
H	5.09440	1.04310	-2.79920
C	4.08290	1.67830	-0.16900
H	3.61370	1.25980	0.72200
H	3.77450	2.72620	-0.24940
H	3.69220	1.14370	-1.03470
C	5.82400	2.02600	2.48620
H	6.48420	1.63450	3.26070
H	5.71930	3.10550	2.64490
H	4.84250	1.57240	2.62650
C	8.90860	1.88890	1.66380
H	8.67530	1.52980	2.66580
H	9.77450	1.33120	1.30670
H	9.19220	2.94460	1.73400

IrCpSTAR_CO_I_CF2CF3 (Figure 4A)

Ir	0.11210	-0.46780	0.37360
C	0.73720	1.17170	1.88410
C	-0.62250	1.47530	1.43240
C	-0.57310	1.72100	0.03850
C	0.80300	1.54470	-0.40960
C	1.60710	1.27740	0.76480
C	1.55380	-1.97620	0.06530
F	2.55380	-1.89650	1.02010
F	1.05890	-3.25430	0.14720
C	2.30850	-1.97610	-1.29480
F	3.20020	-2.97500	-1.36960
F	1.45130	-2.11460	-2.32340
F	2.98880	-0.82270	-1.48710
C	-1.71220	2.16560	-0.82960
H	-1.61910	1.78650	-1.84790
H	-2.67360	1.83780	-0.43440
H	-1.73060	3.25960	-0.88670
C	-1.80550	1.64160	2.33330
H	-2.74420	1.57340	1.78320
H	-1.82190	0.87870	3.11150
H	-1.76750	2.62490	2.81610
C	1.31390	1.91110	-1.77070
H	2.23490	1.38430	-2.01090
H	0.58500	1.67760	-2.54760
H	1.51550	2.98770	-1.81800
C	3.10270	1.23540	0.82850
H	3.54780	1.09000	-0.15250
H	3.46890	2.18630	1.23130
H	3.45520	0.43550	1.47870
C	1.14480	0.98580	3.31280
H	2.13000	0.52590	3.38840
H	1.18260	1.95630	3.82080
H	0.43850	0.34870	3.84640
I	-1.03860	-2.04630	2.33900
O	-1.68850	-1.70120	-1.70870
C	-0.97660	-1.27780	-0.91970

IrCpSTAR_CO_I_CF2CF3_ANION_DOUBLET (Figure 4B)

Ir	0.14420	-0.43610	0.21630
C	0.71610	1.26410	1.79490
C	-0.61410	1.50720	1.30850
C	-0.51850	1.79780	-0.09680
C	0.86230	1.74300	-0.48350
C	1.61580	1.37120	0.68480
C	1.54480	-1.94460	-0.10010
F	2.62800	-1.84260	0.78530
F	1.08360	-3.23970	0.05670
C	2.23450	-1.98680	-1.49230
F	3.15520	-2.97770	-1.58830
F	1.34870	-2.18610	-2.48750
F	2.89410	-0.83410	-1.76510
C	-1.65190	2.21340	-0.99010
H	-1.48030	1.89710	-2.02050
H	-2.59890	1.78010	-0.66480
H	-1.76830	3.30460	-0.99140
C	-1.84260	1.59950	2.16390
H	-2.75350	1.53170	1.56580
H	-1.86850	0.78330	2.88790
H	-1.86790	2.55410	2.70640
C	1.41900	2.12480	-1.82220
H	2.34780	1.59570	-2.03620
H	0.71910	1.89170	-2.62790
H	1.62920	3.20260	-1.87050
C	3.11270	1.30320	0.77540
H	3.56060	1.04840	-0.18480
H	3.51980	2.27120	1.09430
H	3.43340	0.54850	1.49360
C	1.09130	1.04400	3.22830
H	2.05140	0.53290	3.31310
H	1.16900	2.00270	3.75980
H	0.34830	0.42220	3.72830
I	-1.03400	-2.14660	2.81270
O	-1.93170	-1.89140	-1.38910
C	-1.12110	-1.37500	-0.74410

Ir_CPSTAR_CO_I_C2F5_DIANION_SINGLET (Figure 5A)

Ir	4.30980	-4.66430	-5.15790
C	4.73210	-3.52490	-3.11320
C	3.37800	-3.28270	-3.46210
C	3.36590	-2.58390	-4.72660
C	4.72760	-2.32010	-5.11130
C	5.56830	-2.94510	-4.14810
C	5.70970	-6.15710	-5.20590
F	6.62120	-6.07140	-4.11390
F	5.25030	-7.48370	-5.12940
C	6.67080	-6.19690	-6.42530
F	7.62410	-7.16970	-6.32840
F	6.01390	-6.42850	-7.57770
F	7.34610	-5.03110	-6.56610
C	2.14500	-2.04270	-5.41410
H	2.29590	-1.98200	-6.49420
H	1.27800	-2.68510	-5.24540
H	1.89060	-1.03630	-5.05360
C	2.17120	-3.62600	-2.64040
H	1.30740	-3.83770	-3.27380
H	2.34950	-4.51290	-2.02930
H	1.89580	-2.80140	-1.96660
C	5.17250	-1.49820	-6.28310
H	6.14290	-1.83430	-6.65370
H	4.46530	-1.57520	-7.11180
H	5.26290	-0.43360	-6.01970
C	7.06720	-2.88900	-4.10620
H	7.48630	-2.76440	-5.10590
H	7.41440	-2.05400	-3.48220
H	7.47930	-3.81280	-3.69880
C	5.23790	-4.16900	-1.85680
H	6.11170	-4.78800	-2.06390
H	5.52030	-3.41860	-1.10420
H	4.47960	-4.81810	-1.41350
I	-17.15250	14.24730	22.23290
O	2.57270	-6.19290	-7.05630
C	3.26580	-5.60870	-6.31050

Ir(CpSTAR)(CO)_CF2CF3_K (Figure 5B)

IR	-0.24480	-0.78950	0.65580
C	-0.74180	1.10130	-0.63860
C	-1.00900	-0.05090	-1.43530
C	0.23490	-0.76230	-1.60370
C	1.28870	0.01910	-0.99540
C	0.68870	1.14510	-0.37720
C	-0.51410	-0.08260	2.57390
F	-0.87230	1.26300	2.60800
F	-1.59650	-0.69810	3.34900
C	0.65660	-0.17450	3.58790
F	0.35970	0.39330	4.77990
F	0.99700	-1.45190	3.83480
F	1.74520	0.46350	3.11420
C	0.44300	-1.96390	-2.48260
H	1.27340	-2.57930	-2.13190
H	-0.44420	-2.59950	-2.51360
H	0.66830	-1.66120	-3.51270
C	-2.30550	-0.37540	-2.11860
H	-2.43960	-1.45160	-2.24700
H	-3.16220	0.01000	-1.56120
H	-2.34160	0.07600	-3.11910
C	2.75570	-0.28740	-1.05940
H	3.28490	0.10590	-0.19010
H	2.94050	-1.36230	-1.09700
H	3.20970	0.15700	-1.95450
C	1.40510	2.27470	0.30320
H	2.36050	1.95210	0.71870
H	1.60580	3.08680	-0.40660
H	0.81510	2.68890	1.12170
C	-1.70590	2.20970	-0.32760
H	-1.49150	2.66580	0.63850
H	-1.65230	2.99760	-1.08970
H	-2.73710	1.85110	-0.29860
K	-3.05340	-2.21920	1.87110
O	-0.26580	-3.62150	1.62870
C	-0.19190	-2.50810	1.24850

Ir_CpSTAR__CO__CF2CF3_Na (Figure 5C)

Ir	0.15640	-0.31540	0.22620
C	0.77210	1.18010	1.90000
C	-0.58660	1.46240	1.55490
C	-0.60950	1.86750	0.17190
C	0.75450	1.93580	-0.30360
C	1.60040	1.48830	0.74500
C	1.42970	-1.90150	0.54460
F	2.35910	-1.65480	1.54450
F	0.78600	-3.14980	1.04450
C	2.27920	-2.47190	-0.62080
F	3.10420	-3.46360	-0.22230
F	1.50460	-2.96780	-1.60080
F	3.05550	-1.50500	-1.14950
C	-1.81310	2.37660	-0.57030
H	-1.72780	2.20190	-1.64410
H	-2.73080	1.89290	-0.23120
H	-1.93310	3.45650	-0.42030
C	-1.75050	1.52490	2.50170
H	-2.69110	1.27080	2.00990
H	-1.61960	0.85260	3.35200
H	-1.85980	2.53960	2.90660
C	1.19090	2.44900	-1.64370
H	2.12640	1.98860	-1.96440
H	0.44460	2.24900	-2.41420
H	1.34800	3.53450	-1.61120
C	3.10050	1.47170	0.73200
H	3.49220	1.36720	-0.28040
H	3.49730	2.40510	1.14970
H	3.49720	0.64780	1.32570
C	1.29650	0.87780	3.27490
H	2.15950	0.21340	3.23630
H	1.60600	1.79950	3.78330

H	0.53950	0.39860	3.89920
Na	-1.20720	-2.37710	1.55810
O	-1.42040	-1.73530	-1.90040
C	-0.79060	-1.21220	-1.06960

Ir_CpSTAR__CO__CF2CF3_MgI (Figure 5D)

Ir	0.84650	-0.15260	0.46460
C	1.20630	1.19750	2.27290
C	-0.21680	1.23370	1.98780
C	-0.39220	1.79840	0.68260
C	0.91100	2.12510	0.15290
C	1.89400	1.77260	1.14950
C	2.03260	-1.60260	0.74860
F	3.05260	-1.53260	1.63580
F	0.13080	-1.98520	3.57420
C	1.97980	-3.04030	0.23070
F	3.06160	-3.76110	0.50020
F	0.90800	-3.68230	0.86630
F	1.72650	-3.11830	-1.07790
C	-1.71120	2.09060	0.02940
H	-1.63020	2.10400	-1.05810
H	-2.46430	1.34940	0.29880
H	-2.07770	3.07270	0.34670
C	-1.29980	0.90820	2.97170
H	-2.21640	0.58080	2.47870
H	-0.98350	0.13020	3.66830
H	-1.54030	1.80540	3.55420
C	1.18670	2.84910	-1.13100
H	2.15190	2.56690	-1.55290
H	0.42190	2.64540	-1.88090
H	1.20120	3.93120	-0.95860
C	3.36680	2.03210	1.05920
H	3.71510	2.02360	0.02600
H	3.59780	3.01630	1.48200
H	3.93890	1.28950	1.61550
C	1.80740	0.76580	3.57760
H	2.87710	0.58160	3.48180
H	1.66720	1.55310	4.32650
H	1.33590	-0.15080	3.93870
O	-0.50430	-1.20060	-2.03190
C	0.01920	-0.87700	-1.06750
I	-2.97670	-2.71600	0.98120
Mg	-0.57610	-2.17950	1.90830

Ir_CPSTAR_CO_bis_CF3_CARBENE_PLUS_Mg (Figure 6A)

C	0.19700	0.59850	-0.02710
Ir	-1.91060	0.71930	0.10650
C	0.86380	0.00400	-1.00040
F	2.15210	-0.10510	-1.25580
F	0.22300	-0.68340	-2.03060
F	-2.63370	-1.74100	-3.25780
C	1.03760	1.27540	1.03000
F	2.28020	0.76160	1.18290
F	0.46130	1.22520	2.24950
F	1.21160	2.60220	0.74350
C	-4.01000	1.53270	-0.24410
C	-3.19210	2.04210	-1.32070
C	-2.18140	2.87270	-0.73320
C	-2.42570	2.96760	0.69270
C	-3.54300	2.13490	0.98900
O	-1.91280	-1.72360	1.85900
C	-1.90940	-0.79300	1.17070
C	-1.16710	3.67850	-1.49080
H	-0.25370	3.81890	-0.91380
H	-0.89580	3.20200	-2.43390
H	-1.57160	4.66960	-1.72540
C	-3.49360	1.91940	-2.79000
H	-2.59740	2.02750	-3.40320
H	-3.96160	0.96740	-3.04800
H	-4.18750	2.71280	-3.09340
C	-1.72660	3.88730	1.64790
H	-1.72330	3.48690	2.66260
H	-0.69060	4.05900	1.35930
H	-2.23010	4.86130	1.67570
C	-5.28580	0.75560	-0.40660
H	-5.48850	0.12630	0.46080
H	-6.13550	1.43820	-0.52560
H	-5.25890	0.10880	-1.28500
C	-4.20400	1.98980	2.32790
H	-3.49020	2.10770	3.14390
H	-4.97910	2.75530	2.44990
H	-4.68310	1.01650	2.43950
Mg	-1.90300	-0.88110	-1.86030

Ir_CPSTAR_CO_CF2CCF3_PLUS_MgF (Figure 6B)

C	-0.19020	0.26620	0.46830
Ir	-2.16990	0.69700	-0.14120
C	0.96280	0.50360	-0.43590
F	1.19930	1.81480	-0.67260
F	2.13320	-0.05850	-0.13510
F	0.68050	-0.01620	-1.75240
C	0.08270	-0.12440	1.71130
F	1.27570	-0.34250	2.26080
F	-0.83880	-0.34440	2.64110
C	-4.17410	1.77640	0.15140
C	-3.53470	2.30740	-1.02850
C	-2.31660	2.95370	-0.61080
C	-2.24340	2.84690	0.83220
C	-3.39440	2.15650	1.30710
O	-2.85160	-2.22840	-0.00850
C	-2.58490	-1.10260	-0.06930
C	-1.44870	3.83890	-1.46080
H	-0.40590	3.81030	-1.14470
H	-1.48390	3.55310	-2.51380
H	-1.78680	4.87990	-1.39550
C	-4.14830	2.37230	-2.39870
H	-3.39830	2.42430	-3.18980

H	-4.77950	1.50650	-2.60090	H	-6.30620	1.89590	0.32910
H	-4.77740	3.26640	-2.48530	H	-5.75130	0.59660	-0.72940
C	-1.17540	3.46750	1.68220	C	-3.77830	1.92900	2.73900
H	-1.07600	2.95850	2.64170	H	-2.90280	1.84360	3.38360
H	-0.20430	3.44680	1.18710	H	-4.38540	2.76240	3.11290
H	-1.42020	4.51580	1.88760	H	-4.36430	1.01670	2.85830
C	-5.53030	1.13390	0.19320	Mg	-1.30310	0.13250	-2.46980
H	-5.61560	0.42560	1.01880	F	-1.40080	0.08490	-4.26290

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