Supplementary Materials: Comparing the Acidity of $(R_3P)_2BH$-Based Donor Groups in Iridium Pincer Complexes

Leon Maser, Christian Schneider, Lukas Alig and Robert Langer

Content

Spectra

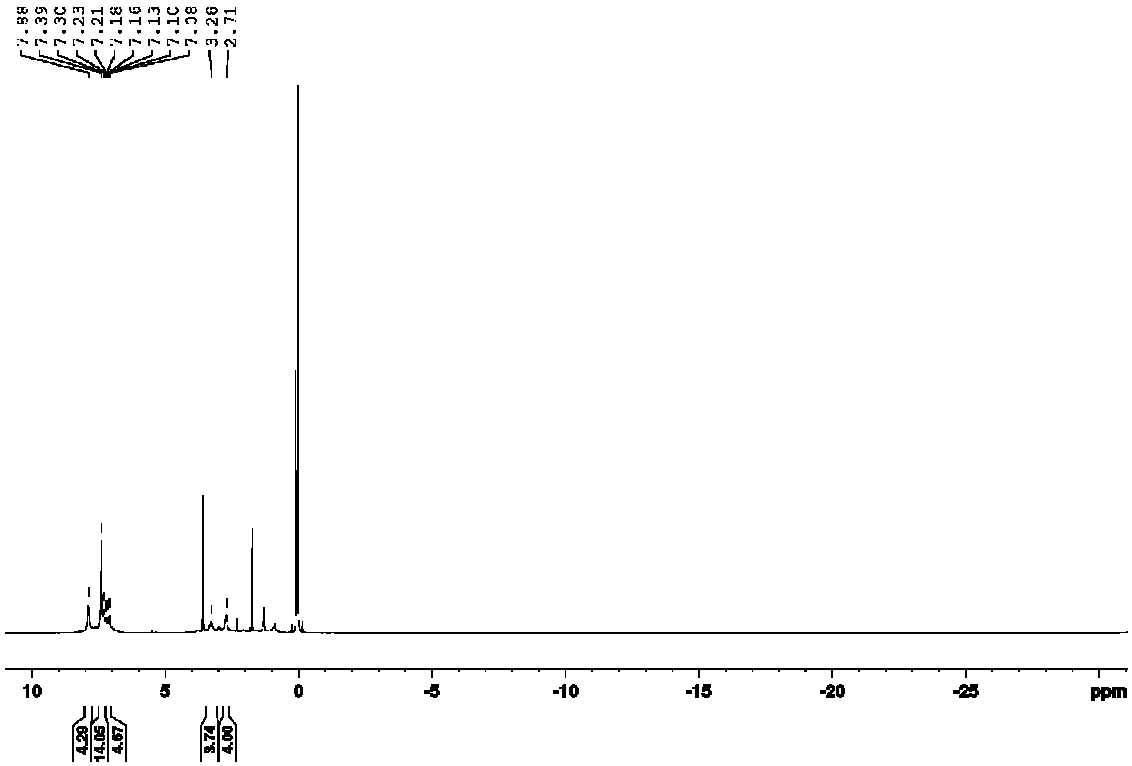

Figure S1. ^{1}H NMR spectrum of [(κ^{3}*P,N,P*-^{Ph}PN^{H}P)Ir(CO)]Cl (**2a**) in THF-d_8 after addition of the first equivalent of LiHMDS.

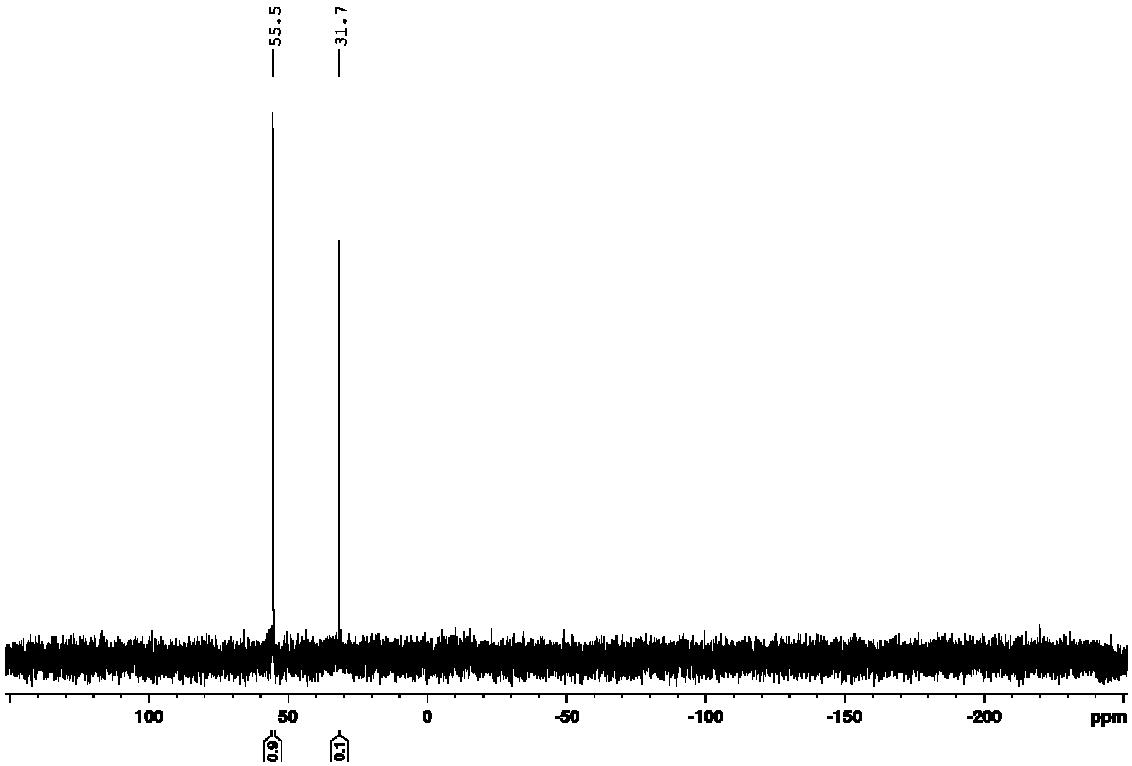

Figure S2. ^{31}P{^{1}H} NMR spectrum of [(κ^{3}*P,N,P*-^{Ph}PN^{H}P)Ir(CO)]Cl (**2a**) in THF-d_8 after addition of the first equivalent of LiHMDS.

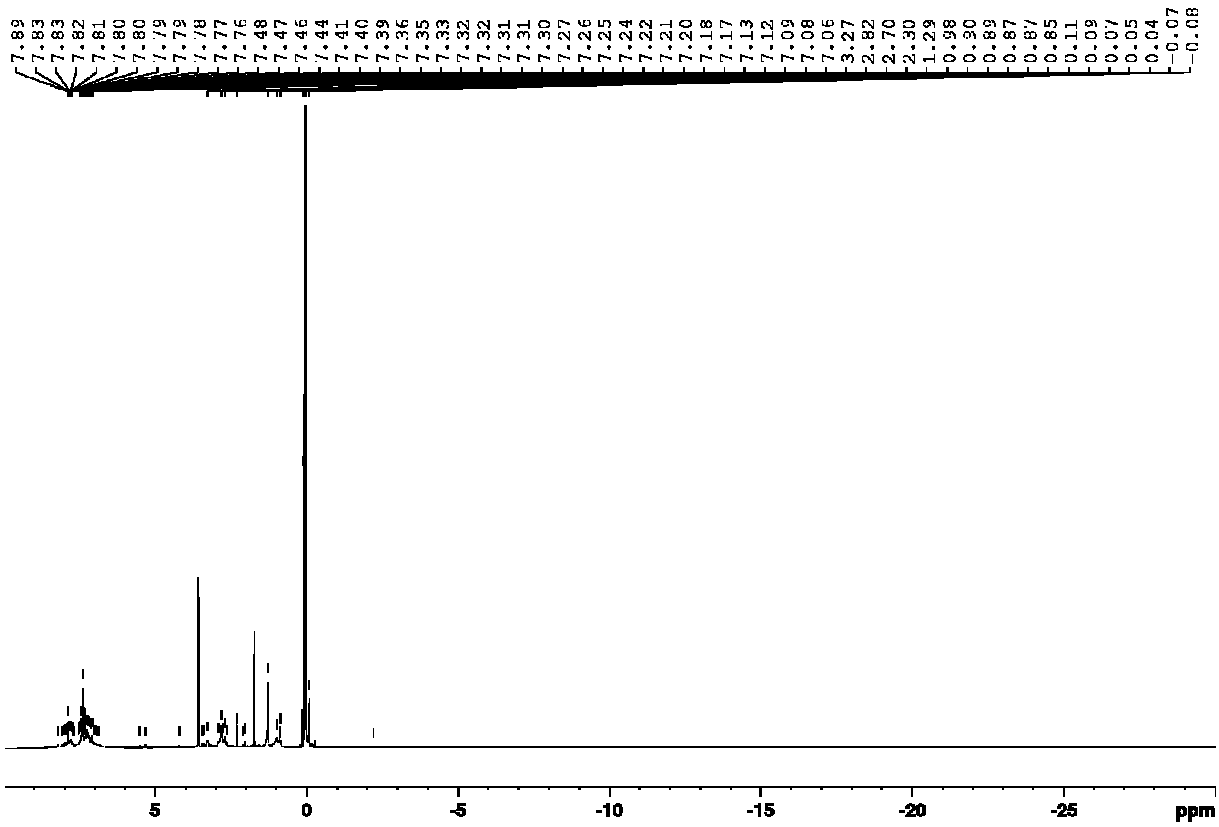

Figure S3. ^{1}H NMR spectrum of [(κ^{3}*P,N,P*-^{Ph}PN^{H}P)Ir(CO)]Cl in (**2a**) THF-d_8 after addition of the second equivalent of LiHMDS.

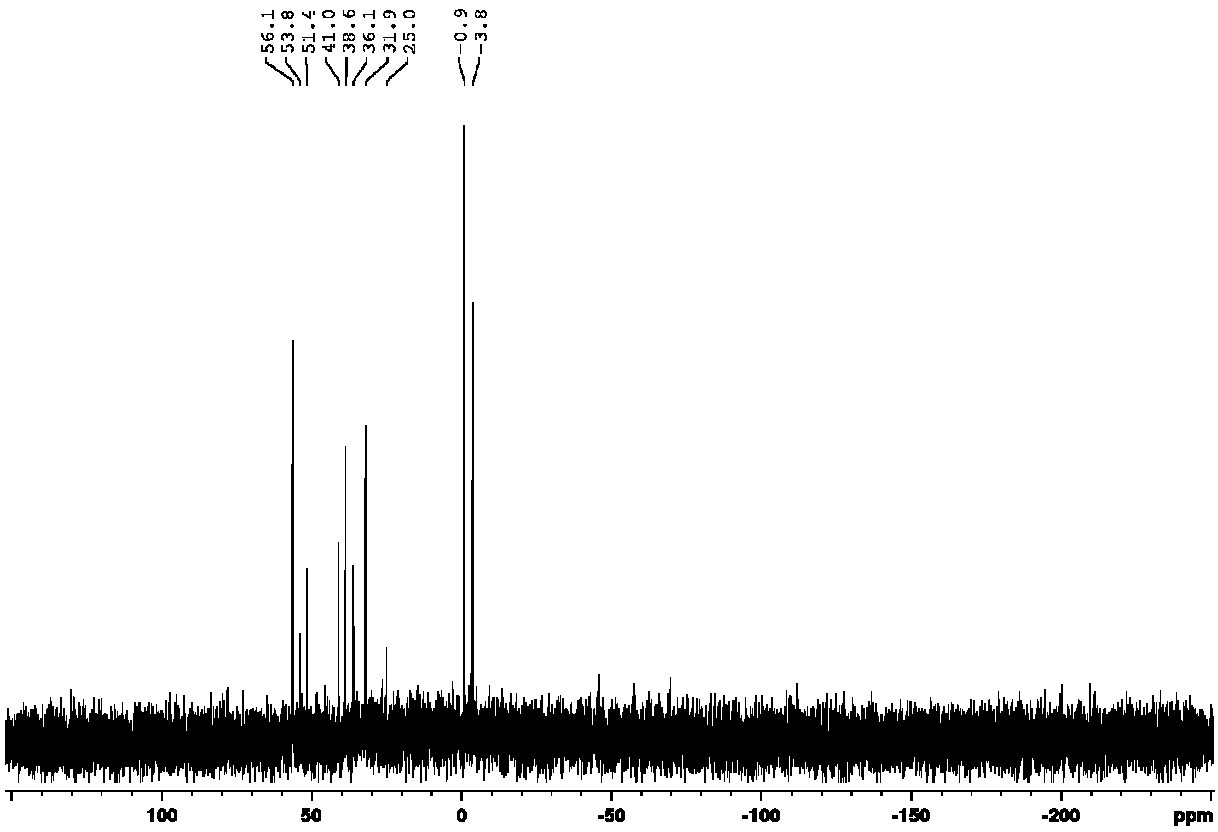

Figure S4. ^{31}P{^{1}H} NMR spectrum of [(κ^{3}*P,N,P*-^{Ph}PN^{H}P)Ir(CO)]Cl (**2a**) in THF-d_8 after addition of the second equivalent of LiHMDS.

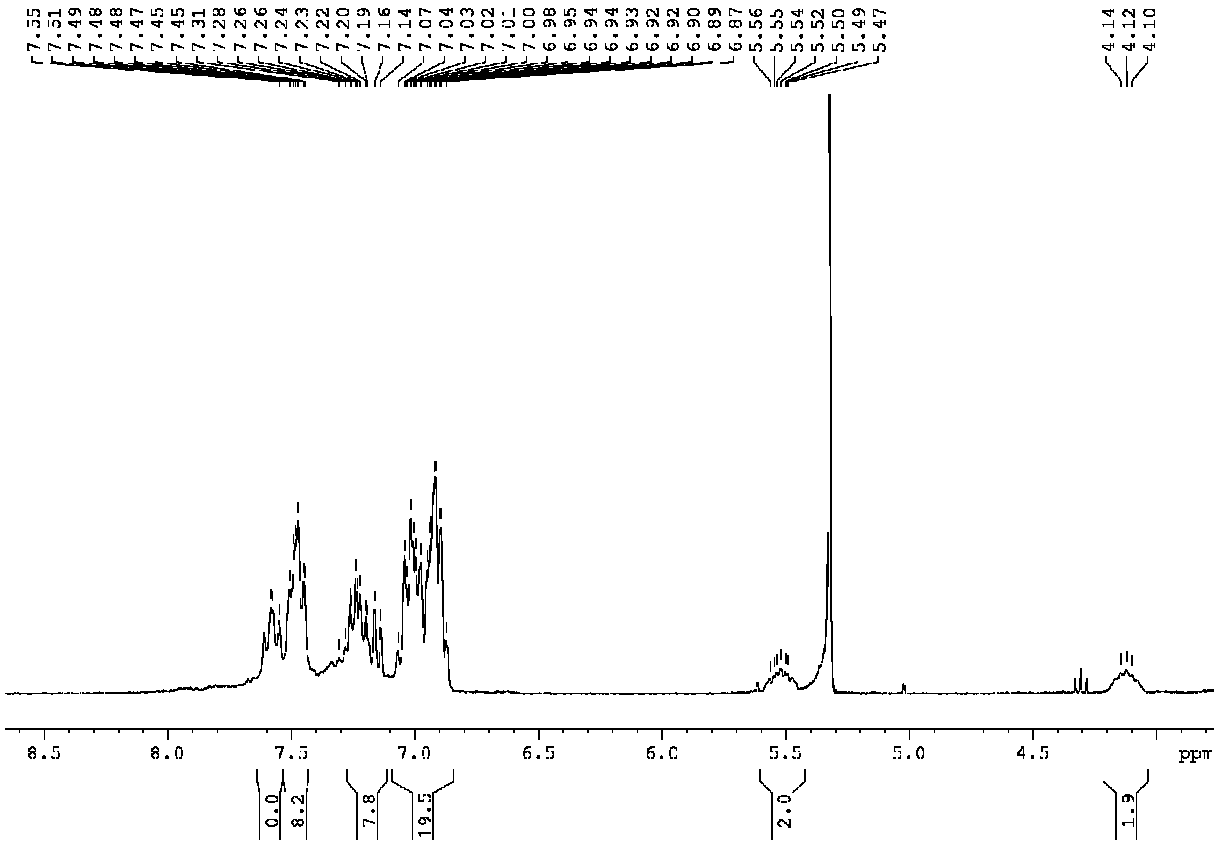

Figure S5. ^{1}H NMR spectrum of [{κ^{3}*P,C,P*-HB(dppm)$_2$}Ir(CO)$_2$]Br (**5c**) in CD_2Cl_2.

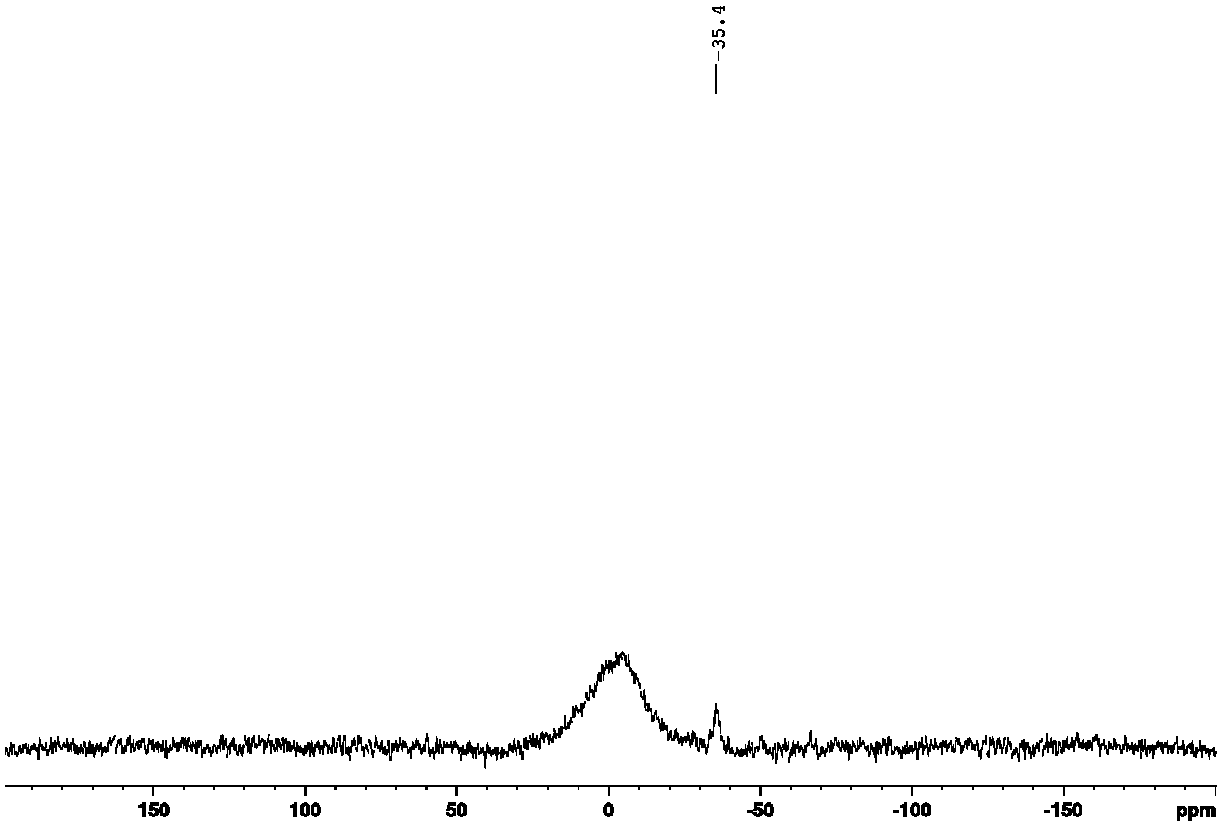

Figure S6. ^{11}B{^{1}H} NMR spectrum of [{κ^{3}*P,C,P*-HB(dppm)$_2$}Ir(CO)$_2$]Br (**5c**) with reduced glass peak in CD_2Cl_2.

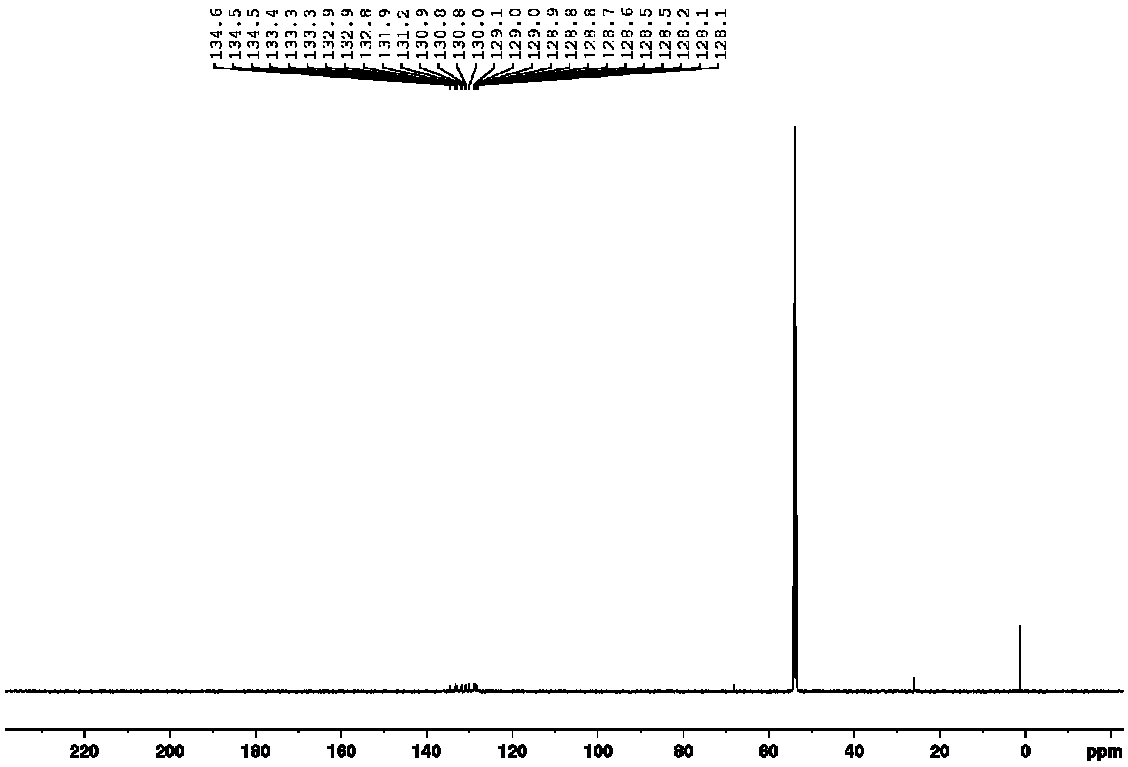

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of [{κ^3*P,C,P*-HB(dppm)$_2$}Ir(CO)$_2$]Br (**5c**) in CD_2Cl_2.

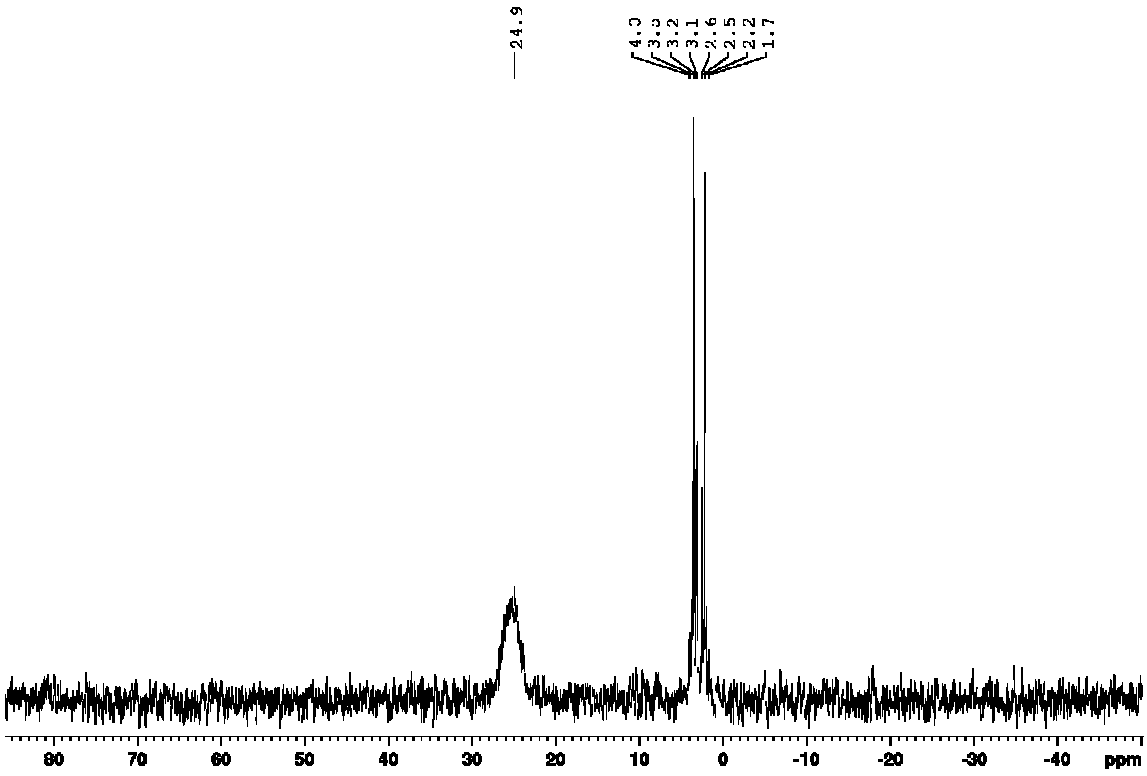

Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of [{κ^3*P,C,P*-HB(dppm)$_2$}Ir(CO)$_2$]Br (**5c**) in CD_2Cl_2.

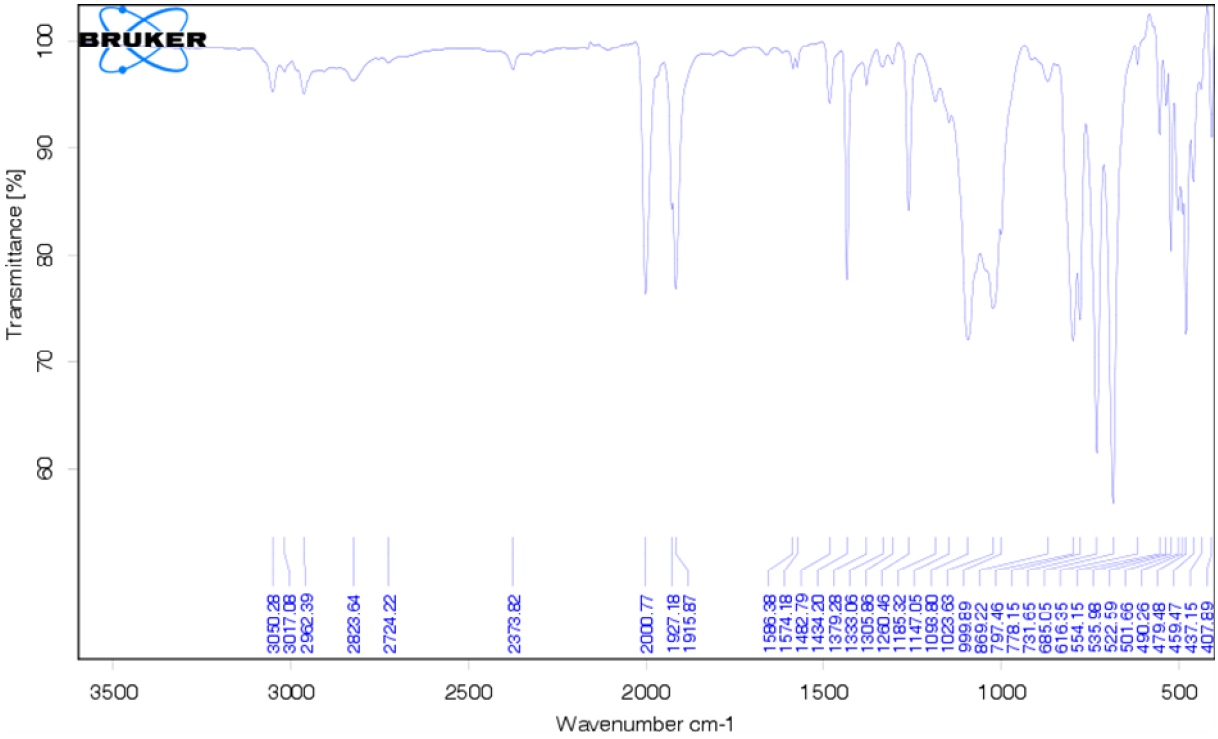

Figure S9. FT-IR spectrum of [{κ³*P,C,P*-HB(dppm)$_2$}Ir(CO)$_2$]Br (**5c**) .

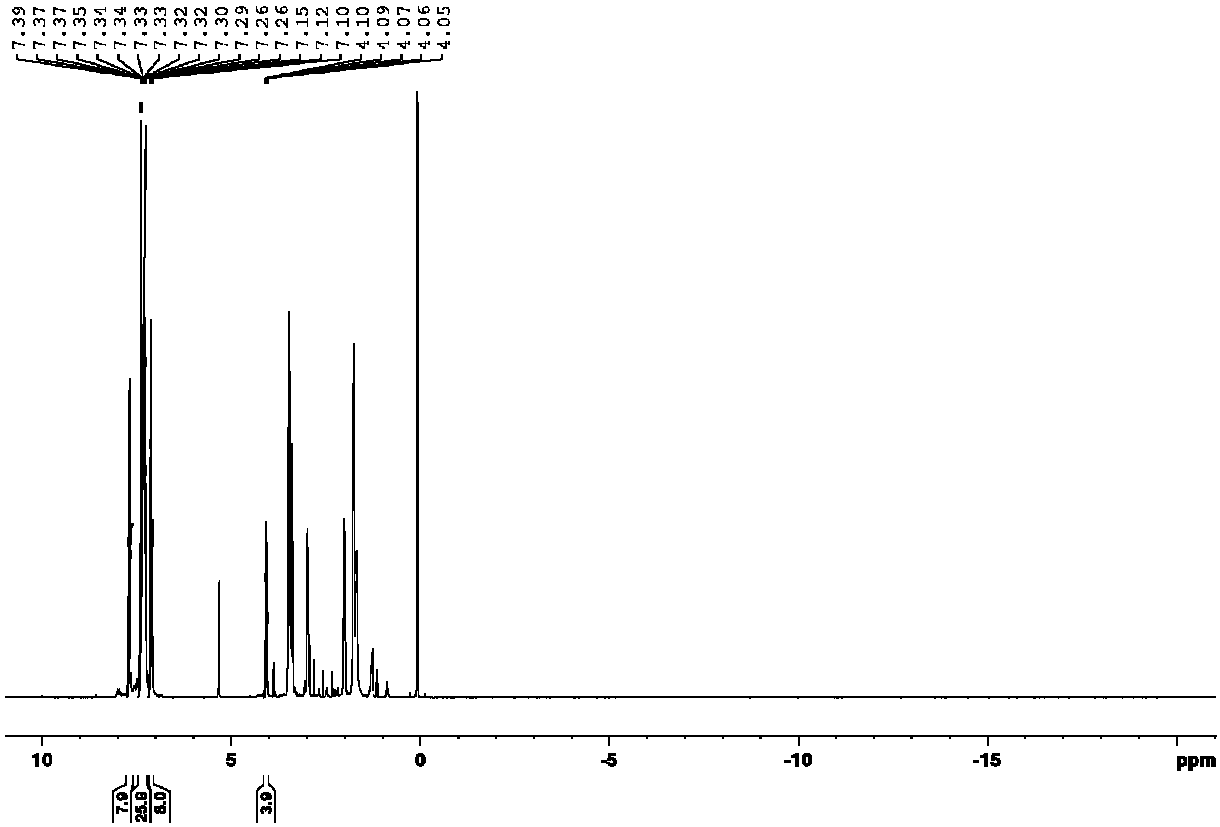

Figure S10. ^{1}H NMR spectrum of [{κ³*P,C,P*-C(dppm)$_2$}Ir(CO)]Cl (**4b**) in CD_2Cl_2.

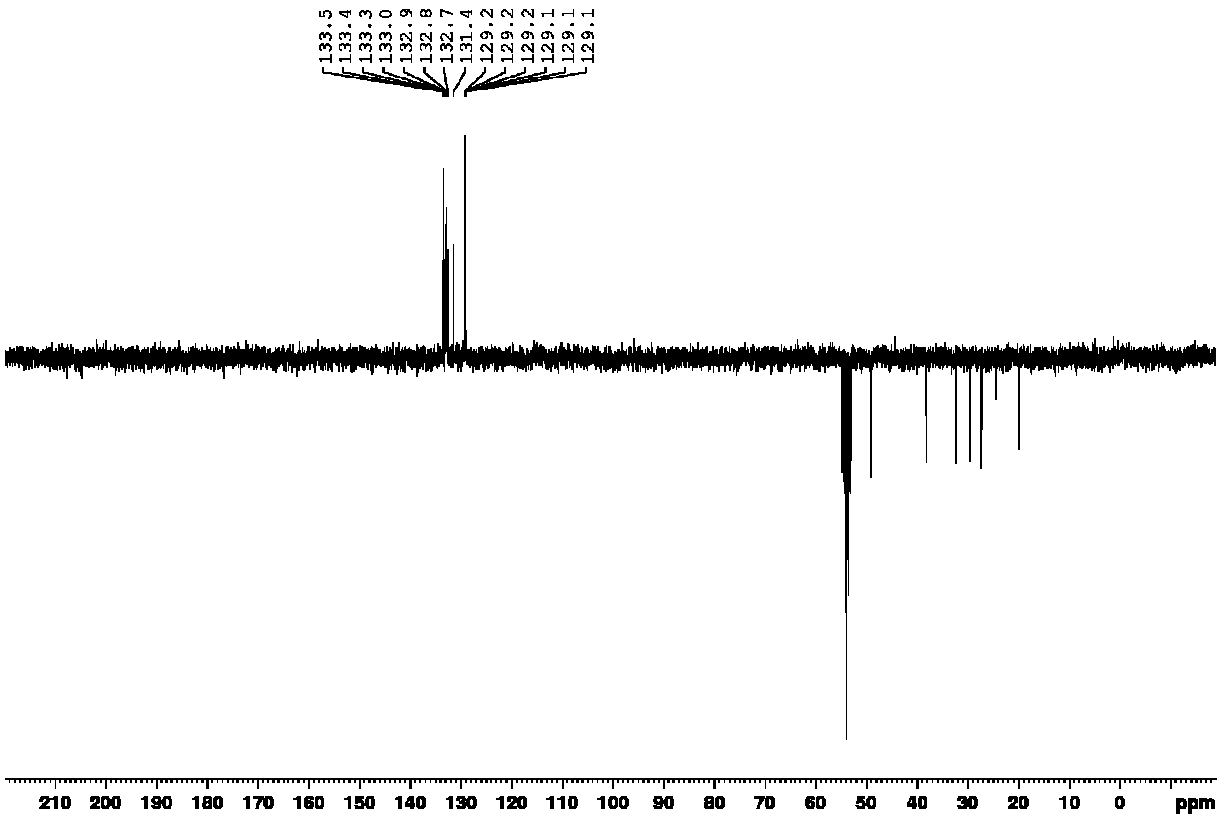

Figure S11. ^{13}C APT NMR spectrum of [{κ^3*P,C,P*-C(dppm)$_2$}Ir(CO)]Cl (**4b**) in CD_2Cl_2.

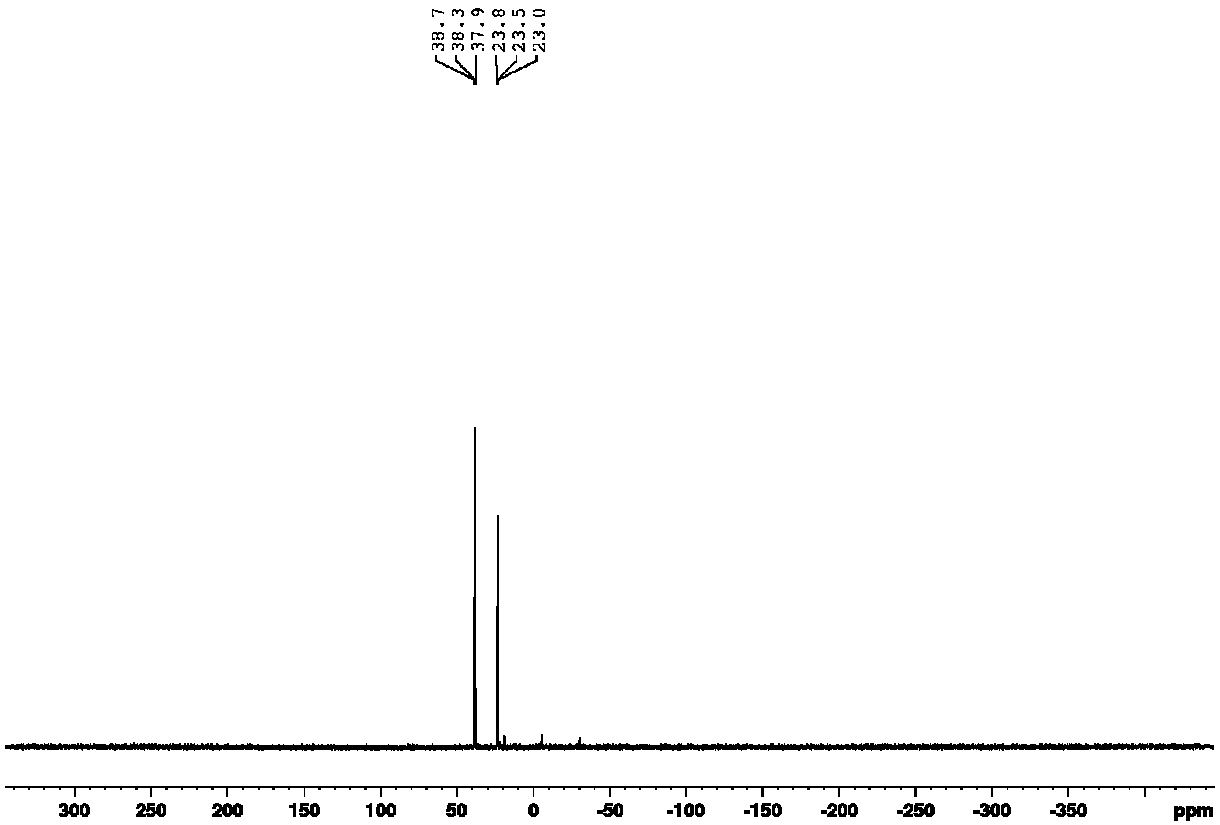

Figure S12. ^{31}P{^{1}H} NMR spectrum of [{κ^3*P,C,P*-C(dppm)$_2$}Ir(CO)]Cl (**4b**) in CD_2Cl_2.

X-Ray Crystallography

The single crystal X-ray diffraction data for the structural analysis were collected using graphite-monochromated Mo-K_α-radiation ($\lambda_{MoK\alpha}$= 0.71073) the pixel detector system Bruker Quest D8. The structures were solved with the Olex2 software by direct methods with SHELXT and refined against F^2 by full-matrix-least-square techniques using SHELXL.[8–11] Crystallographic data for **5c** was deposited at Cambridge Crystallographic Data Centre (CCDC 1906827) and can be obtained free of charge via www.ccdc.cam.ac.uk/.

Table S1. Crystallographic data of complex **5c**.

Complex	**5c**
Formula	$C_{52}H_{45}BIrO_2P_4Br{\cdot}C_4H_8O$
M / g·mol^{-1}	1180.79
T/K	110(2)
Crystal System	monoclinic
Space Group	*C*2/*c*
a / Å	40.6382(15)
b / Å	12.2295(5)
c / Å	24.2274(9)
α / °	90
β / °	125,090(1)
γ / °	90
V / Å^3	9852.3(7)
Z	8
$\rho_{calc.}$ / g·cm^{-3}	1.557
μ / mm^{-1}	3.696
F(000)	4624
Θ_{min}/°	2.220
Θ_{max}/°	31.282
Measured Refl.	142905
Independent Refl.	14758 (R_{Int} = 0.0304)
Ind. Refl. (I>2 (I))	13053
Parameters/Restraints	599/0
R_1	0.0277
R_1 (all data)	0.0354
wR_2	0.0695
wR_2 (all data)	0.0728
GooF	1.023
Max. peak + hole / e·Å^{-3}	0.963/-2.678
CCDC	1906827

DFT Calculations

DFT calculations were performed with Grimme's B97D functional including dispersion[2] and the def2TZVPP basis set after a pre-optimization with the def2SVP basis set[3,4] in Gaussian16.[5,10] Crystal structures were used as starting models, where possible. After optimization, a frequency calculation was performed to ascertain that a ground state was found (no imaginary modes). The proton affinities (PA's) were calculated as the difference in Gibbs energy (E) between a protonated complex and it's deprotonated counterpart:

$$PA = E(\text{complex}) - E(\text{complexH}^+)$$

Not included in the calculations were counter ions and implicit or explicit solvation effects.

Cartesian coordinates of all DFT-optimized geometries

2a

Atomic center	X	Y	Z
C	2.468401	0.037735	2.303634
C	1.252147	0.779264	2.860264
N	0.001002	0.113688	2.364581
Ir	0.000446	-0.216336	0.175704
C	-1.252391	0.772813	2.863327
C	-2.466255	0.028582	2.305156
C	-0.000112	-0.589134	-1.622508
O	-0.000668	-0.843453	-2.753197
H	0.003912	-0.835160	2.748519
P	2.294569	-0.047588	0.442908
C	3.337804	-1.425166	-0.109891
C	4.681199	-1.270876	-0.483591
C	5.422915	-2.385269	-0.882340
C	4.830531	-3.651610	-0.909168
C	3.488352	-3.806530	-0.546563
C	2.739898	-2.696147	-0.154548
C	3.011102	1.509476	-0.162325
C	2.352439	2.194722	-1.195991
C	2.880134	3.386998	-1.695509
C	4.063338	3.907087	-1.163187
C	4.721273	3.233501	-0.128598
C	4.198701	2.039504	0.371092

P	-2.293417	-0.050364	0.444280
C	-3.336744	-1.425990	-0.112932
C	-4.681756	-1.269944	-0.480145
C	-5.424720	-2.382163	-0.882463
C	-4.831803	-3.648022	-0.919451
C	-3.488071	-3.804572	-0.563324
C	-2.738407	-2.696305	-0.167534
C	-3.011007	1.507772	-0.157107
C	-4.193844	2.041059	0.383448
C	-4.717831	3.234941	-0.115148
C	-4.066352	3.904908	-1.156093
C	-2.888031	3.381348	-1.695866
C	-2.358704	2.189496	-1.197172
H	2.495273	-0.994308	2.674996
H	3.397841	0.530144	2.604609
H	1.254009	0.786505	3.958095
H	1.226420	1.813000	2.501470
H	-1.253339	0.776353	3.961166
H	-1.231067	1.807918	2.508241
H	-2.488731	-1.005038	2.672416
H	-3.397404	0.515902	2.609068
H	5.141526	-0.287279	-0.480654
H	6.461562	-2.263022	-1.177921
H	5.410641	-4.514962	-1.224222
H	3.022732	-4.787881	-0.583854
H	1.685362	-2.799508	0.096667
H	1.425091	1.794038	-1.594941
H	2.366195	3.910813	-2.497141
H	4.471898	4.836686	-1.550564
H	5.640581	3.636691	0.287880
H	4.723241	1.523084	1.170935
H	-5.142256	-0.286432	-0.469321
H	-6.464640	-2.258643	-1.172996

H	-5.412808	-4.509728	-1.237356
H	-3.022271	-4.785507	-0.608465
H	-1.682942	-2.800541	0.079311
H	-4.713786	1.527458	1.188051
H	-5.633358	3.640736	0.307092
H	-4.476073	4.834312	-1.542701
H	-2.379092	3.902217	-2.502594
H	-1.435058	1.786263	-1.602072

1a

Atomic center	X	Y	Z
C	-2.469296	0.059318	2.319369
C	-1.256470	-0.662388	2.905861
N	-0.002247	-0.027873	2.382531
Ir	-0.003139	0.062266	0.161027
C	1.240848	-0.675936	2.915386
C	2.471388	0.008612	2.317724
C	0.010061	0.241681	-1.683770
H	-0.027542	1.641908	0.319045
Cl	0.042031	-2.433412	0.254304
O	0.027843	0.368886	-2.828613
H	0.003027	0.941256	2.703126
P	-2.344262	0.100207	0.454922
C	-3.168466	1.638820	-0.053120
C	-4.300666	1.629596	-0.880971
C	-4.890990	2.836543	-1.267716
C	-4.361794	4.051756	-0.828193
C	-3.230181	4.064646	-0.003717
C	-2.631296	2.864636	0.375225
C	-3.324559	-1.267948	-0.200233
C	-2.871544	-1.955626	-1.335076
C	-3.655424	-2.964721	-1.896365
C	-4.887644	-3.295218	-1.325786

C	-5.343529	-2.611415	-0.193587
C	-4.567658	-1.596292	0.366881
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C	3.226714	1.585929	-0.054640
C	4.621402	1.644008	0.121111
C	5.322692	2.791718	-0.246263
C	4.641960	3.881855	-0.801463
C	3.258803	3.822773	-0.988255
C	2.549459	2.677997	-0.614514
C	3.268776	-1.295867	-0.223264
C	3.506735	-2.458313	0.523185
C	4.169182	-3.538288	-0.062347
C	4.582729	-3.467555	-1.395223
C	4.335961	-2.313075	-2.145990
C	3.680040	-1.228612	-1.564676
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H	-1.257492	-0.611116	4.002132
H	-1.226802	-1.707621	2.587599
H	1.242762	-0.605061	4.010538
H	1.186415	-1.725071	2.616464
H	2.545575	1.046539	2.664499
H	3.389139	-0.510313	2.611655
H	-4.718845	0.688258	-1.223599
H	-5.765570	2.823058	-1.912519
H	-4.824369	4.987781	-1.129542
H	-2.812199	5.008946	0.335175
H	-1.733945	2.880977	0.989889
H	-1.901228	-1.724105	-1.758960
H	-3.296570	-3.499688	-2.771190
H	-5.492438	-4.086958	-1.759993
H	-6.302471	-2.865136	0.250128
H	-4.942218	-1.056551	1.232956

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H	2.730984	4.663515	-1.430480
H	1.475551	2.628676	-0.762627
H	3.170896	-2.533215	1.552565
H	4.354253	-4.436370	0.520533
H	5.095235	-4.311174	-1.849719
H	4.656769	-2.256048	-3.182603
H	3.497835	-0.330228	-2.149389

3c

Atomic center	X	Y	Z
Ir	-0.965866	1.107124	-0.147826
H	-0.850549	0.798465	1.382446
P	-2.556850	-0.596921	-0.298809
Cl	-0.991659	1.407128	-2.739964
P	1.018600	2.276305	0.012485
B	0.573522	-0.501111	-0.241563
C	-2.178355	2.565931	0.181128
C	-1.765449	-2.264448	-0.516589
C	-3.782769	-0.501627	-1.651396
C	-3.592732	-0.865309	1.197665
C	0.967537	4.077576	-0.349646
C	1.821427	2.174255	1.646434
C	2.227909	1.610423	-1.218740
P	-0.086009	-2.109868	0.262603
P	2.223386	-0.215901	-0.941173
O	-2.853508	3.454135	0.500146
H	-2.395782	-3.065741	-0.115103
H	-1.590771	-2.420526	-1.585970
C	-4.256062	0.758634	-2.039857
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C	-3.378292	-0.118823	2.361286

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C	0.103768	4.524526	-1.362589
C	3.215512	2.135549	1.801879
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H	3.221294	2.065569	-1.152314
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C	2.681472	-0.975682	-2.564100
C	3.715836	-0.561166	0.087081
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C	-5.346517	-2.102373	2.338412
C	1.669732	6.368187	0.045534
H	2.410827	4.673234	1.148784
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C	0.034439	5.884129	-1.670885
H	3.864208	2.121139	0.933759
C	3.786319	2.074265	3.074130
C	1.582864	2.154396	4.065167
H	-0.068413	2.239650	2.682076
C	1.468699	-4.415770	0.774264
C	1.066021	-3.857341	-1.552990
C	0.024318	-1.295422	2.914723
C	-1.362576	-3.249107	2.562510
C	3.705389	-1.925769	-2.696645
C	1.852187	-0.700770	-3.666229

C	3.561784	-1.256410	1.288782
C	4.982727	-0.070312	-0.265928
C	-5.731842	-0.282304	-3.654009
H	-5.586067	1.848313	-3.331798
H	-5.627099	-2.437213	-3.771154
H	-3.950462	0.211911	4.410033
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H	-6.117068	-2.869826	2.321838
H	2.272305	7.082809	0.601840
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H	-0.637015	6.221273	-2.457162
C	2.972746	2.080651	4.210822
H	4.867062	2.013754	3.172332
H	0.941824	2.173788	4.943784
H	1.310080	-4.217151	1.830664
C	2.283935	-5.478247	0.374547
H	0.626319	-3.204163	-2.302611
C	1.873523	-4.924881	-1.947599
C	-0.295635	-1.312577	4.274267
H	0.662189	-0.519890	2.494646
H	-1.786799	-3.999808	1.899652
C	-1.686777	-3.264286	3.919732
H	4.338984	-2.167218	-1.848874
C	3.905649	-2.583744	-3.914895
C	2.067061	-1.345831	-4.883506
H	1.020159	-0.006144	-3.558350
H	2.567912	-1.598678	1.567835
C	4.655163	-1.465845	2.131856
C	6.072427	-0.251685	0.588747
H	5.118587	0.451727	-1.210905
H	-6.484970	-0.195392	-4.433772
H	-5.702728	-1.556145	4.397712
H	0.749242	7.868626	-1.203489

H	3.417279	2.031520	5.202017
H	2.763292	-6.102897	1.124761
C	2.485447	-5.734499	-0.985121
H	2.037264	-5.110948	-3.005523
H	0.115481	-0.551475	4.933411
C	-1.151907	-2.295741	4.777223
H	-2.362733	-4.022611	4.307759
C	3.092878	-2.293313	-5.012023
H	4.696437	-3.326107	-4.001037
H	1.425848	-1.115218	-5.731505
H	4.524013	-2.012328	3.063109
C	5.909976	-0.952346	1.789529
H	7.047456	0.147536	0.317498
H	3.121917	-6.560472	-1.294268
H	-1.412711	-2.304803	5.833212
H	3.250632	-2.803146	-5.959992
H	6.758574	-1.094046	2.455078

cis-**1b**

Atomic center	X	Y	Z
Ir	-0.967562	1.107539	-0.053154
H	-1.062866	0.993800	1.512120
P	-2.609615	-0.570106	-0.273964
Cl	-0.749647	1.020180	-2.571690
P	0.921039	2.497931	0.161386
C	0.619248	-0.500533	0.108764
C	-2.237381	2.497523	-0.043208
C	-1.650701	-2.000034	-0.971265
C	-3.989662	-0.299105	-1.414457
C	-3.359079	-1.112245	1.284481
C	0.773112	4.220299	-0.356438
C	1.753788	2.443971	1.775831
C	2.145651	1.716360	-1.003978
P	-0.078889	-2.167551	-0.062214

P	2.219142	-0.083635	-0.685854
O	-3.010237	3.345547	-0.014248
H	-2.200106	-2.946427	-0.975012
H	-1.408684	-1.701617	-1.997808
C	-5.217577	0.133969	-0.881917
C	-3.838364	-0.433102	-2.805049
C	-3.502256	-0.186844	2.328255
C	-3.881713	-2.406939	1.425248
C	1.250522	5.272636	0.441666
C	0.124506	4.490255	-1.575892
C	3.128027	2.725672	1.873320
C	1.032503	2.143823	2.940952
H	3.148321	2.146416	-0.932996
H	1.745496	1.868611	-2.010596
C	0.936166	-3.391558	-0.904140
C	-0.442366	-2.787722	1.591731
C	2.718199	-0.917923	-2.207155
C	3.546106	-0.351813	0.517440
H	-5.349049	0.234707	0.191397
C	-6.281212	0.426245	-1.736090
H	-2.889558	-0.731747	-3.235645
C	-4.911941	-0.148381	-3.649275
H	-3.102531	0.816786	2.220383
C	-4.156295	-0.555289	3.505498
H	-3.803874	-3.126962	0.615021
C	-4.515736	-2.777840	2.610659
C	1.085730	6.591866	0.013142
H	1.737990	5.068973	1.390213
H	-0.264276	3.677147	-2.184094
C	-0.025386	5.810983	-1.996127
H	3.703743	2.986917	0.990469
C	3.770390	2.680238	3.110092
C	1.677204	2.102777	4.179024

H	-0.034263	1.954062	2.880900
C	1.930033	-4.068798	-0.175385
C	0.740875	-3.678226	-2.264900
C	-0.603555	-1.917576	2.682290
C	-0.664690	-4.166962	1.755547
C	3.695610	-1.927084	-2.135854
C	2.212436	-0.518134	-3.456140
C	3.361889	-1.041978	1.723317
C	4.818114	0.155159	0.193576
C	-6.131448	0.283065	-3.118532
H	-7.227900	0.758792	-1.319580
H	-4.792418	-0.258192	-4.723542
H	-4.276675	0.169429	4.306245
C	-4.656368	-1.852005	3.650463
H	-4.911196	-3.784023	2.718581
H	1.449783	7.407089	0.632274
C	0.453326	6.861249	-1.203712
H	-0.523610	6.021484	-2.938455
C	3.047492	2.363262	4.264462
H	4.832870	2.897850	3.172702
H	1.107757	1.877433	5.076784
H	2.078006	-3.857470	0.879428
C	2.707629	-5.040192	-0.803669
H	-0.013228	-3.153379	-2.842271
C	1.526467	-4.649025	-2.885015
C	-0.963587	-2.428981	3.928380
H	-0.493304	-0.845093	2.561316
H	-0.544485	-4.848432	0.918254
C	-1.026269	-4.668469	3.005259
H	4.100562	-2.236750	-1.179334
C	4.156002	-2.529808	-3.304464
C	2.681195	-1.130310	-4.618699
H	1.455675	0.255238	-3.523486

H	2.396775	-1.458548	1.993544
C	4.433262	-1.204600	2.605048
C	5.882796	-0.009838	1.076566
H	4.983413	0.668325	-0.750643
H	-6.963333	0.506124	-3.780960
H	-5.162549	-2.140318	4.567807
H	0.326936	7.889108	-1.532679
H	3.548855	2.331365	5.228015
H	3.464886	-5.574127	-0.236391
C	2.501825	-5.334886	-2.155189
H	1.371662	-4.873224	-3.936229
H	-1.094259	-1.752816	4.768012
C	-1.171793	-3.801123	4.092457
H	-1.190195	-5.735086	3.129809
C	3.653392	-2.132394	-4.546803
H	4.914647	-3.304653	-3.242953
H	2.293405	-0.811645	-5.582277
H	4.282270	-1.736433	3.540241
C	5.690634	-0.687143	2.286196
H	6.861604	0.385671	0.820098
H	3.101109	-6.100937	-2.639634
H	-1.452178	-4.194432	5.065734
H	4.023977	-2.596631	-5.456838
H	6.521293	-0.814457	2.974926
H	0.901991	-0.444449	1.164525

trans-**1b**

Atomic center	X	Y	Z
Ir	-1.267291	0.39785	-0.082621
H	-0.853271	0.12866	1.408581
P	-1.879332	-1.88393	-0.212566
Cl	-1.556359	0.67297	-2.582775
P	-0.442835	2.59145	0.017913
C	0.787406	-0.27071	-0.701776

C	-2.974683	0.97329	0.462777
C	-0.341901	-2.81105	-0.718483
C	-3.112680	-2.36684	-1.441699
C	-2.345366	-2.65746	1.368385
C	-1.481175	3.86614	-0.739507
C	0.000770	3.24952	1.652806
C	1.138110	2.57638	-0.968345
P	1.114865	-1.92377	-0.072780
P	2.073044	1.01586	-0.799415
O	-3.996777	1.34443	0.835395
H	-0.350242	-3.84647	-0.367627
H	-0.273161	-2.80060	-1.812324
C	-4.164177	-1.48357	-1.727464
C	-3.066650	-3.62455	-2.067915
C	-2.464675	-1.90064	2.540747
C	-2.596816	-4.04042	1.406525
C	-2.359816	4.58337	0.093371
C	-1.516829	4.06722	-2.128905
C	0.517286	4.55665	1.737145
C	-0.141518	2.48555	2.817223
H	1.778620	3.44212	-0.771294
H	0.834266	2.59437	-2.020767
C	2.582557	-2.70819	-0.761758
C	1.088134	-2.04767	1.714680
C	3.006034	0.79347	-2.327030
C	3.181748	1.07557	0.609675
H	-4.189478	-0.49557	-1.282811
C	-5.170635	-1.86429	-2.615040
H	-2.253232	-4.31780	-1.870498
C	-4.072666	-3.99626	-2.960495
H	-2.285672	-0.83198	2.516338
C	-2.813605	-2.52127	3.742511
H	-2.548323	-4.63480	0.497536

C	-2.938682	-4.65723	2.608985
C	-3.252246	5.50043	-0.461346
H	-2.345301	4.43383	1.169113
H	-0.885590	3.48972	-2.794355
C	-2.405425	4.99521	-2.673254
H	0.598905	5.17197	0.844193
C	0.910743	5.07520	2.969994
C	0.245206	3.01246	4.052651
H	-0.561014	1.48722	2.759339
C	3.495851	-3.39669	0.054134
C	2.794928	-2.62499	-2.149918
C	1.220408	-0.91690	2.532286
C	0.885090	-3.31426	2.289746
C	4.408452	0.81406	-2.350762
C	2.275847	0.62403	-3.519964
C	4.054203	-0.00691	0.830725
C	3.175391	2.16073	1.499167
C	-5.127730	-3.11880	-3.230046
H	-5.980927	-1.17511	-2.835152
H	-4.032152	-4.96835	-3.444153
H	-2.911622	-1.92660	4.646691
C	-3.044897	-3.89790	3.780252
H	-3.137255	-5.72537	2.630448
H	-3.927128	6.05228	0.186940
C	-3.272812	5.71139	-1.843502
H	-2.424271	5.15096	-3.748201
C	0.778166	4.30118	4.129982
H	1.306592	6.08538	3.029418
H	0.118156	2.42140	4.955802
H	3.335551	-3.45562	1.126393
C	4.619213	-3.99351	-0.520501
H	2.100220	-2.08603	-2.788181
C	3.920282	-3.22374	-2.713431

C	1.159643	-1.05532	3.918155
H	1.353433	0.06450	2.097179
H	0.763419	-4.19578	1.666285
C	0.821402	-3.44366	3.676009
H	4.974689	0.96663	-1.437956
C	5.078988	0.63885	-3.563626
C	2.956712	0.45627	-4.724320
H	1.185899	0.62799	-3.515759
H	4.094032	-0.83455	0.132178
C	4.886570	-0.01117	1.947270
C	4.011794	2.14677	2.616701
H	2.524778	3.01009	1.338115
H	-5.910145	-3.40990	-3.925456
H	-3.321794	-4.37845	4.714775
H	-3.964936	6.43052	-2.272873
H	1.074240	4.71148	5.091751
H	5.325837	-4.52806	0.108205
C	4.832249	-3.90663	-1.900274
H	4.085102	-3.15739	-3.784884
H	1.264782	-0.17687	4.548411
C	0.960817	-2.31515	4.490373
H	0.654173	-4.42117	4.118177
C	4.357341	0.45641	-4.746094
H	6.165077	0.65295	-3.582864
H	2.394768	0.33087	-5.645716
H	5.560965	-0.84687	2.111661
C	4.860276	1.06097	2.846707
H	4.000340	2.98966	3.301397
H	5.707572	-4.37388	-2.343104
H	0.908628	-2.41901	5.570734
H	4.883948	0.32545	-5.687574
H	5.511034	1.05498	3.716866
H	0.598283	-0.47403	-1.767572

1c

Atomic center	X	Y	Z
Ir	0.213137	-1.510509	-0.023748
H	0.260533	-1.642447	1.536302
P	2.480829	-1.011548	0.009344
Cl	0.162043	-0.990985	-2.555591
P	-2.108654	-1.621961	0.091296
B	-0.123917	0.727978	0.295365
C	0.489455	-3.416514	-0.222744
C	2.705513	0.589631	-0.885577
C	3.552396	-2.208215	-0.835278
C	3.244981	-0.680511	1.630851
C	-2.887673	-3.118971	-0.590709
C	-2.890834	-1.324307	1.711861
C	-2.744187	-0.245927	-0.968915
P	1.456127	1.771826	-0.241283
P	-1.845841	1.280886	-0.471252
O	0.660082	-4.551102	-0.305792
H	3.728214	0.975473	-0.854283
H	2.414984	0.408387	-1.924686
C	4.150474	-3.245686	-0.101445
C	3.653148	-2.199069	-2.235334
C	2.442879	-0.349197	2.730373
C	4.643503	-0.630541	1.756088
C	-3.816671	-3.882547	0.130706
C	-2.477238	-3.537112	-1.869134
C	-4.243973	-0.949192	1.775946
C	-2.168123	-1.477944	2.901153
H	-3.828476	-0.109073	-0.935182
H	-2.426627	-0.515714	-1.978957
C	1.403490	3.059956	-1.531126
C	2.158119	2.586679	1.226984
C	-1.928184	2.402468	-1.903562

C	-2.950156	2.056598	0.765061
H	4.060128	-3.270740	0.980882
C	4.862572	-4.248183	-0.761001
H	3.149546	-1.434987	-2.818741
C	4.369833	-3.203563	-2.888340
H	1.363446	-0.362347	2.626446
C	3.029776	0.023814	3.941112
H	5.274393	-0.886273	0.909100
C	5.227119	-0.267531	2.970044
C	-4.339550	-5.052214	-0.428102
H	-4.125816	-3.574528	1.124763
H	-1.730839	-2.965205	-2.415909
C	-3.012339	-4.699536	-2.422871
H	-4.825987	-0.838207	0.865715
C	-4.855271	-0.716432	3.006604
C	-2.782081	-1.248072	4.134836
H	-1.125696	-1.775607	2.859531
C	1.631356	4.408188	-1.218022
C	1.183174	2.677184	-2.864864
C	1.280192	3.139937	2.171680
C	3.540964	2.736276	1.401578
C	-1.850261	3.786033	-1.673591
C	-2.080264	1.925526	-3.213077
C	-2.638299	2.083044	2.129919
C	-4.183270	2.574238	0.329485
C	4.977992	-4.226014	-2.154279
H	5.324397	-5.046770	-0.186353
H	4.445617	-3.190060	-3.972424
H	2.399606	0.287546	4.786424
C	4.420347	0.061649	4.064537
H	6.309971	-0.241813	3.061668
H	-5.054156	-5.644959	0.137144
C	-3.942825	-5.459047	-1.704142

H	-2.693246	-5.019456	-3.411429
C	-4.123880	-0.863617	4.189683
H	-5.899564	-0.418260	3.042070
H	-2.211745	-1.372924	5.051819
H	1.806793	4.710474	-0.190193
C	1.655201	5.364652	-2.235854
H	0.979859	1.637772	-3.111541
C	1.215035	3.638043	-3.873592
C	1.780394	3.821419	3.282264
H	0.207553	3.030307	2.044077
H	4.238686	2.325595	0.680032
C	4.038538	3.403120	2.521312
H	-1.731950	4.166244	-0.662622
C	-1.945546	4.678997	-2.738754
C	-2.190531	2.826203	-4.274538
H	-2.091254	0.861382	-3.419887
H	-1.706540	1.658683	2.483693
C	-3.542720	2.624538	3.046603
C	-5.085722	3.109007	1.247688
H	-4.432527	2.570128	-0.728490
H	5.533796	-5.007086	-2.666400
H	4.876103	0.346652	5.009336
H	-4.350267	-6.369770	-2.135515
H	-4.600316	-0.681624	5.149658
H	1.841195	6.406809	-1.989365
C	1.454991	4.980528	-3.563125
H	1.047202	3.337341	-4.903870
H	1.092418	4.248933	4.007136
C	3.160594	3.947278	3.462919
H	5.112462	3.495976	2.657365
C	-2.128617	4.201002	-4.039745
H	-1.880783	5.747258	-2.552365
H	-2.319776	2.448266	-5.285262

H	-3.292929	2.633318	4.104125
C	-4.765080	3.137790	2.609512
H	-6.035417	3.507834	0.900659
H	1.482655	5.724594	-4.355042
H	3.551113	4.467537	4.333653
H	-2.214453	4.899490	-4.868033
H	-5.467764	3.557829	3.324611
H	-0.211315	0.987699	1.465457

6c

Atomic center	X	Y	Z
Ir	-1.089824	0.823382	-0.113372
H	-0.758427	0.326058	1.341282
P	-2.417137	-1.096857	-0.302629
Cl	-1.272914	1.434121	-2.584624
P	0.504294	2.505763	0.055432
B	0.575438	-0.546267	-0.798567
C	-2.513924	1.974352	0.509134
C	-1.384253	-2.600387	-0.704574
C	-3.710963	-1.108198	-1.579075
C	-3.250098	-1.616470	1.245789
C	-0.032263	4.152371	-0.503091
C	1.247744	2.833560	1.692186
C	1.947068	2.065263	-1.029266
P	0.301288	-2.279019	-0.054906
P	2.316523	0.273128	-0.879400
O	-3.330527	2.653718	0.957467
H	-1.826819	-3.521775	-0.317346
H	-1.286061	-2.668578	-1.792829
C	-4.335724	0.104255	-1.903075
C	-4.118909	-2.291785	-2.215596
C	-3.084761	-0.895467	2.433595
C	-4.049753	-2.771708	1.248689
C	-0.619620	5.015938	0.437422

C	0.007082	4.524648	-1.854908
C	2.161903	3.894208	1.826072
C	0.943657	2.046261	2.807063
H	2.821169	2.711612	-0.901924
H	1.567518	2.161264	-2.053547
C	1.397286	-3.597874	-0.659873
C	0.177412	-2.411163	1.744333
C	3.189061	-0.173888	-2.411231
C	3.452485	-0.011059	0.501329
H	-3.990168	1.028181	-1.453994
C	-5.372106	0.127541	-2.837120
H	-3.633467	-3.237782	-1.990123
C	-5.151222	-2.262771	-3.154688
H	-2.473363	-0.001010	2.437022
C	-3.694982	-1.330939	3.612521
H	-4.215616	-3.323344	0.326722
C	-4.654865	-3.208074	2.426822
C	-1.147353	6.241368	0.031227
H	-0.665066	4.733778	1.485767
H	0.407648	3.850708	-2.603123
C	-0.515492	5.756669	-2.253790
H	2.377571	4.535141	0.974494
C	2.781521	4.140040	3.050432
C	1.561908	2.296656	4.035580
H	0.222351	1.242432	2.713166
C	1.832214	-4.650598	0.159854
C	1.867308	-3.498509	-1.981875
C	0.825524	-1.464956	2.548962
C	-0.593410	-3.420298	2.341397
C	4.521646	-0.607025	-2.417850
C	2.462943	-0.102488	-3.614056
C	3.756731	-1.343279	0.833934
C	4.016896	1.033198	1.244897

C	-5.782262	-1.053353	-3.462012
H	-5.846531	1.072410	-3.087836
H	-5.459953	-3.181772	-3.646276
H	-3.558967	-0.762670	4.529077
C	-4.475105	-2.488658	3.614055
H	-5.274511	-4.101222	2.417014
H	-1.600720	6.901733	0.765778
C	-1.091943	6.615946	-1.314961
H	-0.481243	6.037475	-3.303051
C	2.484941	3.336593	4.158453
H	3.485774	4.962683	3.144582
H	1.313616	1.684287	4.898712
H	1.485627	-4.719271	1.186925
C	2.726727	-5.598919	-0.342755
H	1.555255	-2.668545	-2.609964
C	2.758315	-4.450579	-2.477033
C	0.710720	-1.533832	3.937536
H	1.403100	-0.669547	2.093799
H	-1.118253	-4.146803	1.728299
C	-0.713084	-3.481987	3.729579
H	5.085316	-0.659121	-1.491193
C	5.123375	-0.981544	-3.622620
C	3.074831	-0.470051	-4.812280
H	1.425572	0.228159	-3.610787
H	3.338855	-2.162618	0.256406
C	4.597035	-1.621627	1.910341
C	4.850112	0.749455	2.329434
H	3.797668	2.065122	1.000791
H	-6.584492	-1.031047	-4.195087
H	-4.950731	-2.825919	4.531529
H	-1.501649	7.571745	-1.631173
H	2.962794	3.532245	5.115026
H	3.064049	-6.412258	0.294530

C	3.189365	-5.500396	-1.658572
H	3.123087	-4.365146	-3.497102
H	1.219444	-0.798008	4.554170
C	-0.059383	-2.539516	4.528904
H	-1.324901	-4.255967	4.183977
C	4.402337	-0.915583	-4.817440
H	6.155776	-1.321271	-3.625184
H	2.514149	-0.410945	-5.741510
H	4.824653	-2.654163	2.161241
C	5.137859	-0.575430	2.665962
H	5.270686	1.566740	2.908484
H	3.888209	-6.238045	-2.044384
H	-0.156118	-2.586094	5.610545
H	4.873509	-1.205904	-5.753014
H	5.785387	-0.793717	3.511188
H	0.359547	-0.792816	-1.963733

6b

Atomic center	X	Y	Z
Ir	-1.025134	0.998247	-0.145560
H	-1.014310	0.825415	1.411040
P	-2.539616	-0.798014	-0.259847
Cl	-0.955945	1.077687	-2.719252
P	0.775605	2.477876	0.045908
C	0.589783	-0.491096	-0.240011
C	-2.382280	2.306017	-0.059256
C	-1.556606	-2.254102	-0.839069
C	-3.952118	-0.665909	-1.394090
C	-3.264412	-1.261481	1.345031
C	0.536813	4.200055	-0.482624
C	1.547302	2.542426	1.694012
C	2.058354	1.759225	-1.076050
P	0.109881	-2.112183	-0.066550
P	2.171448	-0.036062	-0.698853

O	-3.208562	3.107139	0.010512
H	-2.042591	-3.211325	-0.631164
H	-1.429161	-2.122525	-1.917930
C	-5.221485	-0.342012	-0.885983
C	-3.770803	-0.800168	-2.780412
C	-3.424901	-0.281052	2.333817
C	-3.734424	-2.561404	1.582358
C	1.058617	5.278735	0.249585
C	-0.212238	4.439981	-1.647961
C	2.918566	2.803670	1.839672
C	0.759604	2.362511	2.839668
H	3.033433	2.250667	-1.020575
H	1.642913	1.854922	-2.084888
C	1.191208	-3.352991	-0.820685
C	-0.187382	-2.674944	1.643881
C	2.875468	-0.820055	-2.189437
C	3.474061	-0.166316	0.574714
H	-5.373772	-0.236365	0.184163
C	-6.296975	-0.161630	-1.757180
H	-2.787895	-1.003759	-3.190201
C	-4.853032	-0.625276	-3.643390
H	-3.062843	0.725716	2.155083
C	-4.038878	-0.597778	3.546956
H	-3.641071	-3.328925	0.819432
C	-4.330111	-2.881268	2.802353
C	0.837643	6.587166	-0.186889
H	1.624901	5.102794	1.158931
H	-0.630338	3.608351	-2.209157
C	-0.421495	5.750187	-2.078407
H	3.544966	2.958016	0.967476
C	3.496319	2.854519	3.108207
C	1.336982	2.421896	4.109286
H	-0.304403	2.174519	2.735679

C	2.188779	-3.972352	-0.051770
C	1.087067	-3.639049	-2.190691
C	-0.224006	-1.729978	2.675889
C	-0.465940	-4.022541	1.920073
C	3.999741	-1.655461	-2.134881
C	2.234224	-0.590872	-3.418730
C	3.162850	-0.710231	1.824218
C	4.767711	0.325576	0.333344
C	-6.115676	-0.305652	-3.135544
H	-7.276125	0.087459	-1.356693
H	-4.705230	-0.729030	-4.715045
H	-4.164513	0.171449	4.304581
C	-4.484982	-1.899727	3.786190
H	-4.677953	-3.894987	2.982407
H	1.238521	7.419397	0.385972
C	0.101136	6.824489	-1.350582
H	-1.001492	5.930772	-2.979673
C	2.707325	2.660527	4.245467
H	4.561944	3.041353	3.206207
H	0.716483	2.282929	4.991006
H	2.273521	-3.753590	1.008673
C	3.066212	-4.879519	-0.648484
H	0.336773	-3.145114	-2.800683
C	1.961784	-4.550397	-2.779476
C	-0.542960	-2.127243	3.975741
H	-0.014599	-0.689031	2.448557
H	-0.431440	-4.762339	1.123715
C	-0.775493	-4.418106	3.221213
H	4.490480	-1.853561	-1.188180
C	4.486854	-2.246240	-3.302862
C	2.733525	-1.175567	-4.582198
H	1.339815	0.026580	-3.460800
H	2.157576	-1.072010	2.009944

C	4.131333	-0.762478	2.829497
C	5.732818	0.277371	1.338747
H	5.022222	0.740529	-0.639101
H	-6.955001	-0.167017	-3.812094
H	-4.954933	-2.149717	4.733881
H	-0.070934	7.844042	-1.686020
H	3.158633	2.699212	5.233564
H	3.836089	-5.358608	-0.049326
C	2.949089	-5.173398	-2.009332
H	1.877824	-4.768408	-3.840227
H	-0.580818	-1.388837	4.772350
C	-0.818919	-3.469143	4.248927
H	-0.983813	-5.463301	3.434840
C	3.861839	-2.001414	-4.527382
H	5.354874	-2.898355	-3.252618
H	2.240522	-0.984988	-5.532148
H	3.879915	-1.181576	3.800379
C	5.414791	-0.267133	2.588933
H	6.732177	0.660645	1.148765
H	3.628761	-5.884291	-2.471933
H	-1.067077	-3.777994	5.261138
H	4.248812	-2.455846	-5.436071
H	6.168201	-0.302571	3.371760

3c

Atomic center	X	Y	Z
Ir	0.108846	-1.425129	0.109731
P	2.395399	-1.275351	0.171055
P	-2.110170	-1.043712	-0.338562
B	0.376603	0.822833	0.498066
C	-0.015045	-3.299109	-0.070373
C	2.860501	0.064917	-1.036488
C	3.420287	-2.702038	-0.319833
C	3.140959	-0.722664	1.747013

C	-2.795503	-1.865166	-1.822932
C	-3.283788	-1.432405	1.007048
C	-2.384337	0.759211	-0.731563
P	1.583055	1.396352	-0.874982
P	-1.330083	1.707796	0.429111
O	-0.086636	-4.455424	-0.147187
H	3.866099	0.468366	-0.881736
H	2.796393	-0.352370	-2.046872
C	3.210601	-3.904835	0.373952
C	4.396366	-2.647760	-1.325464
C	2.365090	-0.780982	2.912392
C	4.466257	-0.270039	1.816695
C	-4.173096	-1.846146	-2.092118
C	-1.923611	-2.498208	-2.718894
C	-4.462244	-0.713595	1.253493
C	-2.956851	-2.516991	1.836615
H	-3.434991	1.063259	-0.721341
H	-1.978571	0.912489	-1.738746
C	0.702443	1.501203	-2.457226
C	2.524670	2.929382	-0.610169
C	-1.405610	3.448201	-0.085837
C	-2.109362	1.600870	2.062884
H	2.449818	-3.958411	1.148493
C	3.966950	-5.034805	0.066560
H	4.579541	-1.726610	-1.871342
C	5.147891	-3.784940	-1.636912
H	1.336950	-1.127875	2.841623
C	2.906210	-0.380700	4.135806
H	5.085388	-0.244673	0.922547
C	5.003602	0.139511	3.038263
C	-4.668695	-2.445092	-3.251372
H	-4.860549	-1.384241	-1.387984
H	-0.861151	-2.522336	-2.494586

C	-2.422507	-3.100897	-3.876169
H	-4.731802	0.139588	0.638938
C	-5.297670	-1.070443	2.313206
C	-3.799993	-2.881215	2.886820
H	-2.031642	-3.059979	1.667074
C	0.229181	2.727027	-2.947373
C	0.323714	0.304291	-3.088026
C	2.756610	3.330464	0.714626
C	3.085575	3.661242	-1.668821
C	-0.502017	4.345043	0.507435
C	-2.280023	3.904760	-1.082794
C	-1.720543	0.578226	2.941304
C	-3.134714	2.487333	2.424133
C	4.935469	-4.977687	-0.941865
H	3.795188	-5.961681	0.607375
H	5.899171	-3.735750	-2.421030
H	2.301137	-0.428607	5.037776
C	4.223205	0.085160	4.198659
H	6.030307	0.493313	3.086990
H	-5.737086	-2.433444	-3.451569
C	-3.793616	-3.071837	-4.145675
H	-1.742239	-3.601944	-4.560603
C	-4.970087	-2.156193	3.129884
H	-6.201520	-0.497324	2.502679
H	-3.538040	-3.724817	3.520323
H	0.491248	3.654186	-2.448778
C	-0.603358	2.753372	-4.068928
H	0.637572	-0.650846	-2.672414
C	-0.511395	0.337093	-4.204798
C	3.529713	4.462887	0.976881
H	2.333576	2.753740	1.533261
H	2.921761	3.348616	-2.696259
C	3.849310	4.799077	-1.401545

H	0.179394	3.998651	1.278563
C	-0.463364	5.676807	0.096789
C	-2.241391	5.240725	-1.489517
H	-2.978447	3.221176	-1.555363
H	-0.933539	-0.110753	2.648399
C	-2.367692	0.437845	4.168505
C	-3.773197	2.344863	3.657126
H	-3.425757	3.289608	1.750534
H	5.519900	-5.860977	-1.185745
H	4.644036	0.400209	5.150190
H	-4.182509	-3.546195	-5.043118
H	-5.621822	-2.432277	3.954833
H	-0.966848	3.706566	-4.443259
C	-0.974208	1.561881	-4.698080
H	-0.815062	-0.592982	-4.675648
H	3.708859	4.767758	2.004719
C	4.069932	5.201921	-0.080110
H	4.275194	5.368183	-2.223796
C	-1.330916	6.125773	-0.905536
H	0.246213	6.361133	0.554022
H	-2.920511	5.588091	-2.263843
H	-2.076594	-0.363844	4.841625
C	-3.392865	1.318095	4.526873
H	-4.564234	3.034921	3.938878
H	-1.625558	1.585490	-5.567924
H	4.666557	6.087177	0.124406
H	-1.298777	7.163344	-1.227587
H	-3.894517	1.205749	5.484618
H	0.872370	1.053548	1.572975

4b

Atomic center	X	Y	Z
Ir	-1.039938	1.017908	-0.179121
P	-2.543295	-0.728528	-0.347908

P	0.714589	2.488009	-0.011299
C	0.526554	-0.438256	-0.383928
C	-2.374344	2.309909	-0.069301
C	-1.591907	-2.245923	-0.882167
C	-3.849537	-0.564644	-1.607306
C	-3.377194	-1.193705	1.206550
C	0.501288	4.198339	-0.591524
C	1.472673	2.552469	1.645185
C	2.064548	1.808326	-1.101584
P	0.071507	-2.066059	-0.127868
P	2.130980	0.002368	-0.783589
O	-3.204260	3.123399	-0.011660
H	-2.074655	-3.192198	-0.623117
H	-1.483340	-2.172438	-1.969235
C	-5.078358	-1.234707	-1.515180
C	-3.583510	0.262413	-2.710132
C	-3.622956	-0.170005	2.135477
C	-3.781032	-2.503000	1.507242
C	1.119668	5.299065	0.018887
C	-0.327224	4.392433	-1.708745
C	2.819034	2.890214	1.850798
C	0.673807	2.203404	2.744640
H	3.041754	2.278082	-0.953678
H	1.740639	1.966953	-2.134983
C	1.187200	-3.321370	-0.808625
C	-0.214648	-2.523709	1.615417
C	2.764249	-0.769519	-2.308823
C	3.416606	-0.189275	0.493679
H	-5.298651	-1.854388	-0.650241
C	-6.029661	-1.084510	-2.526790
H	-2.639940	0.803704	-2.749586
C	-4.535623	0.403997	-3.721017
H	-3.288945	0.839779	1.917383

C	-4.267970	-0.451297	3.340118
H	-3.603719	-3.313126	0.806357
C	-4.412603	-2.784995	2.720113
C	0.915853	6.583136	-0.493138
H	1.743000	5.158031	0.897131
H	-0.835594	3.538087	-2.151503
C	-0.519714	5.675259	-2.221326
H	3.453328	3.159210	1.011172
C	3.361044	2.868425	3.136304
C	1.215779	2.189850	4.031093
H	-0.365010	1.929351	2.574267
C	2.250189	-3.800354	-0.026394
C	1.060876	-3.739415	-2.142128
C	-0.403867	-1.507409	2.560304
C	-0.356695	-3.867473	1.994438
C	3.907552	-1.576037	-2.353581
C	2.008658	-0.566267	-3.476818
C	3.049389	-0.666941	1.756392
C	4.740322	0.221177	0.262564
C	-5.758178	-0.269601	-3.630540
H	-6.985056	-1.597158	-2.449461
H	-4.330836	1.049786	-4.571237
H	-4.457322	0.350369	4.049460
C	-4.659490	-1.759849	3.637283
H	-4.711909	-3.805024	2.946788
H	1.388313	7.435994	-0.012563
C	0.102163	6.771708	-1.614025
H	-1.166072	5.822360	-3.082704
C	2.560492	2.517355	4.227681
H	4.407810	3.119496	3.284843
H	0.590637	1.920469	4.878820
H	2.353881	-3.478905	1.005641
C	3.171514	-4.695020	-0.573215

H	0.253100	-3.361950	-2.762202
C	1.981527	-4.636757	-2.682194
C	-0.734109	-1.832835	3.876599
H	-0.307573	-0.469641	2.251145
H	-0.209499	-4.659930	1.264711
C	-0.680404	-4.188649	3.313147
H	4.481431	-1.760575	-1.451793
C	4.299610	-2.163201	-3.559736
C	2.409288	-1.145402	-4.679456
H	1.099465	0.030582	-3.435644
H	2.018462	-0.947194	1.942289
C	3.996612	-0.747815	2.779084
C	5.685039	0.140265	1.285812
H	5.033617	0.601081	-0.713111
H	-6.503219	-0.150722	-4.413096
H	-5.153209	-1.981183	4.580078
H	-0.057026	7.772541	-2.007029
H	2.985138	2.498533	5.228204
H	3.991130	-5.064916	0.037294
C	3.035577	-5.116603	-1.898615
H	1.878633	-4.957696	-3.714951
H	-0.892658	-1.041021	4.603811
C	-0.872345	-3.170894	4.254103
H	-0.785426	-5.230023	3.606432
C	3.558820	-1.943715	-4.722535
H	5.182956	-2.795731	-3.586621
H	1.827079	-0.977115	-5.581884
H	3.701022	-1.111998	3.759454
C	5.313950	-0.346695	2.544747
H	6.708666	0.457246	1.103311
H	3.750396	-5.817490	-2.321871
H	-1.131190	-3.422952	5.279321
H	3.870596	-2.396808	-5.660103

H	6.051321	-0.405807	3.341252

1a

Atomic center	X	Y	Z
C	2.462746	-0.033536	2.284013
C	1.249540	0.682345	2.881989
N	-0.001062	0.066510	2.340398
Ir	0.000261	-0.112881	0.143720
C	-1.250788	0.686289	2.879620
C	-2.464794	-0.027949	2.281527
C	0.002021	-0.258419	-1.709140
Cl	-0.000302	-2.559336	0.693573
H	0.000248	1.466817	0.065465
O	0.003378	-0.337215	-2.857789
H	-0.002644	-0.924430	2.611567
P	2.338588	0.023125	0.429078
C	3.415152	-1.269007	-0.233700
C	4.182908	-1.009819	-1.382663
C	4.957468	-2.024622	-1.945802
C	4.972040	-3.298217	-1.369346
C	4.204441	-3.559724	-0.230286
C	3.420945	-2.553933	0.335841
C	3.081552	1.606898	-0.060955
C	2.419692	2.477435	-0.937351
C	3.027611	3.672251	-1.331942
C	4.296167	4.004553	-0.850543
C	4.964924	3.136221	0.020236
C	4.364756	1.939001	0.408757
P	-2.338961	0.025231	0.426633
C	-3.417983	-1.266670	-0.232523
C	-3.423883	-2.550496	0.339503
C	-4.210619	-3.556203	-0.222198
C	-4.981450	-3.295675	-1.359313
C	-4.966726	-2.023241	-1.938314

C	-4.188806	-1.008525	-1.379617
C	-3.078955	1.609527	-0.066176
C	-4.359863	1.947149	0.405801
C	-4.956768	3.145547	0.015855
C	-4.287130	4.009424	-0.858666
C	-3.020956	3.671496	-1.342462
C	-2.416225	2.475581	-0.946341
H	2.465587	-1.088272	2.579681
H	3.396281	0.425792	2.622176
H	1.237080	1.740250	2.600985
H	1.248155	0.606846	3.976755
H	-1.250731	0.612913	3.974528
H	-1.235631	1.743543	2.596314
H	-3.397708	0.433680	2.618194
H	-2.469986	-1.082227	2.578692
H	4.182506	-0.020444	-1.830928
H	5.551152	-1.818281	-2.832243
H	5.578074	-4.086261	-1.808419
H	4.207489	-4.550770	0.215165
H	2.799202	-2.779925	1.194953
H	1.433779	2.219272	-1.308847
H	2.510711	4.340682	-2.015319
H	4.767010	4.935366	-1.155406
H	5.955025	3.388806	0.390036
H	4.902491	1.258089	1.064235
H	-2.799892	-2.775617	1.197233
H	-4.213801	-4.546370	0.225207
H	-5.590193	-4.083594	-1.794844
H	-5.562969	-1.817703	-2.823219
H	-4.188188	-0.020021	-1.829747
H	-4.898304	1.269869	1.064450
H	-5.945003	3.402556	0.387600
H	-4.755421	4.941209	-1.164484

H	-2.503438	4.336482	-2.028725
H	-1.431961	2.213028	-1.319190

3a

Atomic center	X	Y	Z
C	-2.440215	0.102190	2.342155
C	-1.196042	-0.602406	2.893972
N	-0.000365	-0.017664	2.294689
Ir	-0.000618	-0.044764	0.156490
C	1.200155	-0.592440	2.893946
C	2.438570	0.120075	2.339368
C	-0.001618	0.011489	-1.720324
Cl	0.001377	-2.599834	0.304611
H	-0.002937	1.532117	0.227001
O	-0.002162	0.008247	-2.880036
P	-2.304833	0.075364	0.494390
C	-3.064683	1.632944	-0.085341
C	-4.125941	1.665907	-0.999632
C	-4.632769	2.892217	-1.442810
C	-4.088701	4.089224	-0.972731
C	-3.027064	4.060387	-0.060073
C	-2.512882	2.840121	0.375363
C	-3.379881	-1.246267	-0.135202
C	-2.946602	-2.036656	-1.207787
C	-3.788989	-3.017488	-1.736672
C	-5.061937	-3.217355	-1.196249
C	-5.498050	-2.432100	-0.123390
C	-4.660784	-1.447758	0.403779
P	2.303864	0.081158	0.492100
C	3.378031	-1.245633	-0.128325
C	2.947480	-2.034907	-1.202859
C	3.788143	-3.020129	-1.726114
C	5.056846	-3.225783	-1.177916
C	5.490251	-2.441850	-0.103062

C	4.654687	-1.452962	0.418404
C	3.065184	1.634420	-0.097214
C	2.507737	2.845134	0.347032
C	3.025797	4.062021	-0.093282
C	4.097330	4.083812	-0.994470
C	4.647138	2.883196	-1.448382
C	4.136269	1.660376	-1.000296
H	-3.373005	-0.366008	2.672398
H	-2.440805	1.156547	2.639467
H	-1.161367	-0.462084	3.988904
H	-1.275619	-1.688929	2.701802
H	1.165436	-0.450426	3.988655
H	1.287964	-1.678839	2.703815
H	3.375122	-0.337378	2.673832
H	2.429025	1.176255	2.630203
H	-4.554293	0.738020	-1.366920
H	-5.453107	2.908091	-2.156453
H	-4.484384	5.041340	-1.318112
H	-2.595097	4.989538	0.304275
H	-1.669250	2.816330	1.061258
H	-1.944605	-1.906152	-1.599484
H	-3.442465	-3.633807	-2.562297
H	-5.712638	-3.986887	-1.605109
H	-6.487399	-2.585385	0.301000
H	-5.009620	-0.831819	1.229069
H	1.948479	-1.899985	-1.600580
H	3.443468	-3.635451	-2.553245
H	5.706209	-3.998856	-1.582198
H	6.476214	-2.599691	0.327494
H	5.001894	-0.838441	1.245389
H	1.656829	2.826726	1.023988
H	2.589201	4.993915	0.258304
H	4.496174	5.033208	-1.343681

H	5.475189	2.893517	-2.153166
H	4.569199	0.729716	-1.354947

6c

Atomic center	X	Y	Z
Ir	0.034392	-1.372840	-0.464806
P	-2.163729	-1.347011	0.116934
Cl	0.113102	0.022313	3.475447
P	2.260719	-1.218400	-0.002581
B	-0.015050	0.919901	-0.506608
C	0.073508	-3.229179	-0.795431
C	-2.494818	0.204456	1.086220
C	-2.610142	-2.704843	1.254770
C	-3.466455	-1.372442	-1.168271
C	2.860330	-2.566949	1.075252
C	3.471428	-1.123094	-1.368193
C	2.531743	0.289249	1.041373
P	-1.721829	1.574152	0.149565
P	1.615202	1.655409	0.246341
O	0.094055	-4.350143	-1.107490
H	-3.545737	0.364683	1.348489
H	-1.879957	0.121357	1.999915
C	-3.262793	-3.853371	0.780334
C	-2.151916	-2.662765	2.581253
C	-3.071386	-1.220645	-2.503093
C	-4.828808	-1.503894	-0.859513
C	3.961355	-3.372620	0.756820
C	2.112947	-2.823267	2.237424
C	4.763182	-0.599839	-1.216122
C	3.062774	-1.597379	-2.622604
H	3.581251	0.525195	1.246869
H	1.982379	0.074298	1.976762
C	-1.897746	3.060528	1.200729
C	-2.818958	1.926702	-1.273271

C	1.591354	3.046806	1.416989
C	2.736073	2.226294	-1.089667
H	-3.599609	-3.902977	-0.251137
C	-3.472721	-4.941768	1.629886
H	-1.593864	-1.804007	2.950637
C	-2.372095	-3.752629	3.425843
H	-2.009893	-1.124727	-2.724488
C	-4.029382	-1.183118	-3.519353
H	-5.137489	-1.638539	0.174529
C	-5.784533	-1.476766	-1.875348
C	4.316366	-4.431375	1.599217
H	4.534228	-3.183614	-0.146661
H	1.254690	-2.199882	2.481828
C	2.481747	-3.872813	3.078073
H	5.089523	-0.227951	-0.248640
C	5.630850	-0.540549	-2.307084
C	3.936647	-1.552364	-3.711272
H	2.050174	-1.980973	-2.733086
C	-2.353601	4.273123	0.657615
C	-1.551966	2.989809	2.560221
C	-2.297294	2.412112	-2.479586
C	-4.208814	1.798087	-1.133902
C	1.229598	4.314304	0.931065
C	1.919262	2.886140	2.769441
C	2.574167	1.779704	-2.408307
C	3.832399	3.044160	-0.771350
C	-3.032274	-4.892307	2.955853
H	-3.976138	-5.829009	1.252669
H	-2.013723	-3.708702	4.451683
H	-3.717774	-1.054514	-4.553049
C	-5.385019	-1.311696	-3.206658
H	-6.839239	-1.583308	-1.631479
H	5.166862	-5.059991	1.344975

C	3.579548	-4.681238	2.759693
H	1.904314	-4.061124	3.979980
C	5.219443	-1.019391	-3.555501
H	6.625047	-0.117415	-2.185561
H	3.613532	-1.923921	-4.680998
H	-2.625773	4.336204	-0.391916
C	-2.474755	5.401772	1.470588
H	-1.165031	2.064460	2.987729
C	-1.680310	4.123647	3.363142
C	-3.150388	2.745316	-3.534971
H	-1.224704	2.524976	-2.597112
H	-4.632499	1.431562	-0.205017
C	-5.058998	2.120994	-2.190085
H	0.965417	4.441103	-0.116090
C	1.214600	5.413476	1.785967
C	1.905899	3.994588	3.620827
H	2.136644	1.902441	3.169959
H	1.747793	1.125207	-2.659225
C	3.491416	2.150354	-3.393449
C	4.745313	3.416545	-1.759294
H	3.965965	3.398460	0.247320
H	-3.195671	-5.741274	3.615940
H	-6.130916	-1.285789	-3.997805
H	3.857183	-5.505676	3.412776
H	5.896594	-0.971311	-4.405227
H	-2.834428	6.335299	1.043767
C	-2.143612	5.327760	2.825932
H	-1.406939	4.060014	4.413066
H	-2.732221	3.117596	-4.467160
C	-4.531440	2.595160	-3.394782
H	-6.132017	1.994526	-2.074212
C	1.560656	5.255624	3.132578
H	0.924030	6.389033	1.405410

H	2.153870	3.861837	4.670864
H	3.363170	1.784550	-4.408660
C	4.575662	2.970418	-3.073470
H	5.587158	4.055107	-1.502061
H	-2.241350	6.206685	3.459244
H	-5.194788	2.843160	-4.219962
H	1.545736	6.113695	3.800557
H	5.288818	3.257070	-3.842817
H	0.003539	1.259922	-1.665181

6b

Atomic center	X	Y	Z
Ir	0.387021	-1.251939	0.244220
P	2.532371	-0.551963	-0.242585
Cl	-0.102935	0.193110	-3.107148
P	-1.811682	-1.858684	-0.042953
C	-0.301773	0.926915	0.288616
C	0.923749	-3.002847	0.473659
C	2.334539	1.101445	-1.073983
C	3.378544	-1.587413	-1.477062
C	3.717523	-0.347927	1.122424
C	-2.034593	-3.296845	-1.131889
C	-2.858147	-2.141928	1.415551
C	-2.581153	-0.470149	-1.007824
P	1.067287	2.026247	-0.154305
P	-2.010539	1.110766	-0.310141
O	1.255168	-4.096120	0.676473
H	3.255537	1.688967	-1.145022
H	1.919455	0.875509	-2.068541
C	4.747615	-1.883265	-1.395143
C	2.602787	-2.118715	-2.520778
C	3.576454	-1.207818	2.222564
C	4.768817	0.578728	1.099962
C	-2.739478	-4.438782	-0.728157

C	-1.397804	-3.261922	-2.384565
C	-4.257304	-2.053548	1.375397
C	-2.216452	-2.474022	2.617834
H	-3.675261	-0.497703	-1.029829
H	-2.153777	-0.549148	-2.016267
C	0.698927	3.567004	-1.020972
C	1.885733	2.460141	1.412322
C	-2.458492	2.453879	-1.427890
C	-3.051181	1.332836	1.175426
H	5.348431	-1.489403	-0.580925
C	5.337753	-2.704865	-2.358880
H	1.544851	-1.881039	-2.578667
C	3.203302	-2.930359	-3.482505
H	2.749085	-1.912358	2.246021
C	4.481006	-1.145546	3.283087
H	4.895325	1.246830	0.252754
C	5.662517	0.651080	2.169878
C	-2.811691	-5.544358	-1.580782
H	-3.223007	-4.470547	0.243826
H	-0.841449	-2.377383	-2.689851
C	-1.485282	-4.366070	-3.231277
H	-4.765580	-1.808277	0.446524
C	-5.005126	-2.278891	2.531263
C	-2.967902	-2.714817	3.769759
H	-1.129890	-2.525252	2.640700
C	0.464256	4.747837	-0.294277
C	0.643677	3.578417	-2.424433
C	1.747590	1.660308	2.557504
C	2.802689	3.525405	1.421558
C	-2.589085	3.750354	-0.902422
C	-2.747903	2.208966	-2.778609
C	-2.655225	0.860057	2.436610
C	-4.344366	1.859938	1.015403

C	4.568248	-3.226906	-3.402318
H	6.396905	-2.939288	-2.290102
H	2.602527	-3.334524	-4.293164
H	4.369998	-1.819849	4.128419
C	5.522652	-0.213128	3.259987
H	6.470175	1.378179	2.149924
H	-3.354718	-6.431709	-1.265931
C	-2.188060	-5.508667	-2.830398
H	-0.999861	-4.335859	-4.203450
C	-4.361322	-2.611255	3.728384
H	-6.088573	-2.199526	2.498476
H	-2.467366	-2.978406	4.698041
H	0.496086	4.740811	0.790897
C	0.209159	5.939290	-0.970620
H	0.772642	2.657101	-2.986493
C	0.374050	4.775708	-3.088835
C	2.488090	1.948303	3.704507
H	1.112069	0.779916	2.546800
H	2.938450	4.138181	0.535415
C	3.537422	3.809457	2.571813
H	-2.382675	3.940940	0.146433
C	-3.004420	4.794250	-1.725140
C	-3.171296	3.260744	-3.592888
H	-2.608848	1.221343	-3.200969
H	-1.690460	0.385833	2.579390
C	-3.527021	0.940214	3.522882
C	-5.213209	1.935407	2.104507
H	-4.670550	2.221674	0.044989
H	5.030635	-3.867627	-4.149003
H	6.223553	-0.158862	4.089070
H	-2.246703	-6.370253	-3.490606
H	-4.946902	-2.790665	4.626489
H	0.041212	6.853031	-0.406706

C	0.168739	5.954961	-2.368021
H	0.326287	4.782187	-4.174157
H	2.383605	1.315004	4.580563
C	3.377204	3.024198	3.717066
H	4.237138	4.640840	2.570821
C	-3.300734	4.549311	-3.069905
H	-3.098596	5.796165	-1.316514
H	-3.394165	3.068417	-4.638665
H	-3.210085	0.562012	4.490220
C	-4.804244	1.480753	3.361253
H	-6.207582	2.352457	1.969569
H	-0.028987	6.885443	-2.894040
H	3.954360	3.242581	4.611561
H	-3.631127	5.364470	-3.708682
H	-5.481426	1.540950	4.209152
H	-0.423050	1.173587	1.348210

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