Supporting Information

Rhodium and Iridium Complexes with a New Scorpionate Phosphane Ligand

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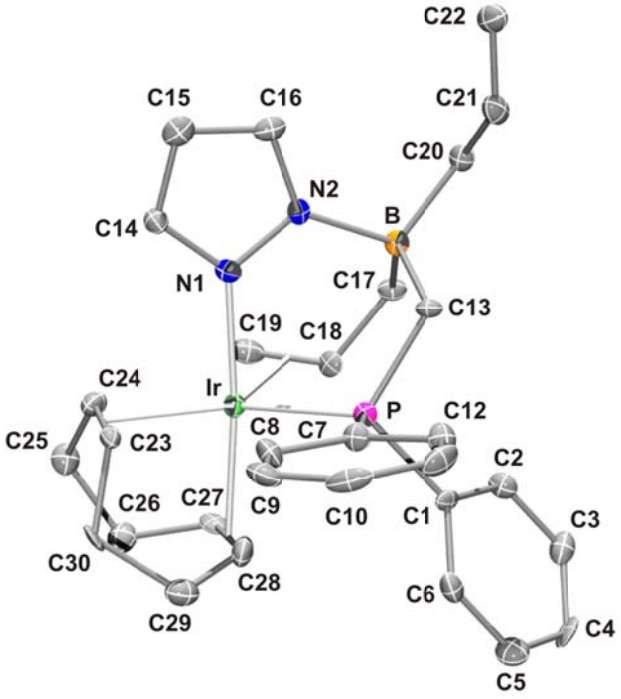

Figure S1. Molecular structure (ORTEP at 50% level) of [(κ^3-A_2BPN)Ir(cod)] (**3**) showing the labeling scheme used (hydrogen atoms have been omitted for clarity).

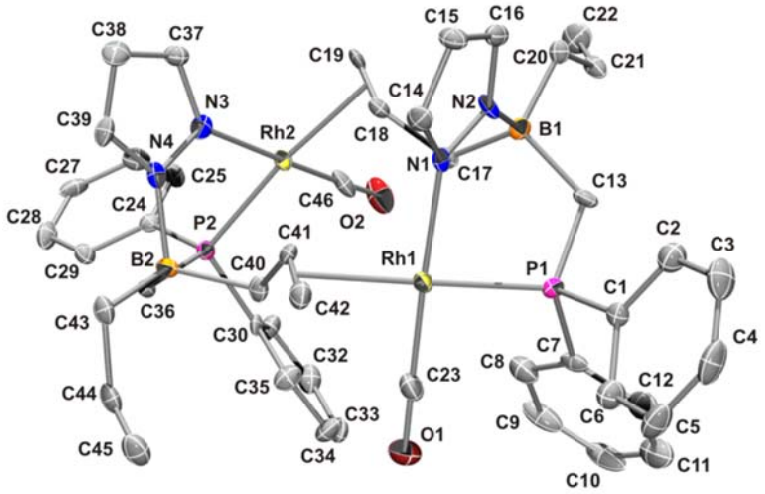

Figure S2. Molecular structure (ORTEP at 50% level) of [{(A_2BPN)Rh(CO)}$_2$] (**8**) showing the labeling scheme used (hydrogen atoms have been omitted for clarity).

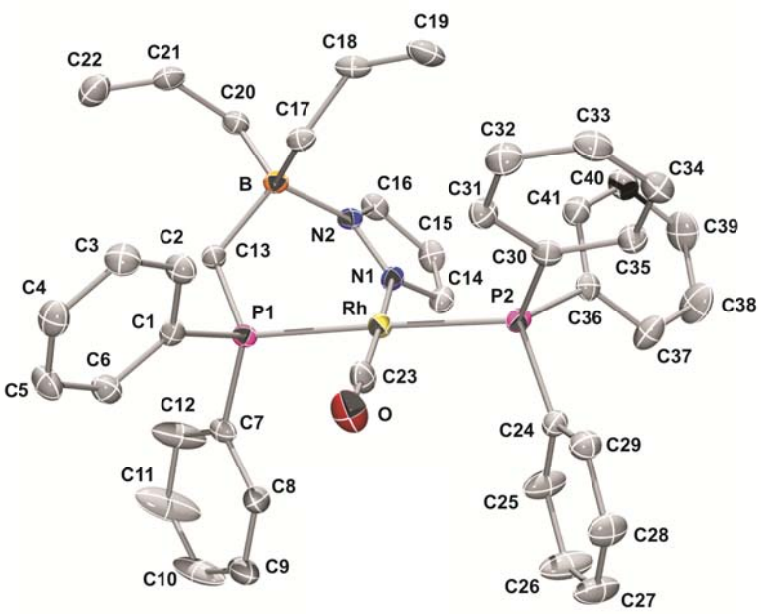

Figure S3. Molecular structure (ORTEP at 50% level) of [(κ^2-A_2BPN)Rh(CO)PPh_3] (**11**) showing the labeling scheme used (hydrogen atoms have been omitted for clarity).

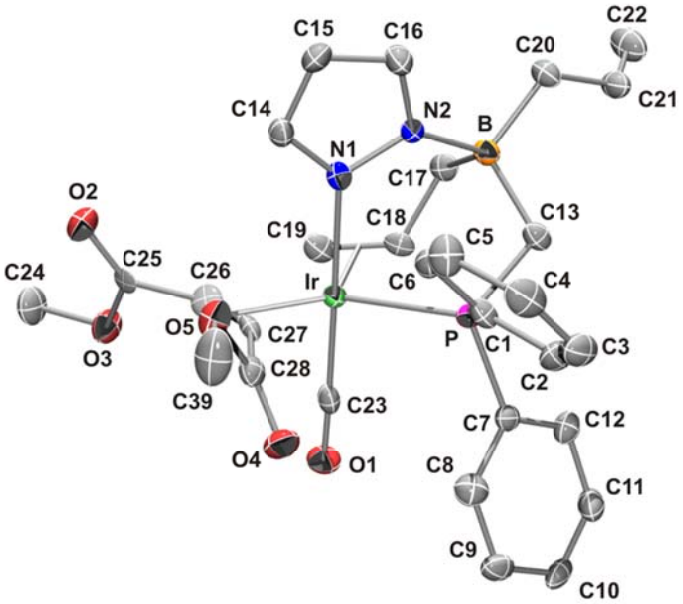

Figure S4. Molecular structure (ORTEP at 50% level) of [(κ^3-A_2BPN)Ir(CO)($MeO_2CC{\equiv}CCO_2Me$)] (**18**) showing the labeling scheme used (hydrogen atoms have been omitted for clarity).

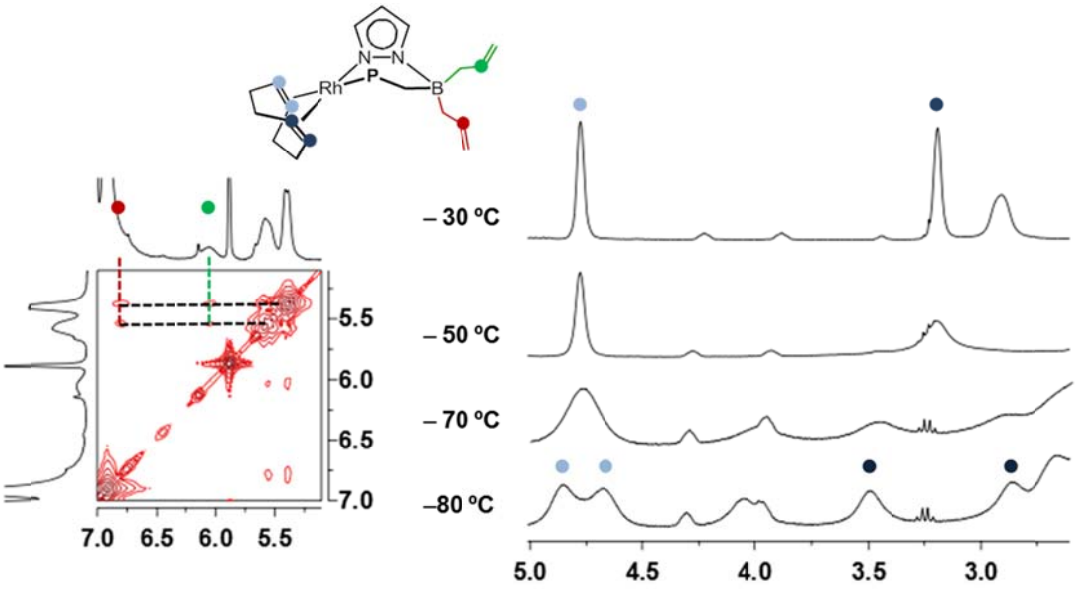

Figure S5. Selected region of the ^{1}H,^{1}H-cosy spectrum of [(κ^2-A$_2$BPN)Rh(cod)] (**2**) in d$_8$-toluene at –80 ºC showing the two inequivalent HC= protons from the two free allyl arms of the ligand (left) and VT ^{1}H NMR of [(κ^2-A$_2$BPN)Rh(cod)] (**2**) in region of the olefinic-cod protons (right).

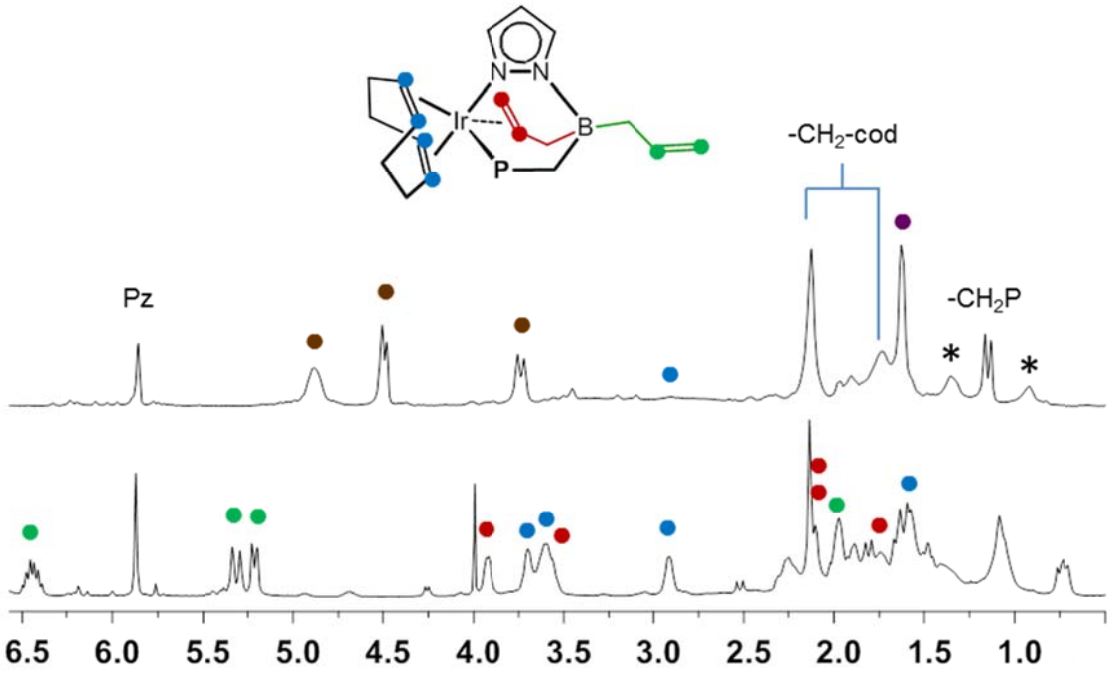

Figure S6. ^{1}H NMR spectra of [(κ^3-A$_2$BPN)Ir(cod)] (**3**) in d$_8$-toluene showing the frozen spectra (–80 ºC, down) and the fast exchange between the two allyl arms at 100 ºC (up). The asterisk denotes hexane.

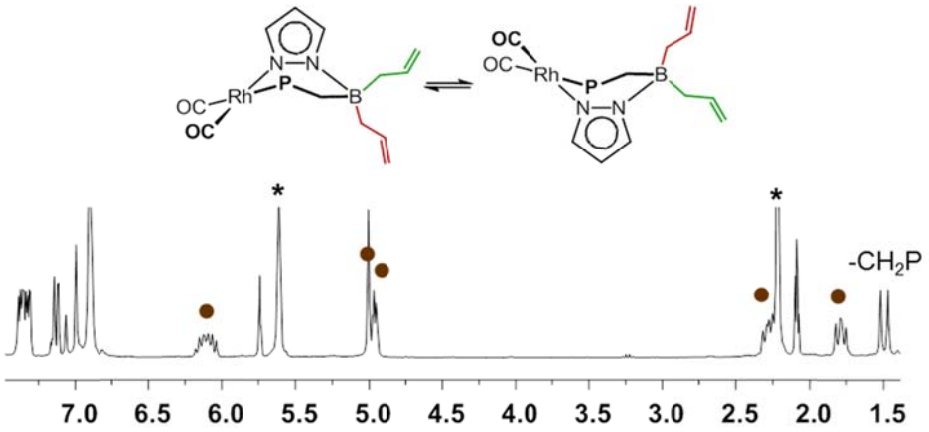

Figure S7. ^{1}H NMR spectra of [(κ^2-A_2BPN)Rh(CO)$_2$] (**6**) in C_6D_6 at 25 ºC showing the fast inversion of the metallacycle, which makes equivalent the two free allyl arms. The asterisk denotes free cod.

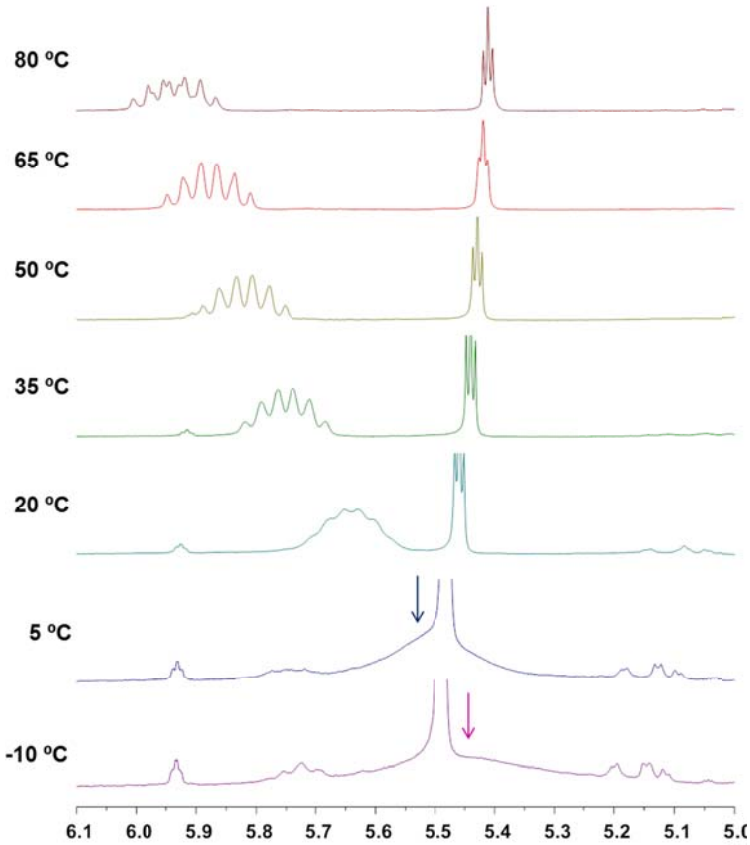

Figure S8. Selected VT ^{1}H NMR spectra of complex [(A_2BPN)Ir(CO)PPh$_3$] (**13**) in the region corresponding to the allyl HC= proton.

Table S1. Estimated Keq values for the equilibrium:

[(κ^3-A_2BPN)Ir(CO)PPh_3] (**13a**) ⇌ [(κ^2-A_2BPN)Ir(CO)PPh_3] (**13b**) obtained from the chemical shifts of the 'olefinic HC=' proton of the coordinated allyl arm in the VT ^{1}H NMR spectra of complex **13**. Full optimization of the data gives a chemical shift value of 6.390 ppm for pure **13b**.

				TBPY-5	*SP*-4		
			HC=	**13a**	**13b**	Keq=X_{13b}/X_{13a}	
	T (K)	**1/T**	**δobs**	**X_{13a}**	**X_{13b}**	**Keq**	**Ln(Keq)**
13b pure			**6,390**				
	353	0,0028	5,936	0,309	0,691	2,238	0,806
	338	0,0030	5,873	0,352	0,648	1,843	0,612
	323	0,0031	5,820	0,388	0,612	1,579	0,457
	308	0,0032	5,751	0,435	0,565	1,300	0,263
	298	0,0034	5,704	0,467	0,533	1,143	0,134
	293	0,0034	5,656	0,499	0,501	1,003	0,003
	278	0,0036	5,525	0,588	0,412	0,699	-0,358
	263	0,0038	5,433	0,651	0,349	0,536	-0,624
	193	0,0052	5,043	0,916	0,084	0,091	-2,393
13a pure			**4,920**				

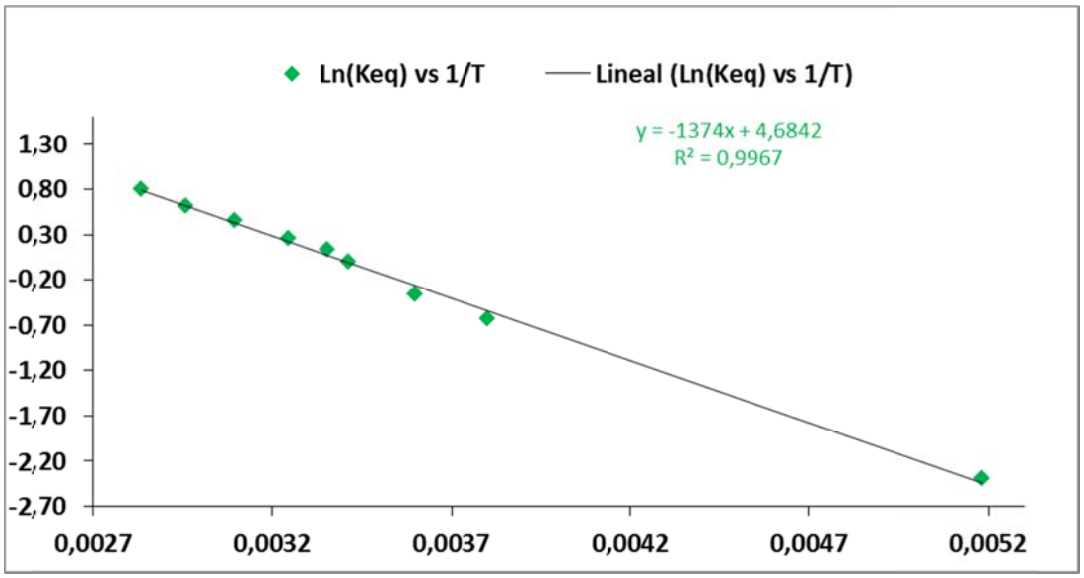

Figure S9. Van't Hoff plot for the equilibrium **13a** ⇌ **13b** and estimated thermodynamic parameters: $\Delta H° = +2.7 \pm 0.1$ kcal mol^{-1}, $\Delta S° = +9.3 \pm 0.5$ cal mol^{-1} K^{-1}, $\Delta G°_{298.15} = -0.045$ kcal mol^{-1}.

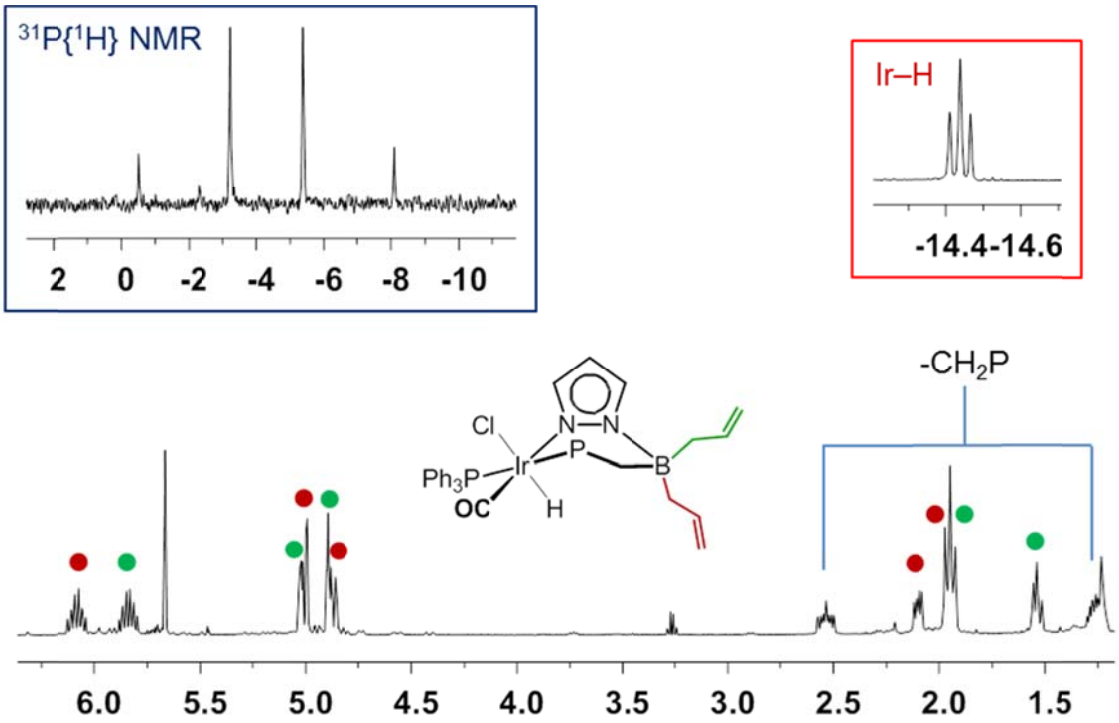

Figure S10. ^{1}H NMR in C_6D_6 of complex [(κ^2-A_2BPN)Ir(CO)(Cl)(H)PPh_3] (**15**). The hydride ligand is shown in the red inset. The $^{31}P\{^{1}H\}$ NMR spectra is shown in the blue inset.

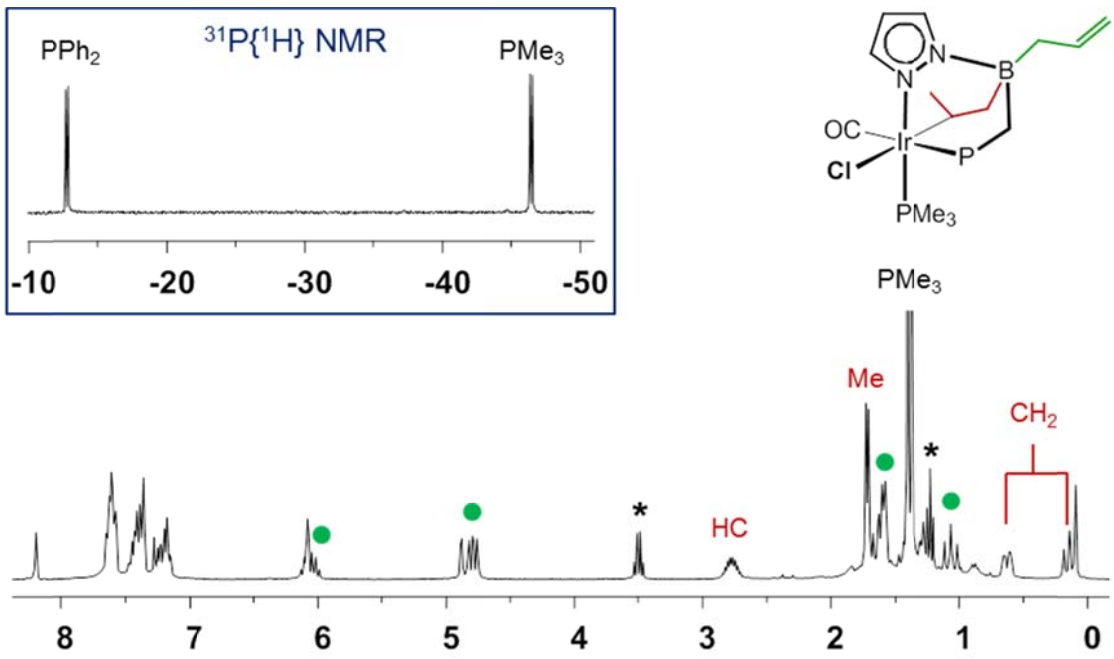

Figure S11. ^{1}H NMR of complex [(κ^3-AB(CH_2CHCH_3)PN)Ir(CO)(Cl)PMe_3] (**16**) in C_6D_6. The $^{31}P\{^{1}H\}$ NMR spectra is shown in the blue inset. The asterisk denotes diethyl ether.

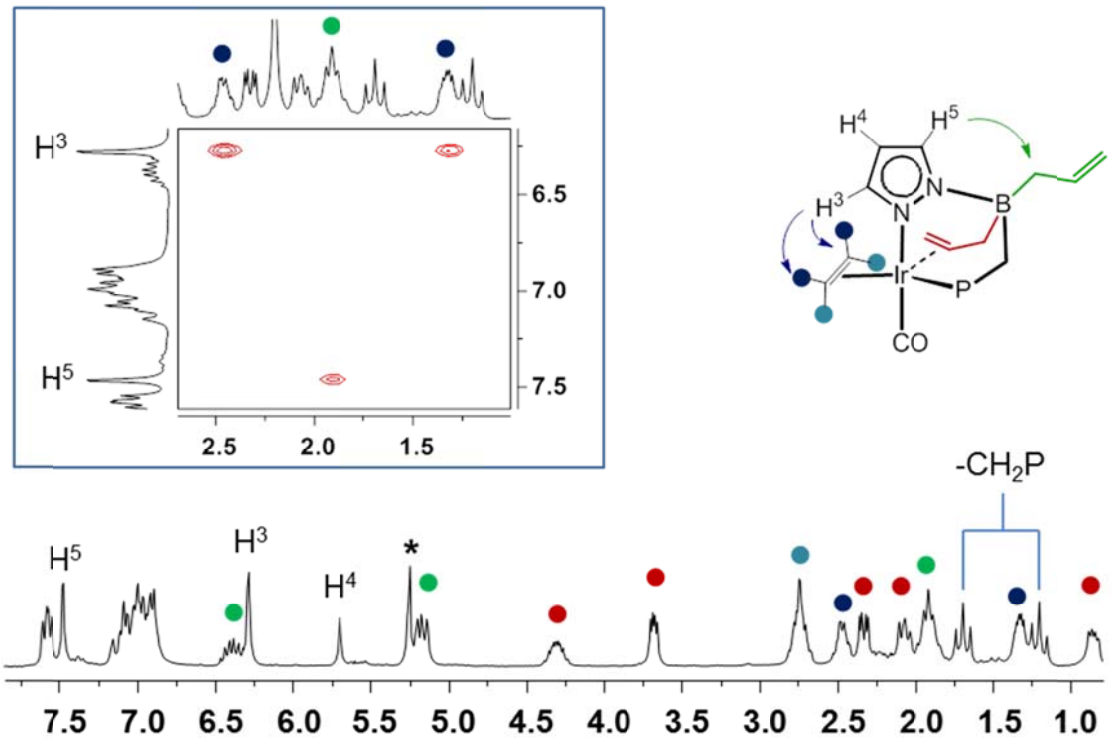

Figure S12. ^{1}H NMR of complex [(κ^3-A_2BPN)Ir(CO)($H_2C{=}CH_2$)] (**17**) in C_6D_6. The blue inset contains a selected region of the ^{1}H,^{1}H-noesy spectrum showing the nOe peaks indicated in the Figure. The asterisk denotes dichloromethane.

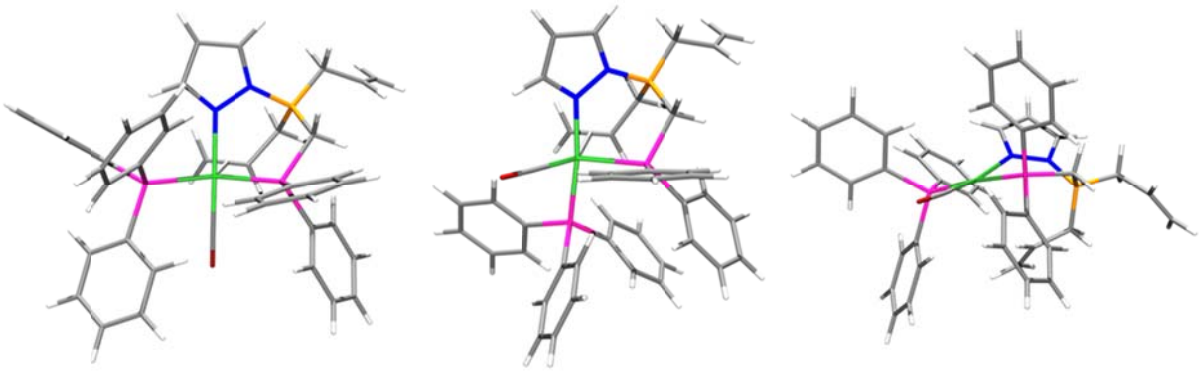

Figure S13. Optimized geometries of [(A_2BPN)Ir(CO)PPh_3] (**13**) in the *TBPY*-5-34_COax (left), *TBPY*-5-31_COeq (middle) and *SP*-4 (right). Relative enthalpies/free energies values were found to be 0/0, 3.6/4.8, and 3.3/–0.2 kcal mol^{-1}, respectively. Code color: Ir (green), N (blue), P (pink), B (orange) and O (red).

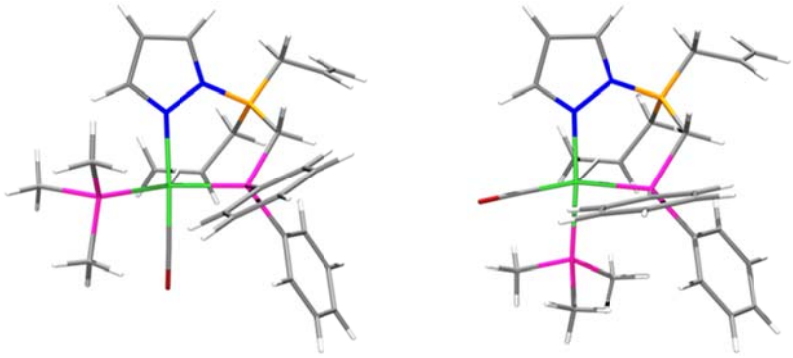

Figure S14. Optimized geometries of [(κ^3-A_2BPN)Ir(CO)PMe_3] (**14**) in the *TBPY*-5-34_COax (left), and *TBPY*-5-31_COeq (right). Relative enthalpies/free energies values were found to be 2.8/2.5 and 0/0 kcal mol^{-1}, respectively. Code color: Ir (green), N (blue), P (pink), B (orange) and O (red).

Table S2. Coordinates (xyz-coordinates) for the optimized geometry of complex *TBPY*-5-34-[(A_2BPN)Ir(CO)PPh_3] (**13**).

Ir	-0.14975	-0.55066	-0.72332
P	-1.92761	0.70905	0.33757
P	2.15309	-0.04067	-0.10588
O	-0.00371	1.28247	-3.09697
N	-0.31321	-2.0582	0.79739
N	-1.50539	-2.53804	1.2519
C	-2.86864	1.66528	-0.93947
C	-3.88149	1.05533	-1.69651
H	-4.159	0.02401	-1.50796
C	-4.54856	1.76656	-2.6959
H	-5.33356	1.27823	-3.26657
C	-4.21339	3.09517	-2.95878
H	-4.73349	3.64725	-3.73632
C	-3.20625	3.71066	-2.2134
H	-2.93995	4.74617	-2.4064
C	-2.53978	3.00252	-1.21345
H	-1.76877	3.50065	-0.63333
C	-1.75515	2.00148	1.65746
C	-0.52236	2.6101	1.91557
H	0.35537	2.28422	1.37018
C	-0.40535	3.61151	2.8842
H	0.56295	4.06566	3.07394
C	-1.52538	4.013	3.61042
H	-1.4377	4.78824	4.36646
C	-2.76307	3.41092	3.36436
H	-3.64007	3.71917	3.92682
C	-2.87786	2.41545	2.39571
H	-3.84626	1.96078	2.21022
C	-3.12934	-0.51404	1.01702
H	-3.04833	-0.44107	2.10879
H	-4.13893	-0.17523	0.75936
C	0.6612	-2.76689	1.40708
H	1.69904	-2.58271	1.18381
C	0.10433	-3.69708	2.28045
H	0.62145	-4.40341	2.91163
C	-1.2684	-3.51684	2.14445
H	-2.08876	-4.03308	2.61661
C	-2.73985	-2.43663	-1.00198
H	-2.58758	-3.52373	-1.07859
H	-3.70551	-2.24939	-1.48944
C	-1.65494	-1.74114	-1.81374
C	-0.3348	-2.26523	-2.05755
C	-4.08576	-3.0239	1.27105
H	-3.88798	-4.08689	1.0711
H	-4.0738	-2.90021	2.36698
C	-5.46382	-2.69235	0.78176
H	-5.86699	-1.73021	1.1057
C	-6.22579	-3.44414	-0.01914

H	-5.89194	-4.41694	-0.37408
H	-7.20864	-3.11751	-0.34807
C	2.90649	1.30297	-1.14114
C	2.30496	2.57328	-1.13746
H	1.40748	2.74622	-0.55181
C	2.84031	3.61854	-1.88697
H	2.35979	4.59246	-1.8702
C	3.98284	3.41205	-2.66365
H	4.39665	4.2249	-3.25331
C	4.58506	2.15501	-2.6802
H	5.47294	1.98279	-3.28195
C	4.05481	1.10763	-1.9217
H	4.5415	0.13926	-1.94143
C	3.34741	-1.44532	-0.35695
C	3.18385	-2.24894	-1.49826
H	2.35953	-2.04758	-2.17403
C	4.0565	-3.30565	-1.75584
H	3.91725	-3.91316	-2.64549
C	5.09471	-3.5914	-0.86594
H	5.76687	-4.42239	-1.05971
C	5.2584	-2.80876	0.27698
H	6.05927	-3.02718	0.9778
C	4.39565	-1.73883	0.52887
H	4.54087	-1.13909	1.42036
C	2.5788	0.54539	1.60624
C	3.71663	1.33406	1.85129
H	4.35769	1.63235	1.028
C	4.03047	1.74564	3.1473
H	4.91184	2.35746	3.31821
C	3.21464	1.37462	4.21842
H	3.45927	1.69585	5.22693
C	2.07939	0.59772	3.98547
H	1.43175	0.31489	4.81007
C	1.75976	0.19121	2.68866
H	0.86344	-0.39277	2.51586
C	-0.04097	0.60374	-2.15718
B	-2.89553	-2.09618	0.59749
H	-2.04494	-1.11303	-2.61438
H	-0.03984	-3.19697	-1.57925
H	0.11127	-2.11437	-3.03856

Table S3. Coordinates (xyz-coordinates) for the optimized geometry of complex *TBPY*-5-31-[(A_2BPN)Ir(CO)PPh_3] (**13**).

Ir	0.15624	-1.03196	-0.47103
P	1.60033	0.89901	-0.09194
P	-1.99306	-0.23053	0.05531
O	-0.72384	-1.28492	-3.38497
N	1.9258	-2.08175	-1.01319
N	3.08025	-2.11327	-0.29615
C	1.0453	2.24987	1.04826
C	1.16892	2.08013	2.43775
H	1.57327	1.15656	2.83958
C	0.79319	3.09529	3.31744
H	0.90981	2.94643	4.38707
C	0.2773	4.29667	2.8281
H	-0.00216	5.092	3.51338
C	0.12384	4.46779	1.45167
H	-0.27774	5.39766	1.05796
C	0.50031	3.45278	0.56973
H	0.39316	3.61417	-0.4975
C	2.18071	1.86278	-1.5711
C	1.83841	1.47721	-2.87268
H	1.18178	0.62859	-3.02469
C	2.34031	2.16825	-3.98037
H	2.06249	1.85065	-4.98138
C	3.19501	3.25392	-3.79965
H	3.58619	3.79151	-4.65882
C	3.55196	3.6446	-2.50543
H	4.22233	4.48639	-2.35546
C	3.05307	2.95423	-1.40284
H	3.34127	3.26727	-0.40382
C	3.18814	0.29948	0.66137
H	3.97219	0.52232	-0.07176
H	3.39405	0.92814	1.53384
C	2.0832	-2.89548	-2.0786
H	1.28277	-3.03093	-2.78878
C	3.35638	-3.45854	-2.06017
H	3.78512	-4.14688	-2.77228
C	3.94846	-2.93566	-0.91464
H	4.93017	-3.09999	-0.50026
C	2.05824	-1.7939	2.06718
H	2.244	-2.85115	2.31011
H	2.18115	-1.25823	3.0184
C	0.60523	-1.65281	1.62616
C	-0.11461	-2.67692	0.92657
C	4.73743	-1.66248	1.68558
H	4.8065	-2.7442	1.87199
H	5.51572	-1.41851	0.94334
C	5.06381	-0.93392	2.95447
H	5.22318	0.14253	2.85792
C	5.15724	-1.46628	4.17715

H	5.01768	-2.532	4.34625
H	5.37637	-0.85969	5.05187
C	-0.41337	-1.17859	-2.26386
B	3.25082	-1.29616	1.06526
H	0.00582	-1.03197	2.28706
H	0.42456	-3.56592	0.60411
H	-1.15855	-2.87112	1.1602
C	-3.30775	-1.54878	-0.04399
C	-4.50428	-1.4462	0.68758
C	-3.14242	-2.64726	-0.90085
C	-5.50789	-2.40683	0.5542
H	-4.65371	-0.62268	1.37714
C	-4.14808	-3.60564	-1.03476
H	-2.2146	-2.76335	-1.44767
C	-5.33415	-3.48862	-0.30975
H	-6.42254	-2.30965	1.13215
H	-3.99661	-4.44889	-1.70234
H	-6.11382	-4.23815	-0.41069
C	-2.65544	1.07831	-1.0824
C	-1.77773	1.82876	-1.87573
C	-4.03165	1.35274	-1.15956
C	-2.25743	2.83157	-2.7213
H	-0.71649	1.61948	-1.84407
C	-4.50988	2.35451	-2.00269
H	-4.73815	0.77869	-0.57128
C	-3.6241	3.09797	-2.78634
H	-1.55749	3.39482	-3.33164
H	-5.57748	2.54853	-2.05234
H	-3.99983	3.87411	-3.44693
C	-2.30885	0.46937	1.73835
C	-2.51397	1.84134	1.93539
C	-2.35074	-0.38812	2.85323
C	-2.76291	2.34385	3.21433
H	-2.48155	2.52362	1.09433
C	-2.59525	0.11782	4.12908
H	-2.21562	-1.45707	2.72639
C	-2.80557	1.48623	4.3126
H	-2.91977	3.40991	3.34652
H	-2.6281	-0.55982	4.97722
H	-3.00252	1.87915	5.30595

Table S4. Coordinates (xyz-coordinates) for the optimized geometry of complex *SP*-4-[(A_2BPN)Ir(CO)PPh_3] (**13**).

Ir	-0.02620200	-0.38700392	-0.16907242
P	-2.37390246	-0.48112736	-0.12808854
P	2.34371470	-0.18762797	0.06945176
O	0.12147508	-3.08676759	1.11917688
N	-0.19507243	1.30875055	-1.43823402
N	-1.06878627	2.36513650	-1.40436518
C	-3.03184219	-1.06804945	1.49434476
C	-3.36578568	-0.15450663	2.50596722
H	-3.27779772	0.91197240	2.33107283
C	-3.81532512	-0.60538187	3.74845638
H	-4.07222451	0.11637436	4.51853131
C	-3.93707981	-1.97266070	3.99820505
H	-4.28918735	-2.32224518	4.96455230
C	-3.60660131	-2.88940752	2.99821409
H	-3.70043410	-3.95586249	3.18217554
C	-3.15637507	-2.44224561	1.75624713
H	-2.90891230	-3.16747814	0.98792911
C	-3.13007039	-1.66037469	-1.32849666
C	-2.32553312	-2.36458841	-2.23364172
H	-1.24854028	-2.22831337	-2.19486990
C	-2.90132043	-3.22654761	-3.17088949
H	-2.26680854	-3.76745036	-3.86734404
C	-4.28537954	-3.39145201	-3.21166739
H	-4.73363595	-4.06135097	-3.94002938
C	-5.09660372	-2.69253891	-2.31255519
H	-6.17525275	-2.81855536	-2.34060301
C	-4.52403192	-1.83253778	-1.37749476
H	-5.16231172	-1.29690868	-0.68041085
C	-3.16693184	1.14245663	-0.45454107
H	-3.52855496	1.06383722	-1.48768756
H	-4.05940072	1.20244537	0.17793997
C	0.54414747	1.43582477	-2.56164236
H	1.30381526	0.70674633	-2.79473981
C	0.17306575	2.57689803	-3.26158210
H	0.58247778	2.95222569	-4.18661764
C	-0.84244998	3.13056042	-2.49003739
H	-1.42023027	4.02445321	-2.65584718
C	-1.76768277	3.03732389	1.12711848
H	-1.50204990	4.10198262	1.05084588
H	-2.67080705	3.02626246	1.76011581
C	-0.66538223	2.34386476	1.86416762
C	0.43811505	2.93318558	2.34523399
C	-3.25723552	3.75288809	-0.95891154
H	-2.69842106	4.69906569	-1.00230350
H	-3.54883466	3.50732714	-1.99304519
C	-4.51002482	3.98584899	-0.16854886
H	-5.25369624	3.18666761	-0.20518702
C	-4.79304004	5.06007290	0.57505112

H	-4.10349249	5.89825703	0.65066087
H	-5.72071552	5.14187300	1.13503346
C	2.91675375	-0.00443013	1.82044209
C	2.12940307	-0.48346297	2.87853681
H	1.16218162	-0.92624292	2.67458061
C	2.57266485	-0.37516015	4.19761152
H	1.94743070	-0.74727322	5.00382253
C	3.80402090	0.21751956	4.47982390
H	4.14438084	0.30684830	5.50745381
C	4.59236394	0.70379041	3.43551846
H	5.54851315	1.17440541	3.64595511
C	4.15244782	0.59630806	2.11563943
H	4.76919949	0.99197710	1.31551428
C	3.21487423	1.20724507	-0.77066982
C	2.82812164	2.52054807	-0.45215871
H	2.03034908	2.69380327	0.26512805
C	3.45755196	3.60376238	-1.06186714
H	3.14993176	4.61385136	-0.80751423
C	4.46996828	3.39386801	-2.00215898
H	4.95543635	4.24078883	-2.47881317
C	4.85276002	2.09333847	-2.32861492
H	5.63878068	1.92153182	-3.05856923
C	4.23009774	1.00248323	-1.71543839
H	4.54153416	-0.00407772	-1.97316053
C	3.22534441	-1.69331238	-0.54377161
C	4.40581596	-2.17776661	0.03910501
H	4.82656561	-1.68342352	0.90810715
C	5.04130036	-3.30461408	-0.48526862
H	5.95031871	-3.67377354	-0.01909254
C	4.51001683	-3.95774594	-1.59862655
H	5.00536371	-4.83594444	-2.00273990
C	3.33449691	-3.48455153	-2.18451714
H	2.90988458	-3.99349228	-3.04505946
C	2.69256052	-2.36403649	-1.65675405
H	1.76177163	-2.01178112	-2.09296775
C	0.06936633	-2.01803820	0.65442969
B	-2.28415557	2.54398725	-0.35875093
H	-0.78010669	1.27258583	2.04231975
H	0.60653869	4.00216719	2.22316327
H	1.19392572	2.37808499	2.89281291

Table S5. Coordinates (xyz-coordinates) for the optimized geometry of complex *TBPY*-5-34-[(A_2BPN)Ir(CO)PMe_3] (**14**).

Ir	0.83724102	-0.51245184	-0.78037946
P	-0.76148582	0.82631812	0.43805248
P	3.14183327	-0.10569241	-0.22725998
O	1.06901581	1.40971607	-3.07599303
N	0.68324261	-2.02679334	0.73218743
N	-0.49978736	-2.44963016	1.25509413
C	-1.73352279	1.90571938	-0.71122549
C	-2.81576817	1.37344469	-1.43148629
H	-3.11795034	0.34275529	-1.28105845
C	-3.51808267	2.16071731	-2.34517956
H	-4.35566995	1.73145695	-2.88784485
C	-3.15043980	3.48984553	-2.55937662
H	-3.69807039	4.10144818	-3.27061101
C	-2.07504878	4.02768934	-1.85109069
H	-1.78226903	5.06243246	-2.00605646
C	-1.37225096	3.24327177	-0.93570753
H	-0.54714363	3.68382551	-0.38516226
C	-0.30822876	2.03204490	1.77266006
C	0.92707580	2.69296768	1.72537779
H	1.61314438	2.46645225	0.91539075
C	1.27911192	3.63346828	2.69591995
H	2.23980064	4.13794986	2.63863385
C	0.39842567	3.91896270	3.74023617
H	0.67113116	4.64325928	4.50237455
C	-0.83580455	3.26852934	3.79982770
H	-1.52816988	3.48849991	4.60764594
C	-1.18914747	2.33742094	2.82208048
H	-2.15689713	1.84945777	2.87763646
C	-1.99337866	-0.32608860	1.17959336
H	-1.82256212	-0.30720644	2.26284790
H	-2.99251933	0.09118935	1.01364487
C	1.65335153	-2.78906656	1.27823684
H	2.68150563	-2.66432382	0.98413512
C	1.10584846	-3.69820558	2.17930880
H	1.62229151	-4.43697348	2.77276862
C	-0.26147039	-3.44602541	2.12772303
H	-1.07765481	-3.92234052	2.64672205
C	-1.87206006	-2.22121154	-0.91229656
H	-1.80809859	-3.31482963	-1.01890102
H	-2.85236055	-1.95518649	-1.32929576
C	-0.79491455	-1.58794109	-1.78782653
C	0.47150452	-2.19489307	-2.11900326
C	-3.09847969	-2.77431067	1.43711103
H	-2.98083458	-3.84356439	1.20916389
H	-3.00874242	-2.67256503	2.53183162
C	-4.48181011	-2.34945643	1.04374250
H	-4.79887549	-1.36661298	1.39969563
C	-5.34291869	-3.04253741	0.29204324

H	-5.09733378	-4.03098066	-0.09057874
H	-6.32226697	-2.64990662	0.03211553
C	3.85185363	1.44721574	-0.94624035
C	4.38304526	-1.32822669	-0.87158190
C	3.64961732	0.06433468	1.54745429
C	0.97586532	0.67859463	-2.17696566
B	-1.89918616	-1.90930885	0.70077557
H	-1.19378816	-0.93130958	-2.56079108
H	0.73167003	-3.15074777	-1.66887043
H	0.87434329	-2.05920301	-3.11992488
H	3.75458502	1.42837685	-2.03448947
H	3.31090223	2.32103601	-0.57534077
H	4.91017521	1.54754428	-0.68616735
H	3.37052095	-0.82692374	2.11212870
H	4.72990348	0.22114932	1.63308332
H	3.12374342	0.91362294	1.98929357
H	4.17110834	-2.33353969	-0.50079021
H	4.30343454	-1.35591908	-1.96174365
H	5.40555507	-1.05271996	-0.59106800

Table S6. Coordinates (xyz-coordinates) for the optimized geometry of complex *TBPY*-5-31-[(A_2BPN)Ir(CO)PMe_3] (**14**).

Ir	-0.00770619	-1.33721733	-0.14153270
P	0.23882929	1.00834382	0.40039703
P	1.96120107	-1.68725497	-1.31558553
O	1.11492127	-3.25251880	1.96055312
N	-1.86982929	-1.28374974	0.88900879
N	-2.83284831	-0.33968758	0.72204825
C	1.29888657	2.02730700	-0.72761739
C	0.80693167	2.40607104	-1.98960713
H	-0.20351977	2.13777611	-2.28088729
C	1.59968157	3.13787169	-2.87542382
H	1.19542599	3.42823192	-3.84118657
C	2.90108489	3.50207188	-2.52166322
H	3.51594042	4.07374299	-3.21073426
C	3.40030247	3.13469411	-1.27155919
H	4.40632713	3.42338250	-0.97961957
C	2.60665276	2.40618123	-0.38201749
H	3.00200739	2.15128596	0.59633865
C	0.90137153	1.47690185	2.06543465
C	1.46116764	0.51773107	2.91737139
H	1.50728815	-0.51699155	2.59589519
C	1.94341445	0.87887829	4.17906321
H	2.36978085	0.12016865	4.82920836
C	1.87023426	2.20500471	4.60275284
H	2.24141959	2.48621252	5.58424278
C	1.31203573	3.17214612	3.76141921
H	1.24925240	4.20688829	4.08656419
C	0.83121732	2.81143583	2.50422573
H	0.39886993	3.57131751	1.85960925
C	-1.42902548	1.80796693	0.30195738
H	-1.68490354	2.10909296	1.32487347
H	-1.32017932	2.73137337	-0.27711240
C	-2.33137639	-2.18834097	1.77648615
H	-1.72724424	-3.03776850	2.05549875
C	-3.60894371	-1.82783324	2.19851066
H	-4.24316946	-2.34432127	2.90260952
C	-3.88372374	-0.65395676	1.50361735
H	-4.76121586	-0.02736941	1.51285351
C	-2.35547341	0.19898878	-1.76801738
H	-3.25587745	-0.36210068	-2.06061374
H	-2.28334853	1.01579286	-2.49949148
C	-1.14227597	-0.71091735	-1.94834097
C	-1.17718363	-2.13881782	-1.79034963
C	-4.05867703	1.73046173	-0.32078026
H	-4.88702446	1.07869707	-0.63459997
H	-4.29422628	2.07136661	0.70116365
C	-4.02741893	2.93366070	-1.21451514
H	-3.38189925	3.75258967	-0.88863580
C	-4.68980608	3.08864846	-2.36534926

H	-5.35633868	2.31795169	-2.74685606
H	-4.59273565	3.98878599	-2.96651687
C	2.14044424	-0.95850049	-2.99830569
C	2.28239457	-3.47752649	-1.63392543
C	3.51965697	-1.17262835	-0.47746989
C	0.67040319	-2.52291128	1.16278161
B	-2.64884697	0.87005256	-0.30269217
H	-0.43888483	-0.35337562	-2.69773535
H	-2.09456156	-2.60671062	-1.43887616
H	-0.61295958	-2.76771645	-2.47673056
H	1.35150944	-1.33451917	-3.65413192
H	2.06559661	0.12949539	-2.94817588
H	3.11132672	-1.23633956	-3.41951145
H	3.55987345	-1.62436457	0.51679841
H	4.39360500	-1.49188921	-1.05390694
H	3.53877528	-0.08659543	-0.37129612
H	2.35734412	-4.00567950	-0.68039929
H	1.44875130	-3.90594493	-2.19450356
H	3.20967087	-3.61664681	-2.19872201