H/D Exchange Under Mild Conditions in Arenes and Unactivated Alkanes with C_6D_6 and D_2O Using Rigid, Electron-rich Iridium PCP Pincer Complexes

Joel D. Smith,[a] George Durrant,[b] Daniel H. Ess[b], Benjamin S. Gelfand[a] and Warren E. Piers[a]*

[a]*Department of Chemistry, University of Calgary, 2500 University Drive NW, Calgary, Alberta, T2N 1N4, Canada*

[b]*Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah, 84602, USA*

Email: wpiers@ucalgary.ca

Supporting Information

Table of Contents

Characterization Data used for Determining Polyhydride Isomers Present in Solution

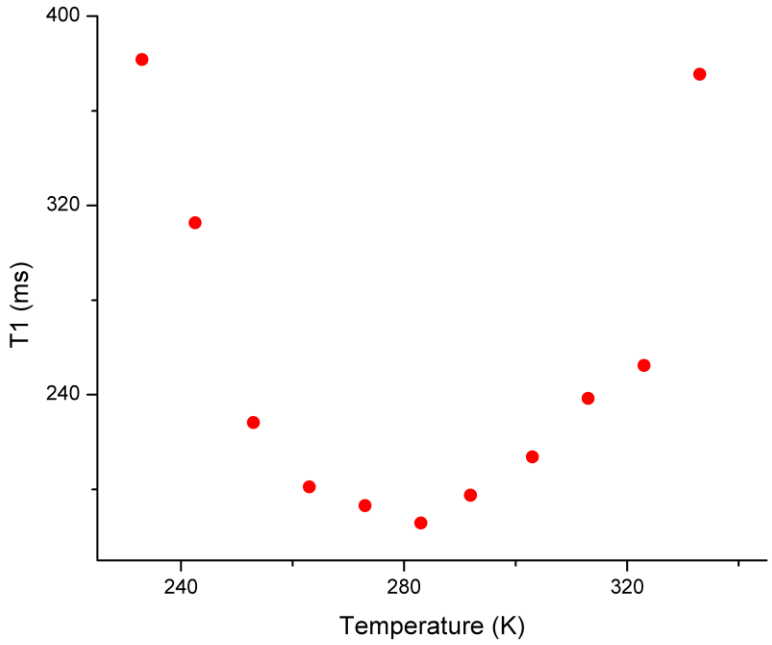


Figure S1. Variable Temperature T_1 data for **Ir-H$_4$**. Measured in methylcyclohexane-d_{14} using ^{1}H NMR at 600 MHz.

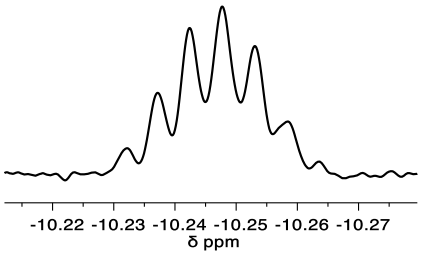
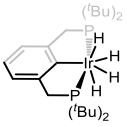
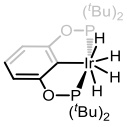
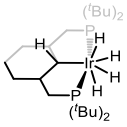
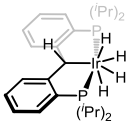
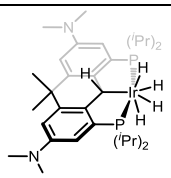


Figure S2. ^{1}H{^{31}P} NMR spectrum (50 °C, methylcyclohexane-d_{14}, 600 MHz) for hydridic region of **Ir-D$_4$** (< 97 %) and **Ir-HD$_3$** (< 3 %).

Table S1. T1 (min) relaxation times, H-D Coupling constants and calculated H-H distances for **Ir-H$_4$** and related complexes.

	Compound				
					
			Ir$^{(Cyc)}$-H$_4$	**Ir$^{(Ph)}$-H$_4$**	**Ir-H$_4$**
	Heinekey		Wendt	Piers	
T_1(min), ms	130 (-53 ºC)[a]	110 (-53 ºC)[a]	154 (-50 ºC)[b]	158 (-30 °C)[c]	155 (10 °C)[bc]
$J_{obs,HD}$, Hz; (Ir-HD_3)	3.5 ± 0.1	4.4 ± 0.1	3.0 ± 0.1	3.0 ± 0.1	3.1 ± 0.1
$^1J_{HD,}$ Hz; (Ir-HD_3)	25 ± 5	22 ± 5	18 ± 5	18 ± 5	19 ± 5 [d]
r(H-H), Å	0.96-1.179	0.9-1.08	1.04-1.28	1.04-1.28	1.02-1.25 [d]

T1 (min) measurements were performed in [a] toluene-d_8 and [b] methylcyclohexane-d_{14}. [c] Values were determined on a 600 MHz spectrometer and adjusted to 500 MHz field. [d] Calculated using methods outlined by Heinekey and Wendt.[1,2]

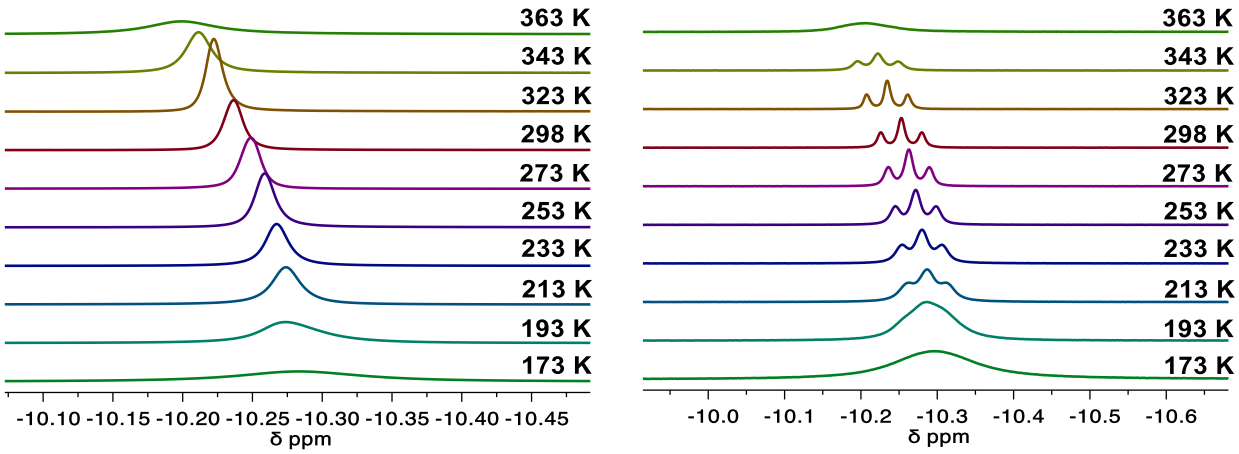


Figure S3. Variable temperature ^{1}H {^{31}P} (left) and ^{1}H NMR (right) spectra (methycyclohexane-d_{14}, 400 MHz) of the hydridic protons of **Ir-H$_4$.**

NMR Data Demonstrating the Formation of Ir-H_3 under Vacuum

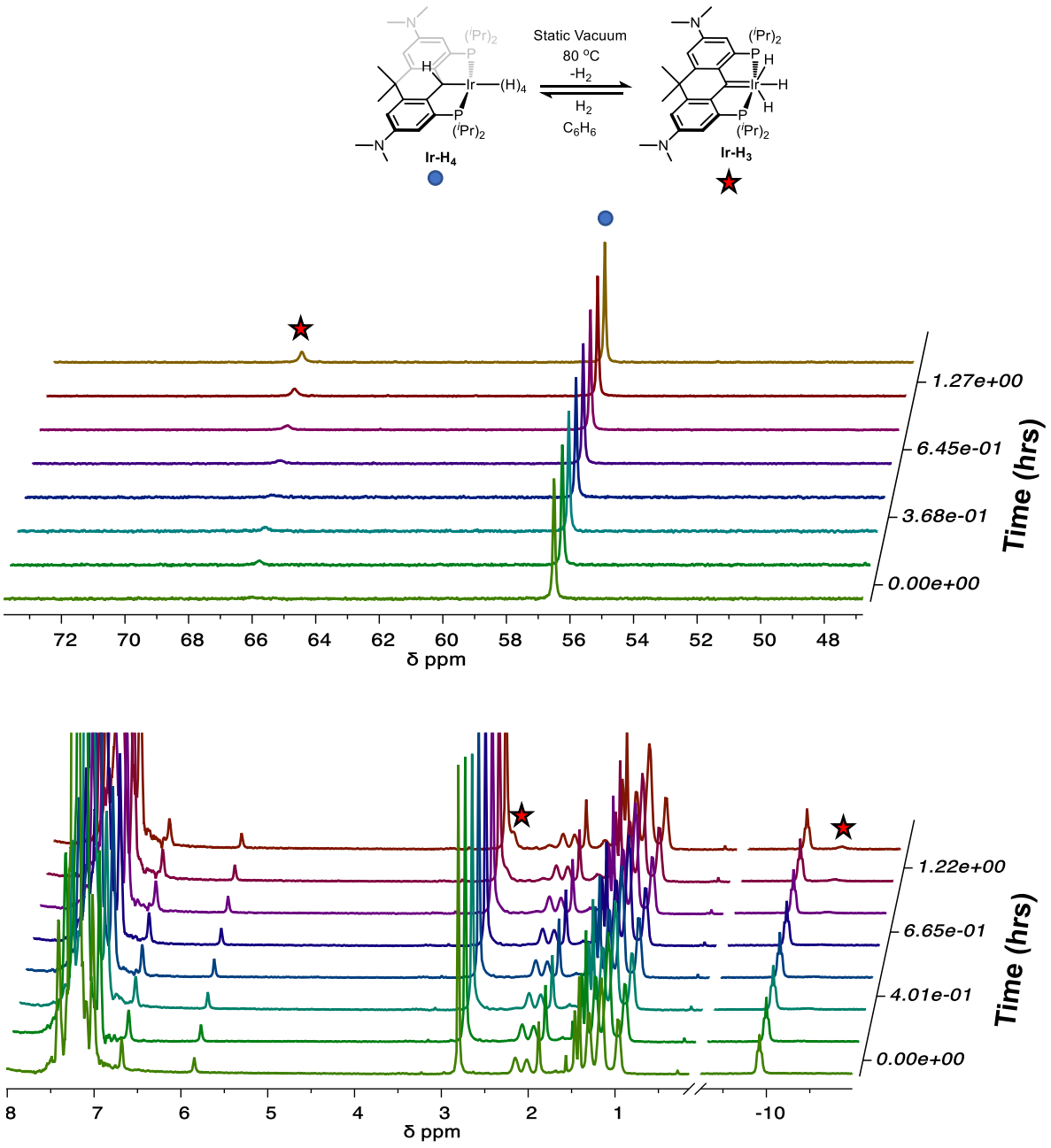


Figure S4. ^{31}P {^{1}H} (162 MHz, top) and ^{1}H NMR (400 MHz, bottom) spectra of **Ir-H_4** heated under static vacuum to 80 °C for 1.6 hours in benzene (spiked with 0.05 mL of cyclohexane-d_{12}).

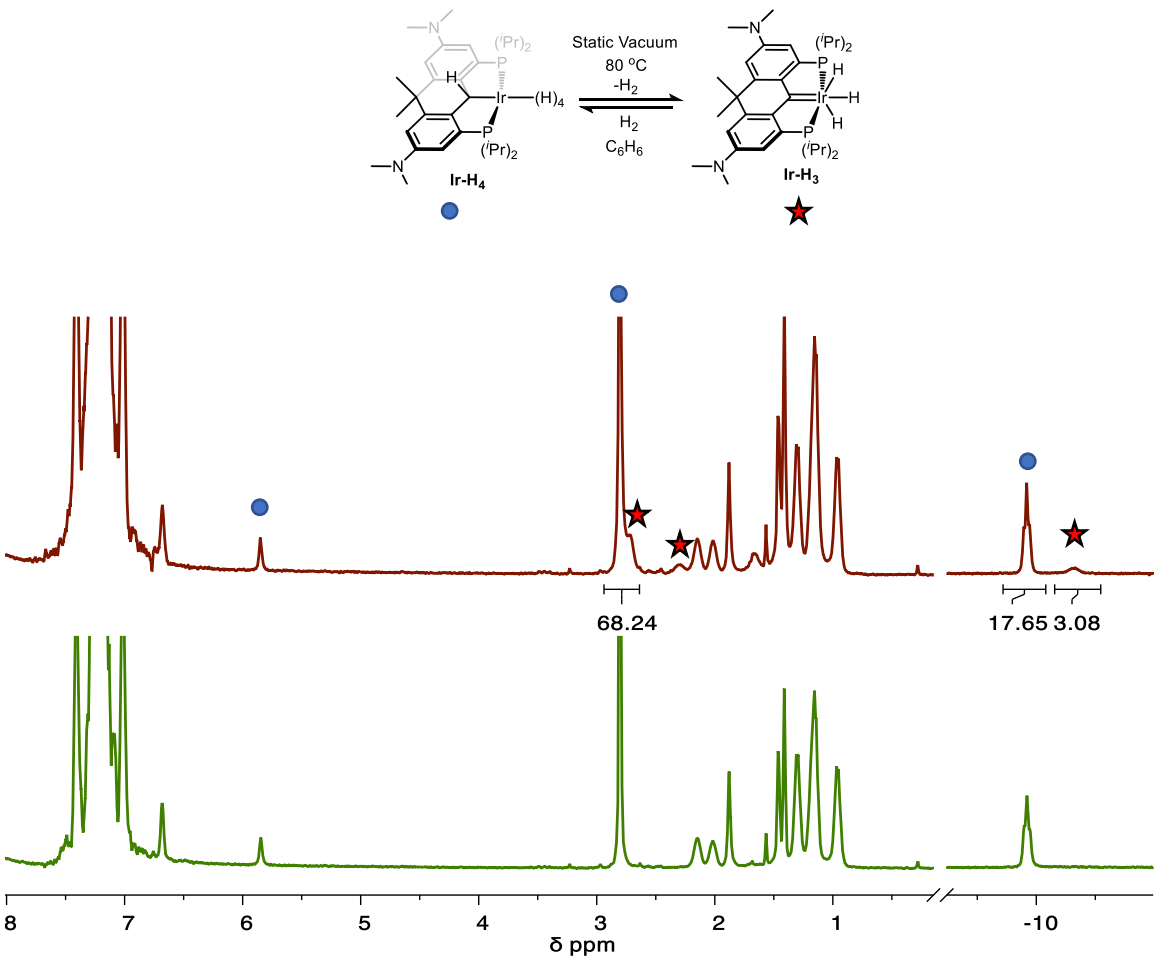


Figure S5. ^{1}H NMR (400 MHz) spectra of **Ir-H$_4$** heated under static vacuum to 80 °C at 0 hrs (bottom) and 1.6 hrs (top) in benzene (spiked with 0.05 mL of cyclohexane-d_{12}).

Relative integrations of selected peaks for **Ir-H$_3$** show NMe_2 protons (2.71 ppm) and hydride protons (-10.30 ppm) have relative integrations of ~ 14 : 3 (slightly greater than 12: 3) when taking into account the overlapping NMe_2 from **Ir-H$_4$** (2.81 ppm) .

Reactions demonstrating H/D exchange within Ir-H$_4$, Ir-Ph and Ir-H$_3$

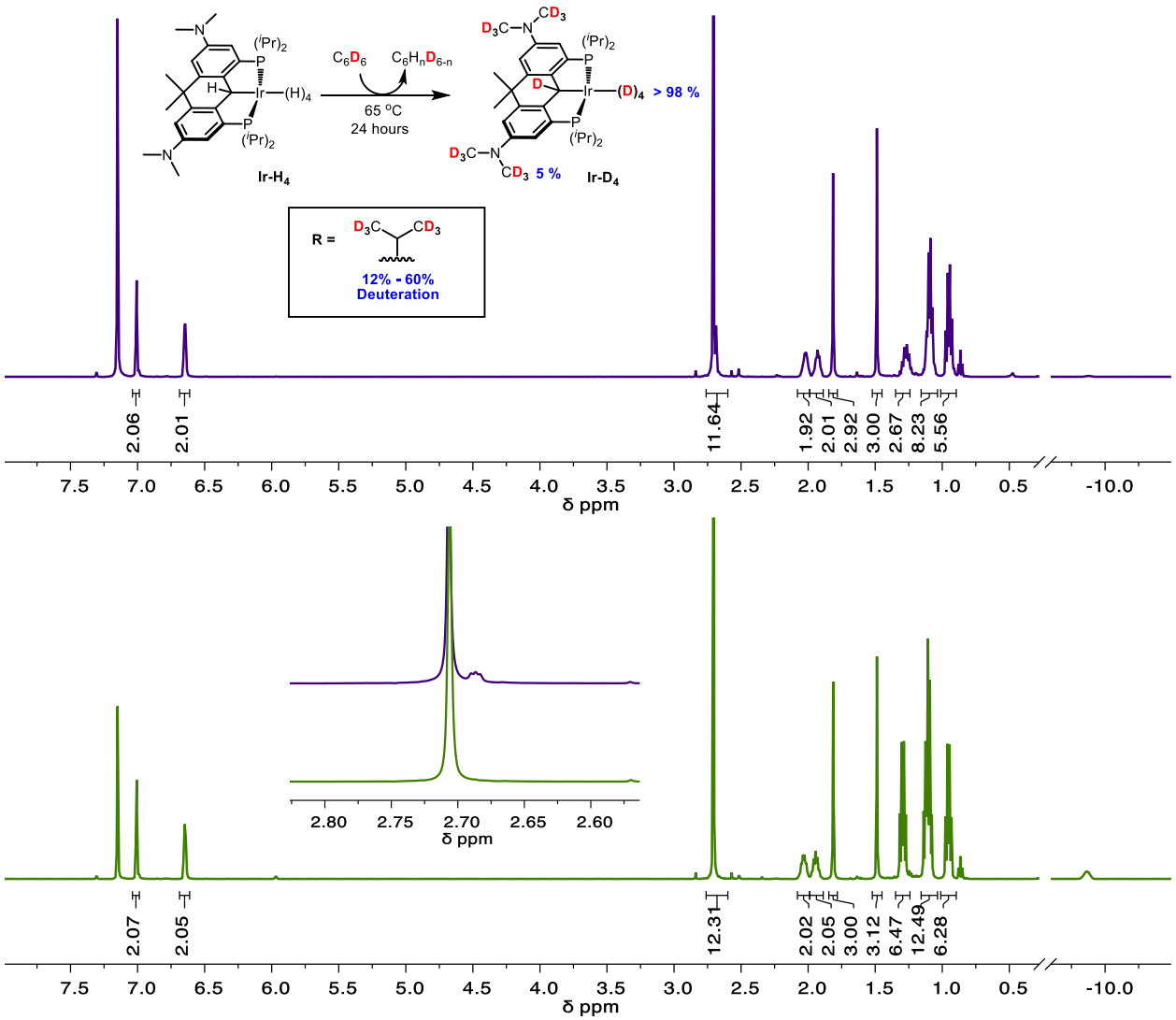


Figure S6. ^{1}H NMR (500 MHz) spectra of **Ir-H$_4$** before (bottom) and after (top) being heated to 65 °C in C_6D_6 for 24 hours.

After heating **Ir-H$_4$** for 24 hours under 1 atmosphere of argon, deuteration of the methyl groups within the P^{i}Pr$_2$ (1.31 ppm, 1.12 ppm and 0.96 ppm) and NMe$_2$ (2.72 ppm) functionalities is inferred from the loss of signal intensity relative to the non-exchange -PC**H**(CH$_3$)$_3$ (2.04 ppm and 1.96 ppm), -C(C**H**$_3$)$_2$- (1.82 ppm,1.50 ppm) and aryl sites (7.02 ppm, 6.65 ppm). The increase in residual C_6D_5H signal is further indication of deuterium incorporation.

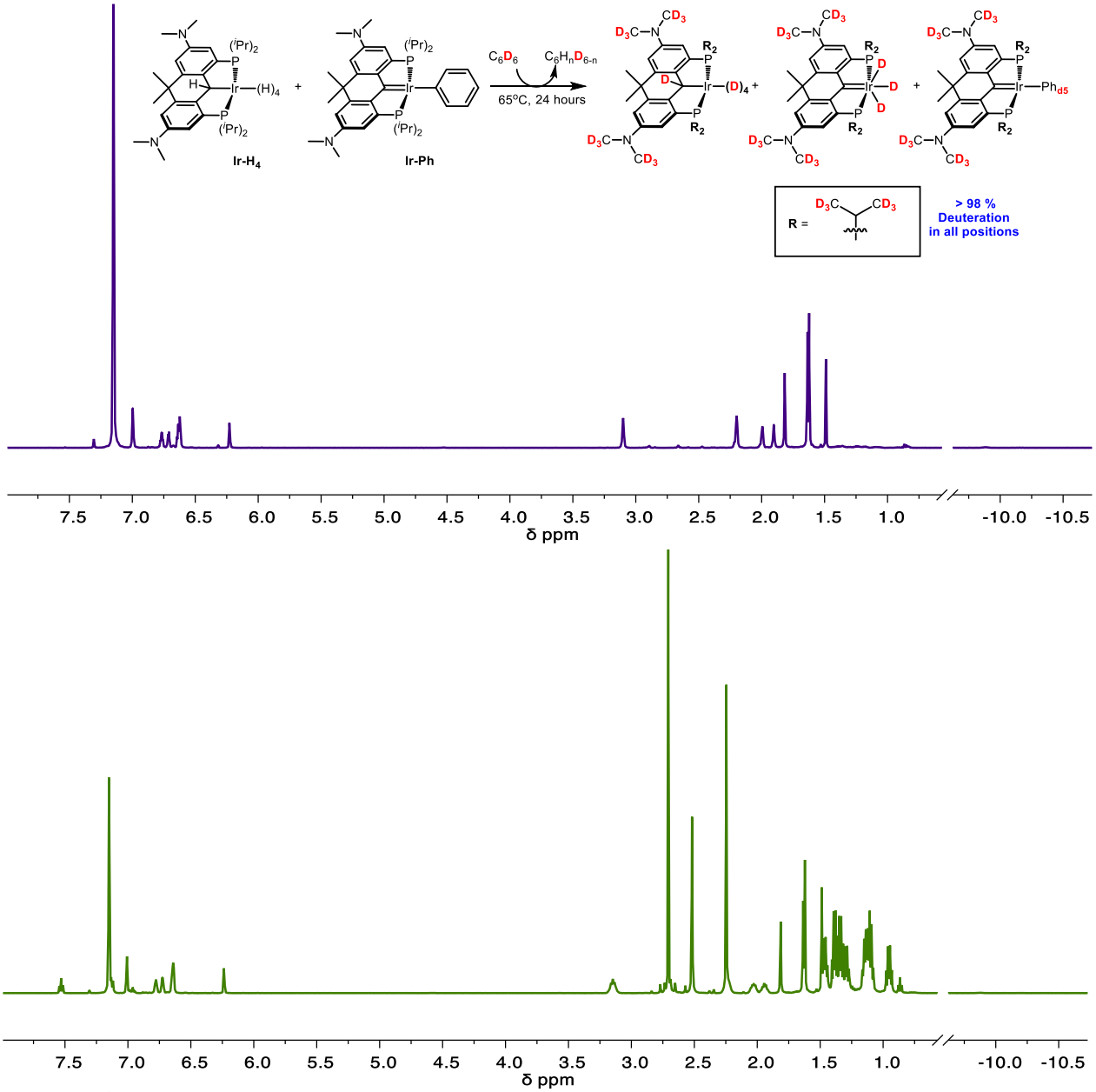


Figure S7. ^{1}H NMR (500 MHz) spectra of **Ir-H$_4$** (0.006 g, 0.008 mmol) and **Ir-Ph (**0.005 g**,** 0.006 mmol) before (bottom) and after (top) being heated to 65 °C in C_6D_6 for 24 hours.

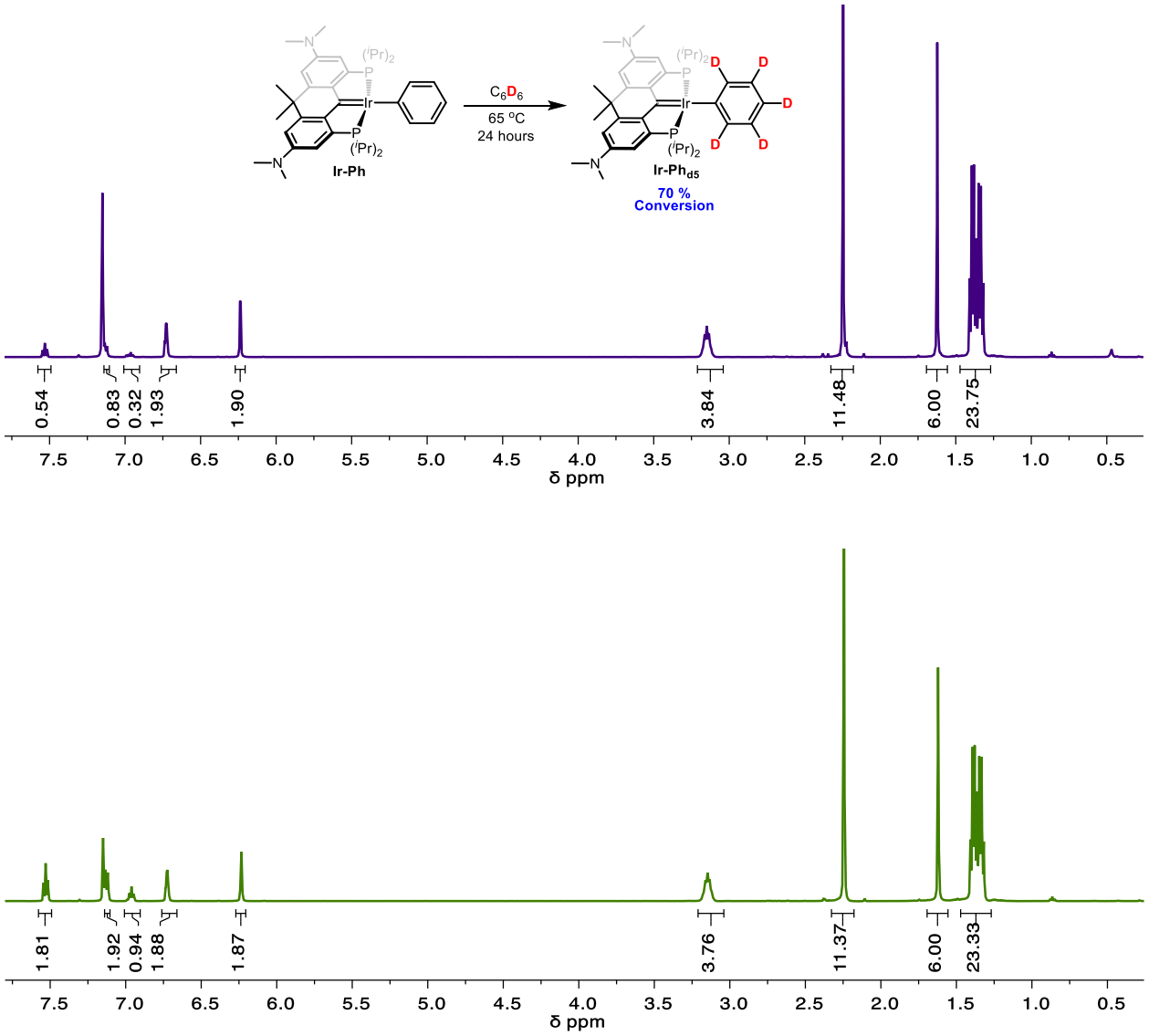
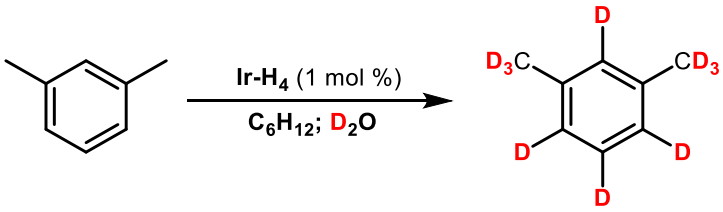


Figure S8. ^{1}H NMR (500 MHz) spectra of **Ir-Ph** before (bottom) and after (top) being heated to 65 °C in C_6D_6 for 24 hours.

After heating **Ir-Ph** for 24 hours under 1 atmosphere of argon, deuteration is limited to phenyl ligand (7.54 ppm, 7.14 ppm and 6.97) as indicated by a loss of more than half of resonance signal intensity relative to all other C-H sites.

Hydrogen Isotope Exchange with D_2O

Table S2. Optimization of conditions for deuteration of *meta*-xylene with D_2O.



Entry	Catalyst	Temp. (°C)	Position % Deuteration			
			Benzyl	2	4 & 6	5
1	Ir-OH	65	0	0	0	0
2	Ir-H_4	65[a]	0	0	0	0
3	Ir-H_4	65	0	0	4	85
4	Ir-H_4	65[b]	5	0	24	94
5	Ir-H_4	80	2	0	20	95
6	Ir-H_4	80[b]	14	0	35	84

Reactions were performed using D_2O (0.4 mL) along with *meta*-xylene (0.38 mmol) and **Ir-H_4** (1 mol %) dissolved in 0.75 mL of cyclohexane. Performed with [a] no D_2O and in cyclohexane-d_{12} [b] under static vacuum.

Characterization Data for Ir-OH

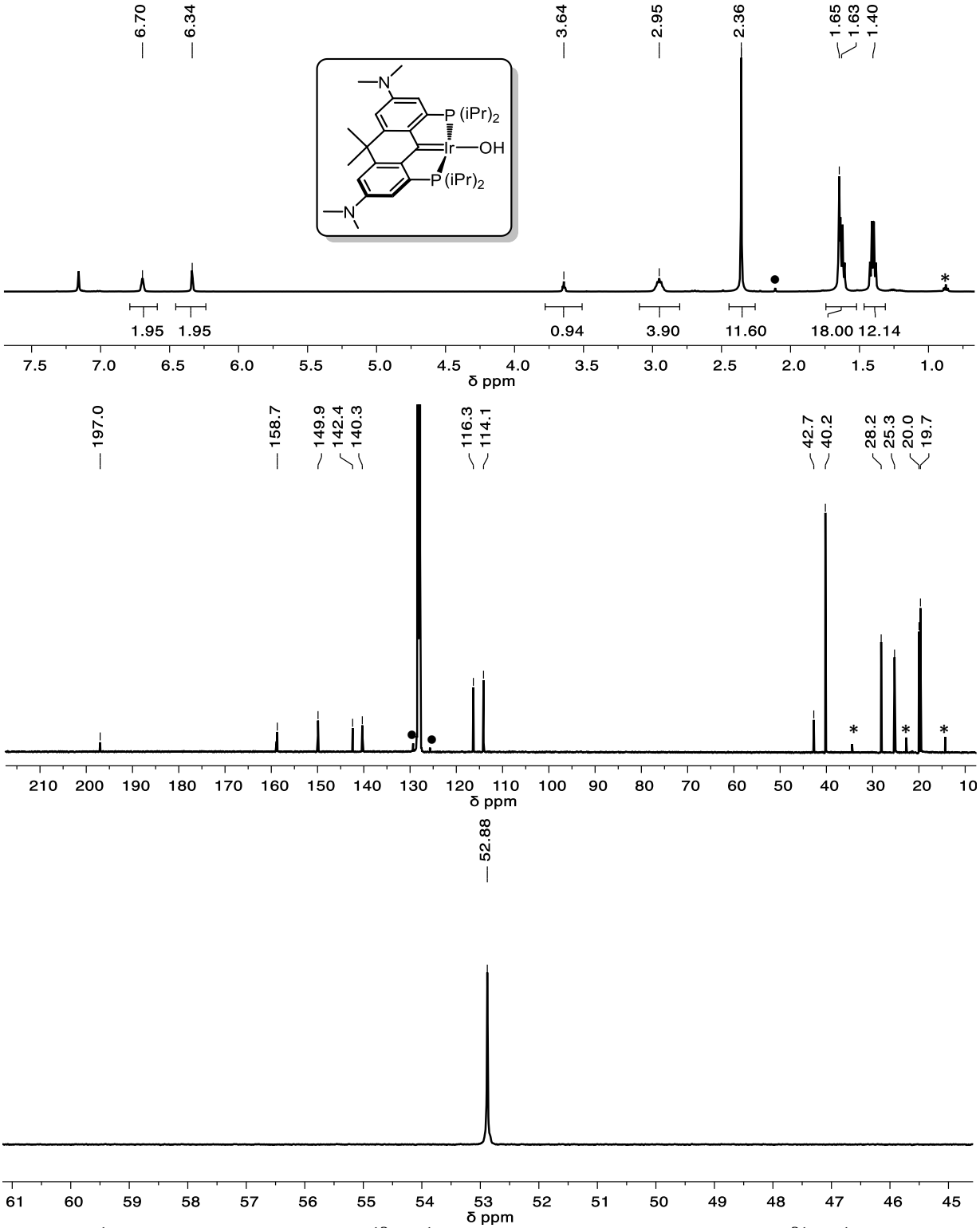


Figure S9. ^{1}H NMR (500 MHz, top), ^{13}C {^{1}H} NMR (126 MHz, middle), and ^{31}P {^{1}H} NMR (203 MHz, bottom) spectra for **Ir-OH** in C_6D_6. Asterisk (*) denotes residual pentane impurity. Bullet (•) denotes toluene impurity**.**

Characterization Data for Ir-H$_4$

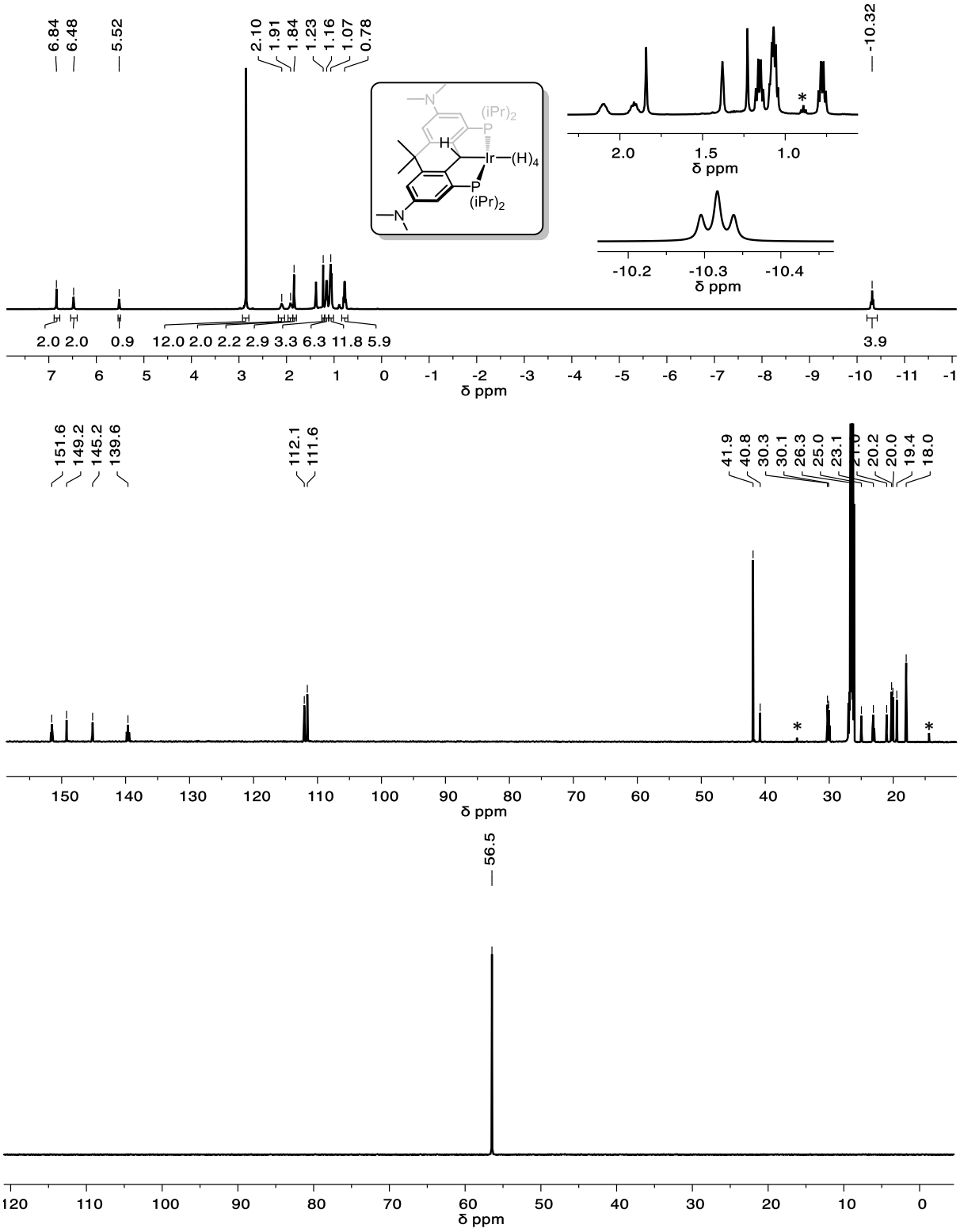


Figure S10. ^{1}H NMR (500 MHz, top), ^{13}C {^{1}H} NMR (126 MHz, middle), and ^{31}P {^{1}H} NMR (203 MHz, bottom) spectra for **Ir-H$_4$** in C_6D_{12}. Asterisk (*) denotes residual pentane impurity.

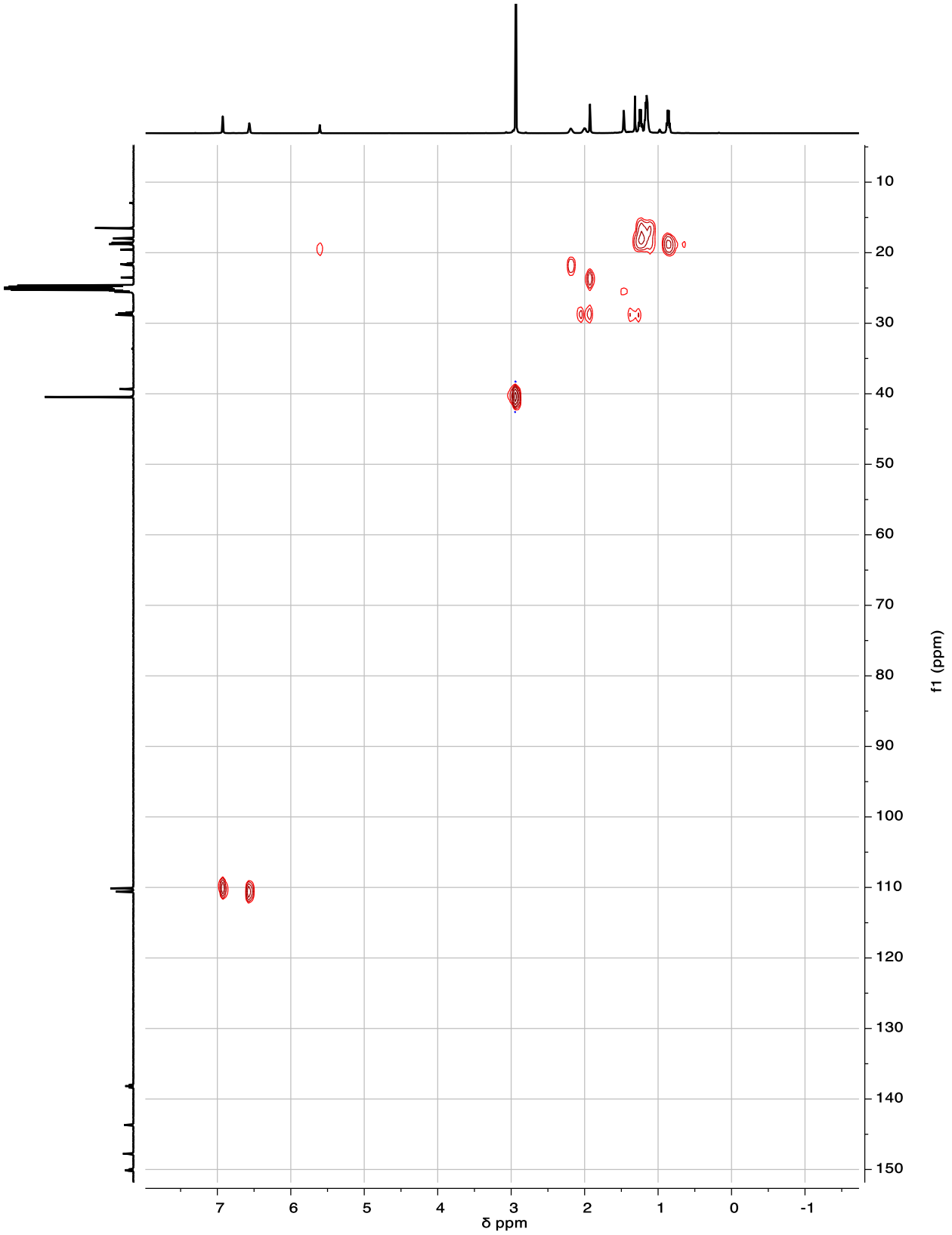


Figure S11. ^{1}H-^{13}C HSQC data for **Ir-H$_4$.**

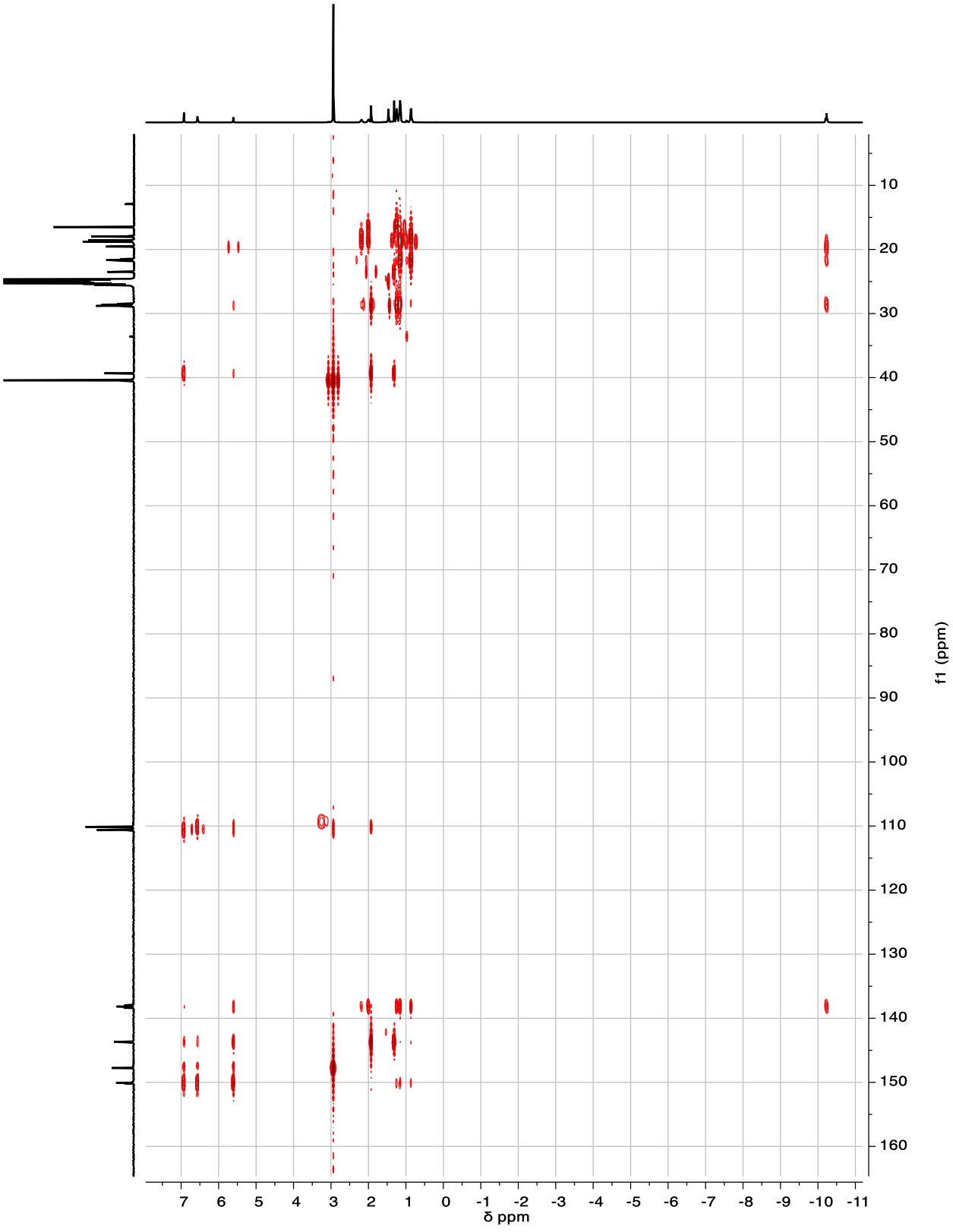


Figure S12. ^{1}H-^{13}C HMBC data for **Ir-H$_4$.**

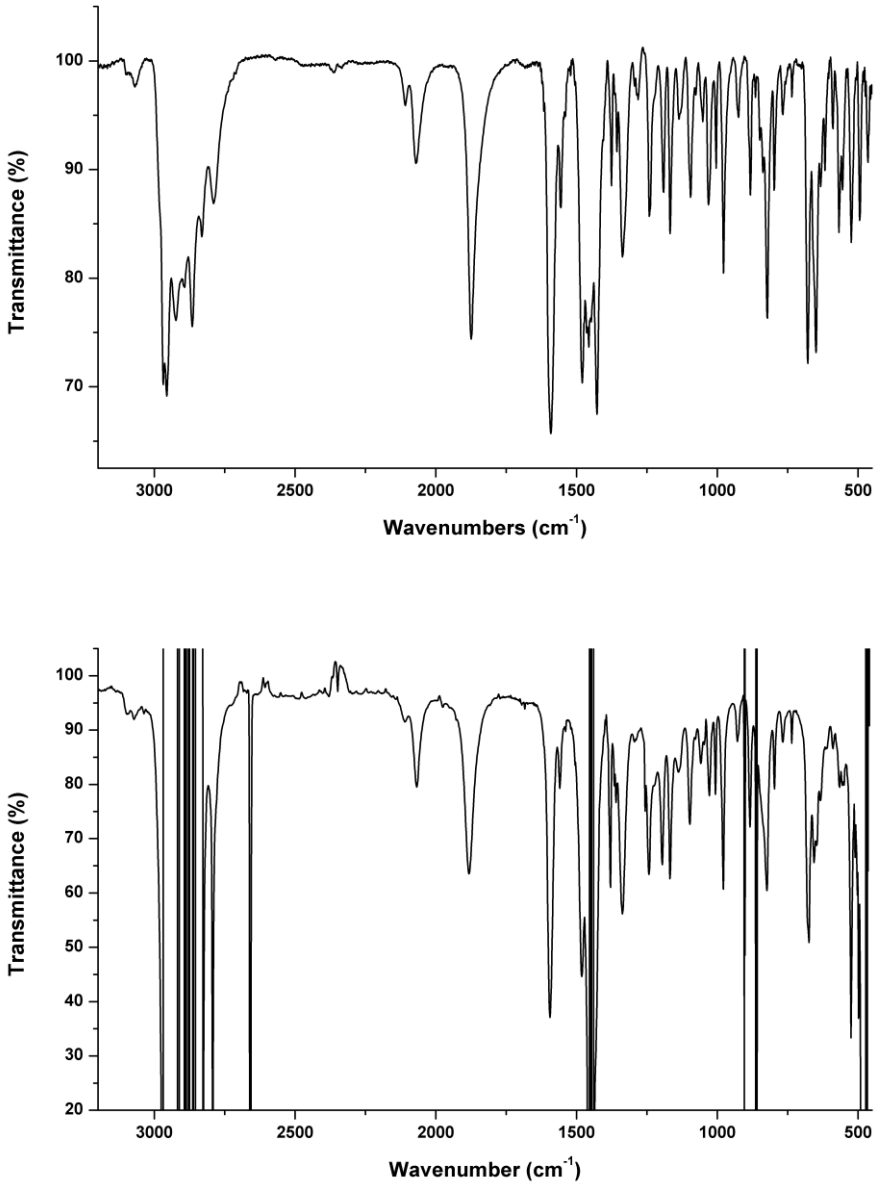


Figure S13. Infrared spectra of **Ir-H$_4$** in KBr (top) and in cyclohexane (bottom).

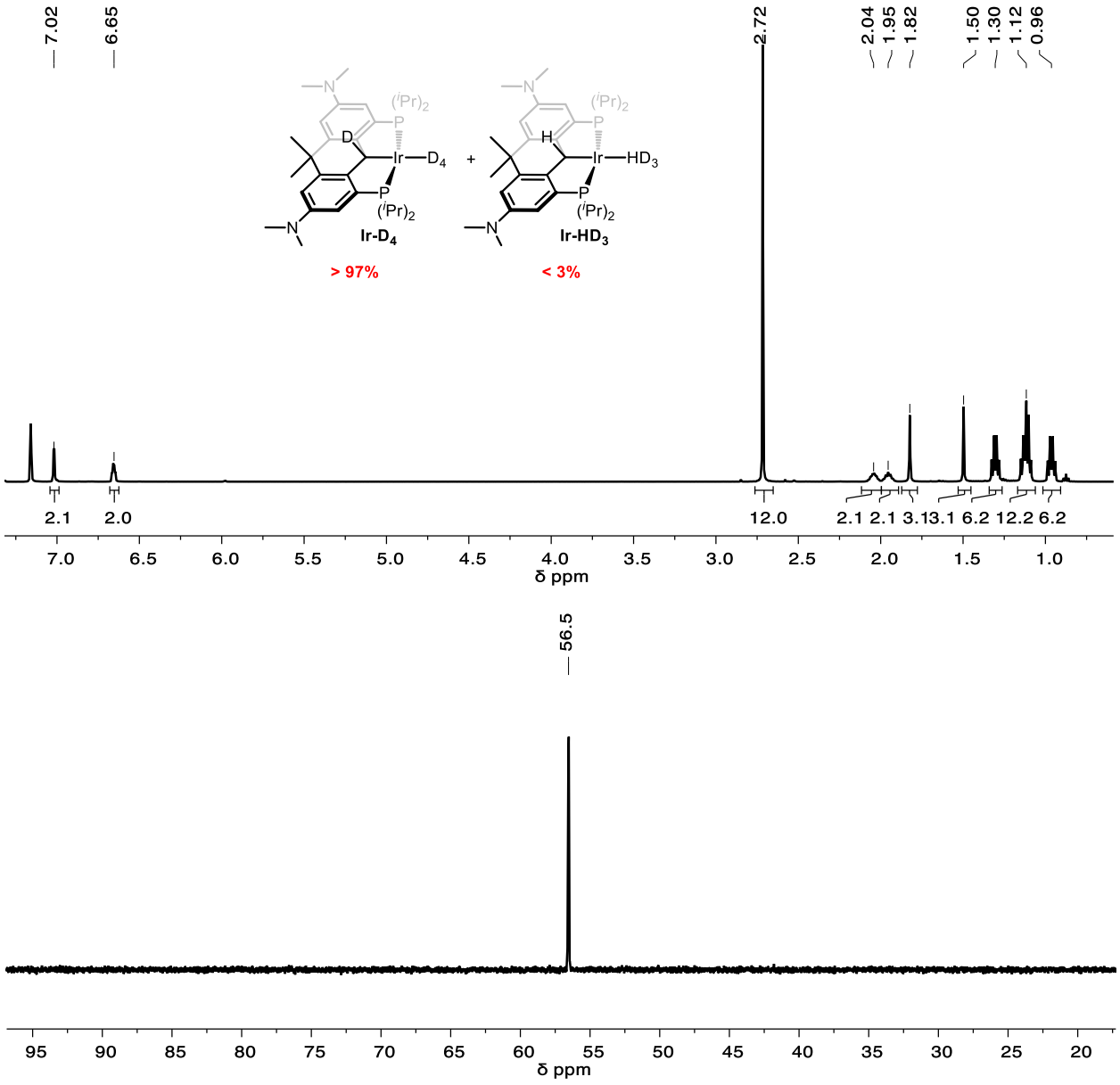


Figure S14. ^{1}H (500 MHz, top) and $^{31}P\{^{1}H\}$ (203 MHz, bottom) NMR spectra for a mixture of **Ir-D4** (> 97 %) and **Ir-HD3** (< 3%) in C_6D_6.

Characterization Data for Ir-Ph

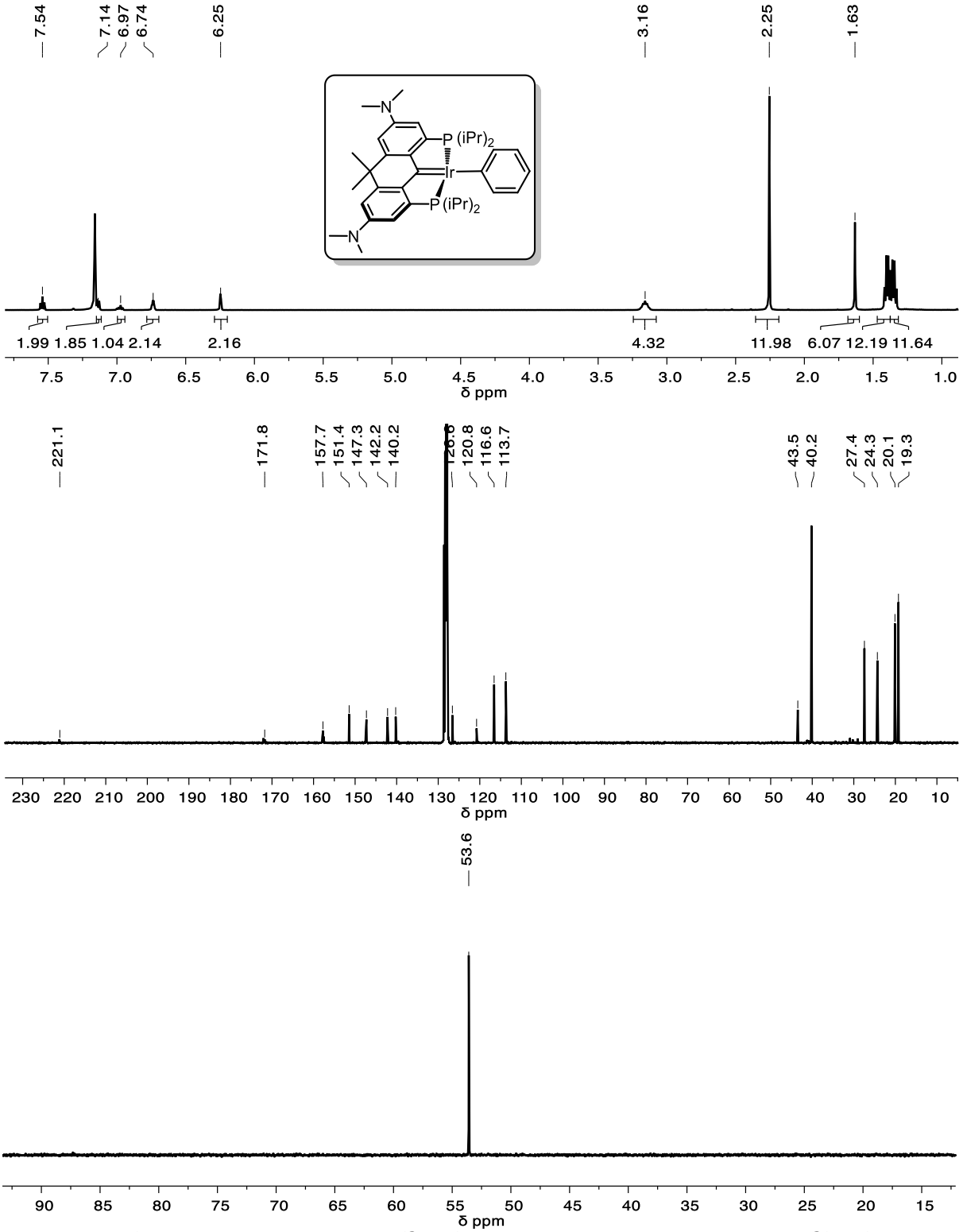


Figure S15. ^{1}H NMR (500 MHz, top), ^{13}C {^{1}H} NMR (126 MHz, middle), and ^{31}P {^{1}H} NMR (203 MHz, bottom) spectra for **Ir-Ph** in C_6D_6.

Figure S16. ^{1}H-^{13}C HSQC data for **Ir-Ph**.

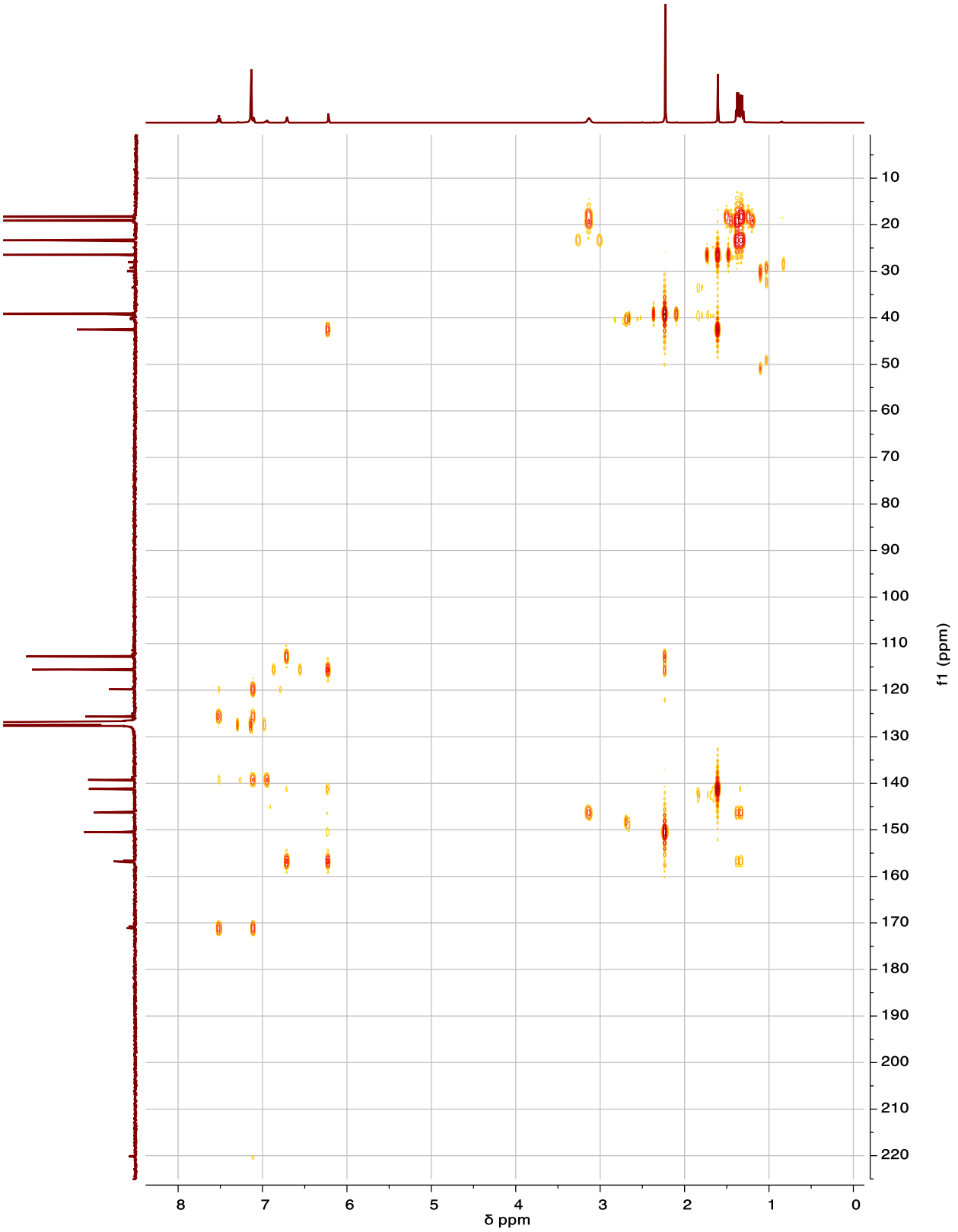


Figure S17. ^{1}H-^{13}C HMBC data for **Ir-Ph**.

Characterization Data for Ir-H$_3$

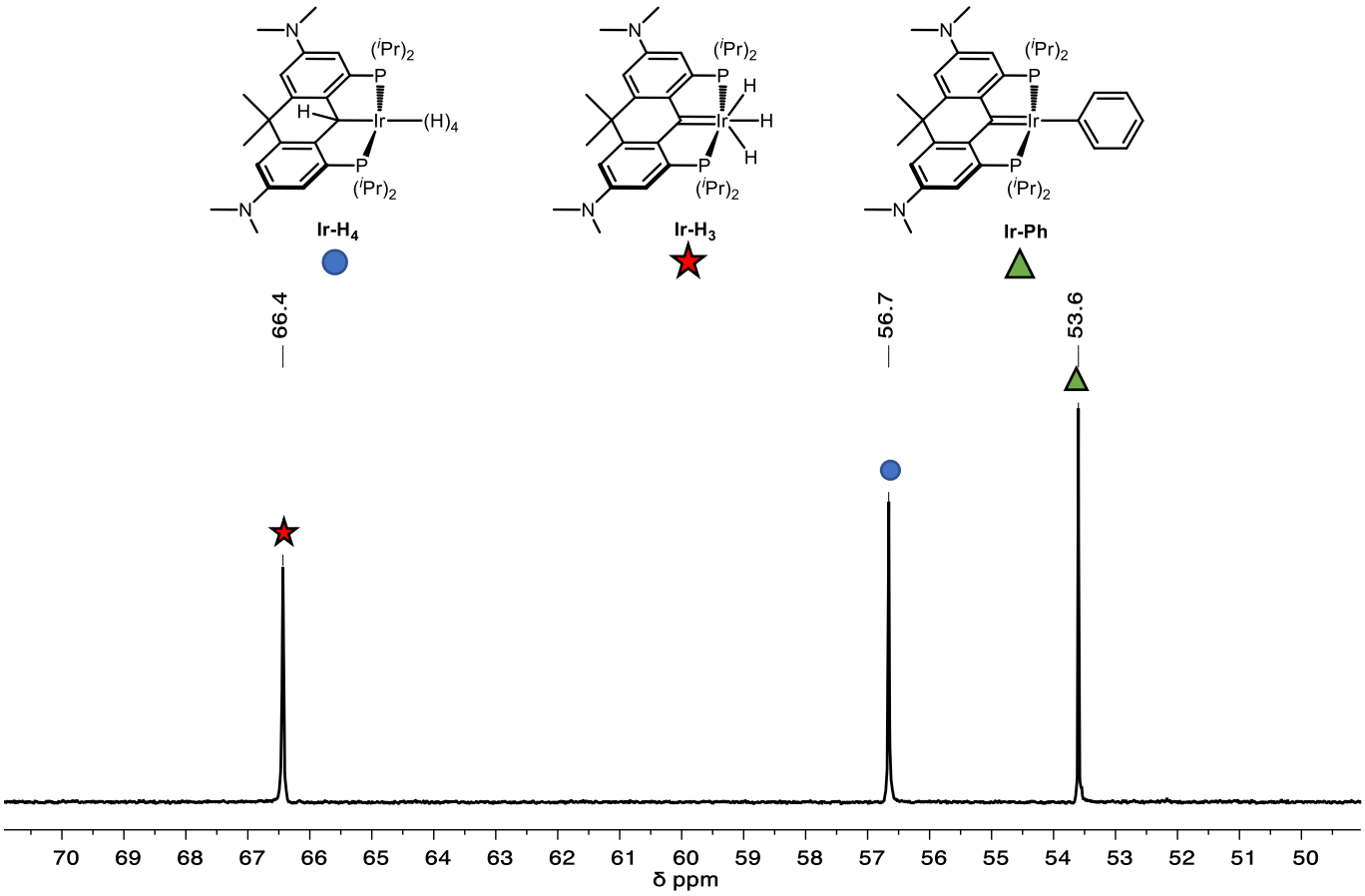


Figure S18. ^{31}P {^{1}H} NMR (203 MHz) resulting from a mixture of **Ir-H$_4$** and **Ir-Ph** in C_6H_6 spiked with C_6D_{12} for locking and shimming.

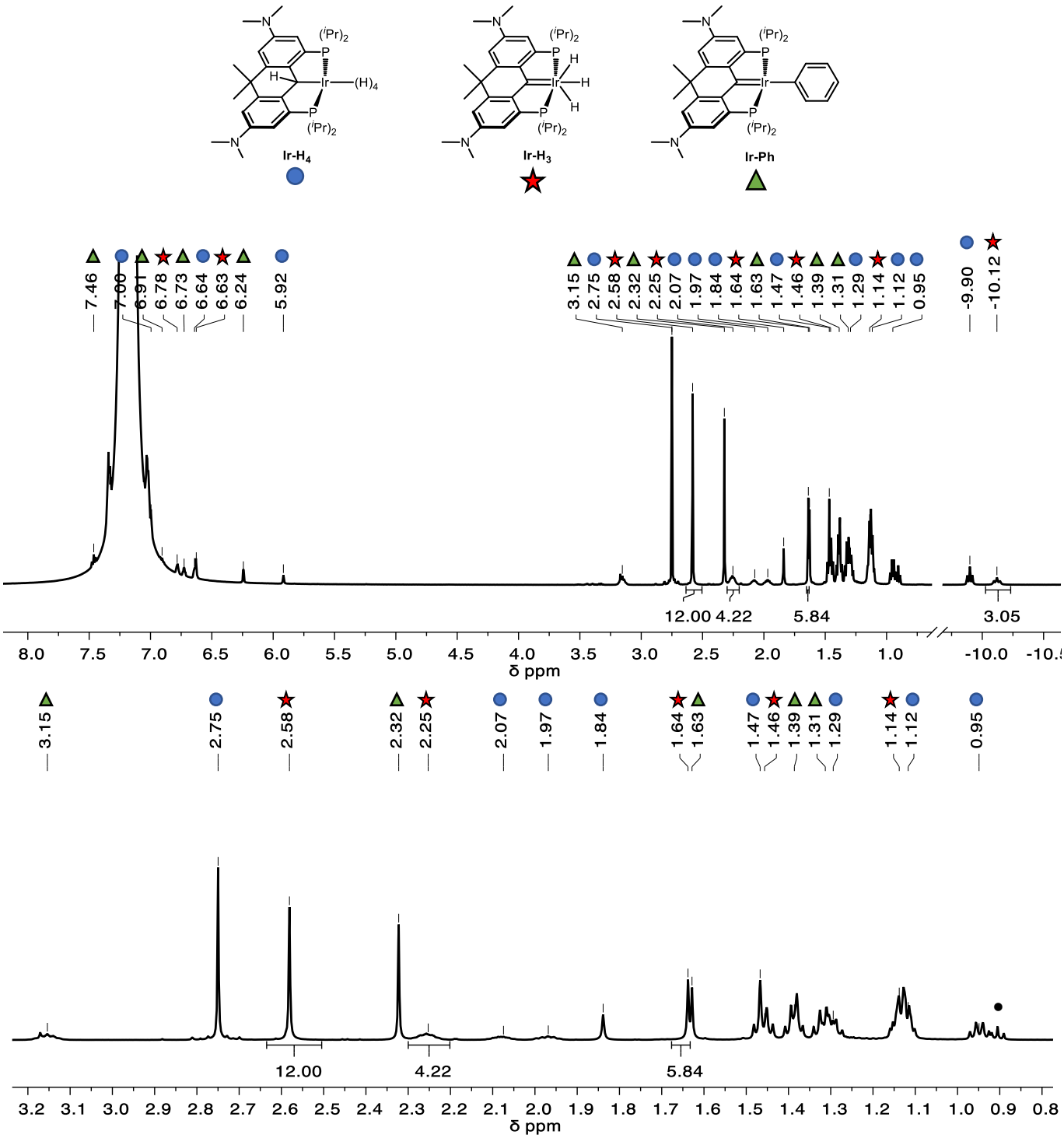


Figure S19. ^{1}H NMR (500 MHz) resulting from a mixture of **Ir-H$_4$** and **Ir-Ph** in C_6H_6 spiked with C_6D_{12} for locking and shimming. Integration -C(CH$_3$)$_2$- protons at 1.64 ppm is underestimated due to peak overlap. Bullet(•) indicates pentane impurity.

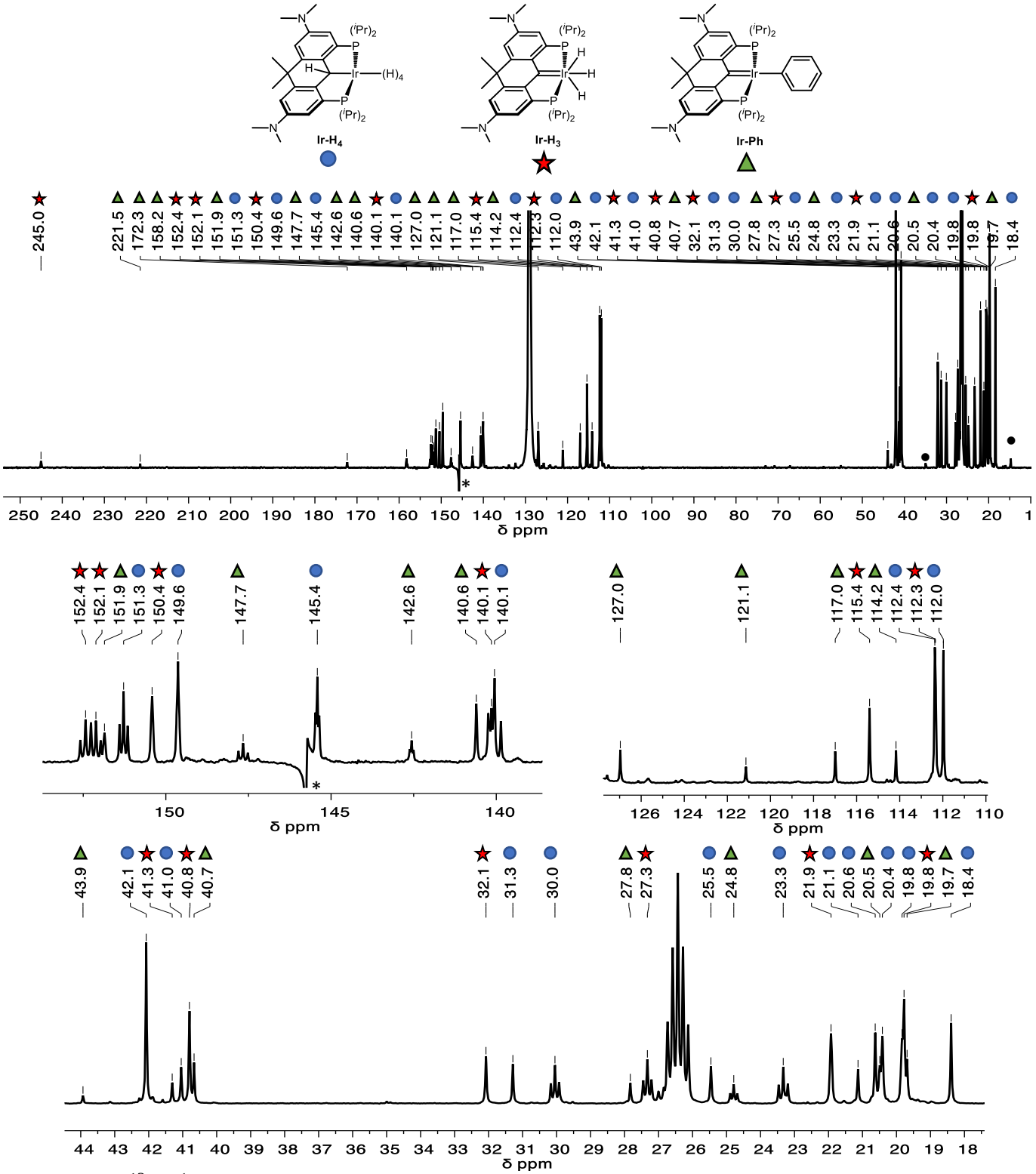


Figure S20. ^{13}C {^{1}H} (126 MHz) resulting from a mixture of **Ir-H$_4$** and **Ir-Ph** in C_6H_6 spiked with C_6D_{12} for locking and shimming. Asterisk (*) indicates NMR "clipping" at the centre of the spectral window. Bullet (•) indicates n-pentane impurity.

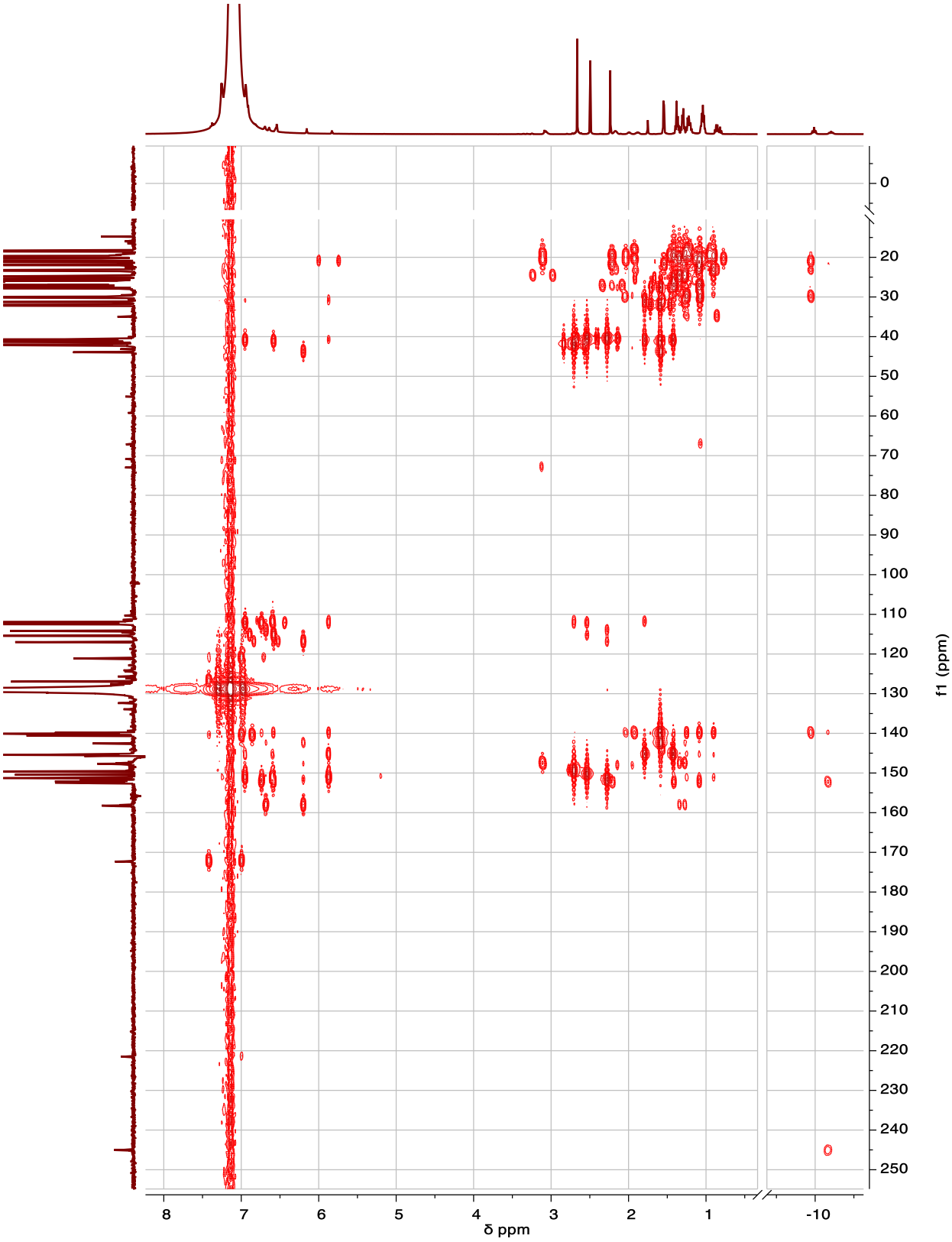


Figure S21. ^{1}H-^{13}C HMBC resulting from a mixture of **Ir-H$_4$** and **Ir-Ph** in C_6H_6 spiked with C_6D_{12} for locking and shimming.

Deuteration of *m*-xylene (Example in Figure 4)

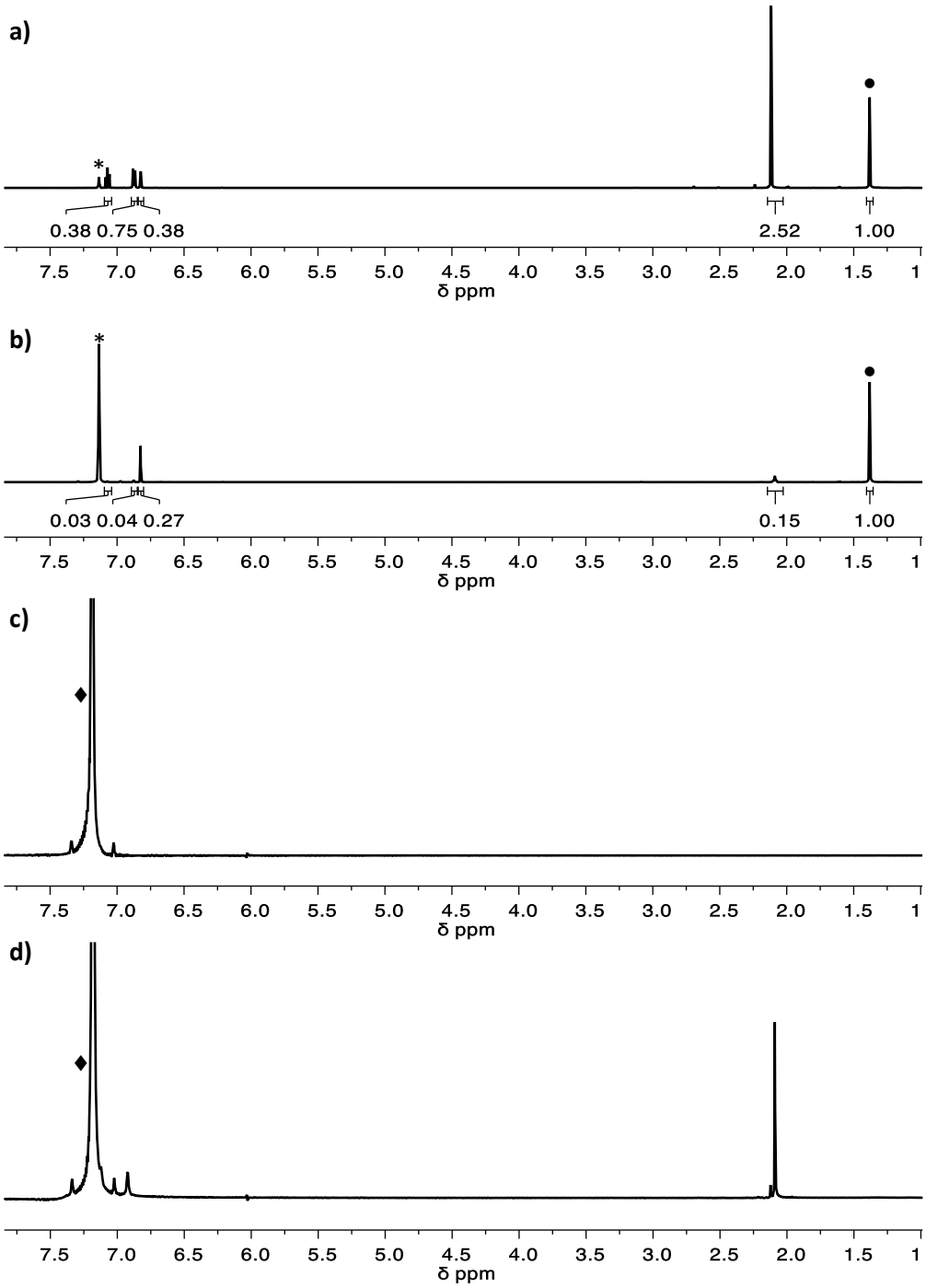


Figure S22. ^{1}H NMR (500 MHz, C_6D_6) spectra of *m*-xylene (a) before and (b) after exhaustive deuteration under the conditions outlined for method [1] in Figure 4. ^{2}H NMR (77 MHz, C_6D_6) spectra of *m*-xylene (c) before and (d) after exhaustive deuteration under the conditions outlined for method [1] in Figure 4. Asterisk (*) denotes residual solvent, bullet (●) denotes C_6H_{12} internal standard, and diamond (♦) denotes C_6D_6.

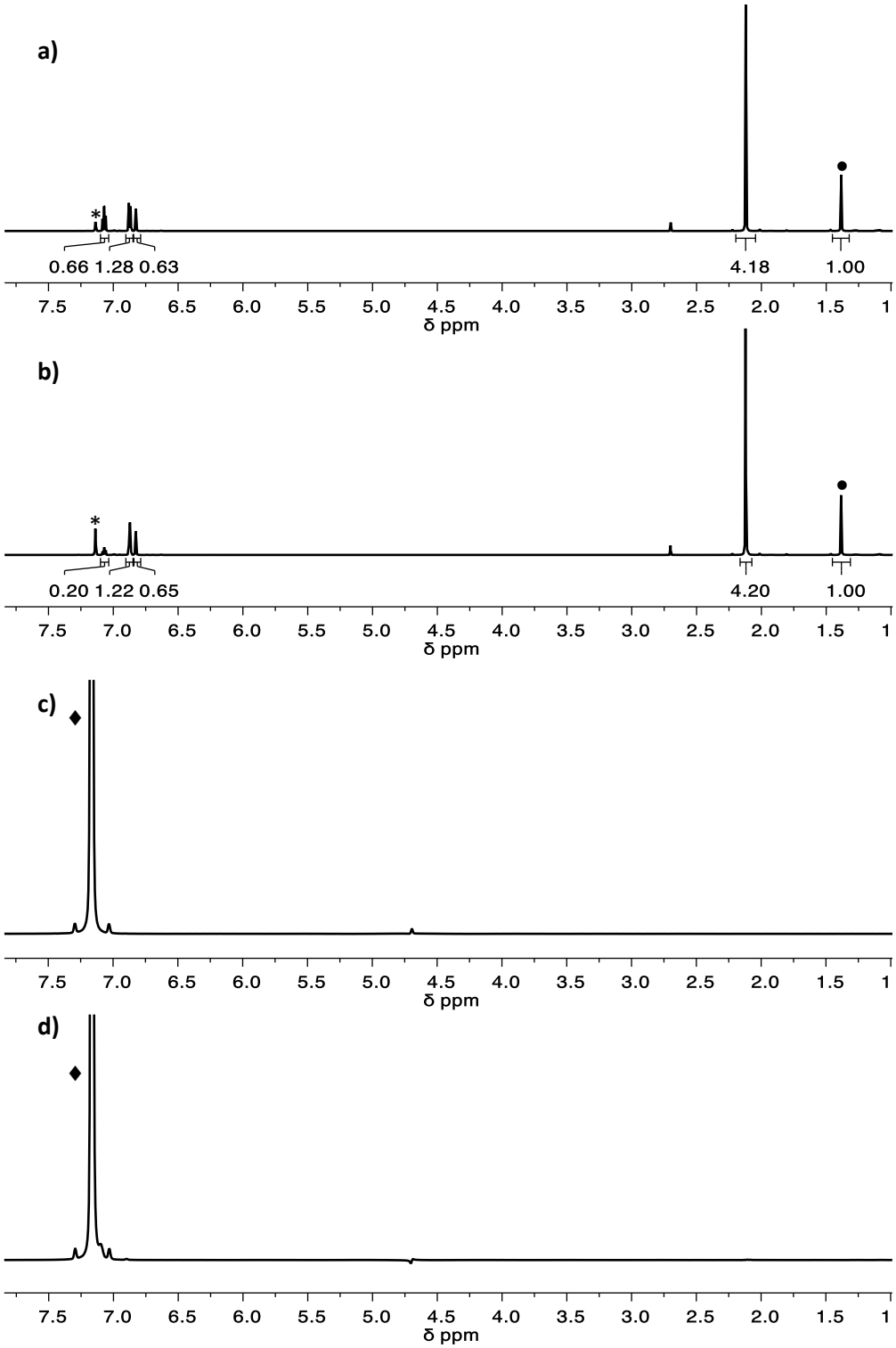


Figure S23. ^{1}H NMR (600 MHz, C_6D_6) spectra of *m*-xylene (a) before and (b) after selective deuteration under the conditions outlined for method [2] in Figure 4. ^{2}H NMR (92 MHz, C_6D_6) spectra of *m*-xylene (c) before and (d) after selective deuteration under the conditions outlined for method [2] in Figure 4. Asterisk (*) denotes residual solvent, bullet (●) denotes C_6H_{12} internal standard, and diamond (♦) denotes C_6D_6.

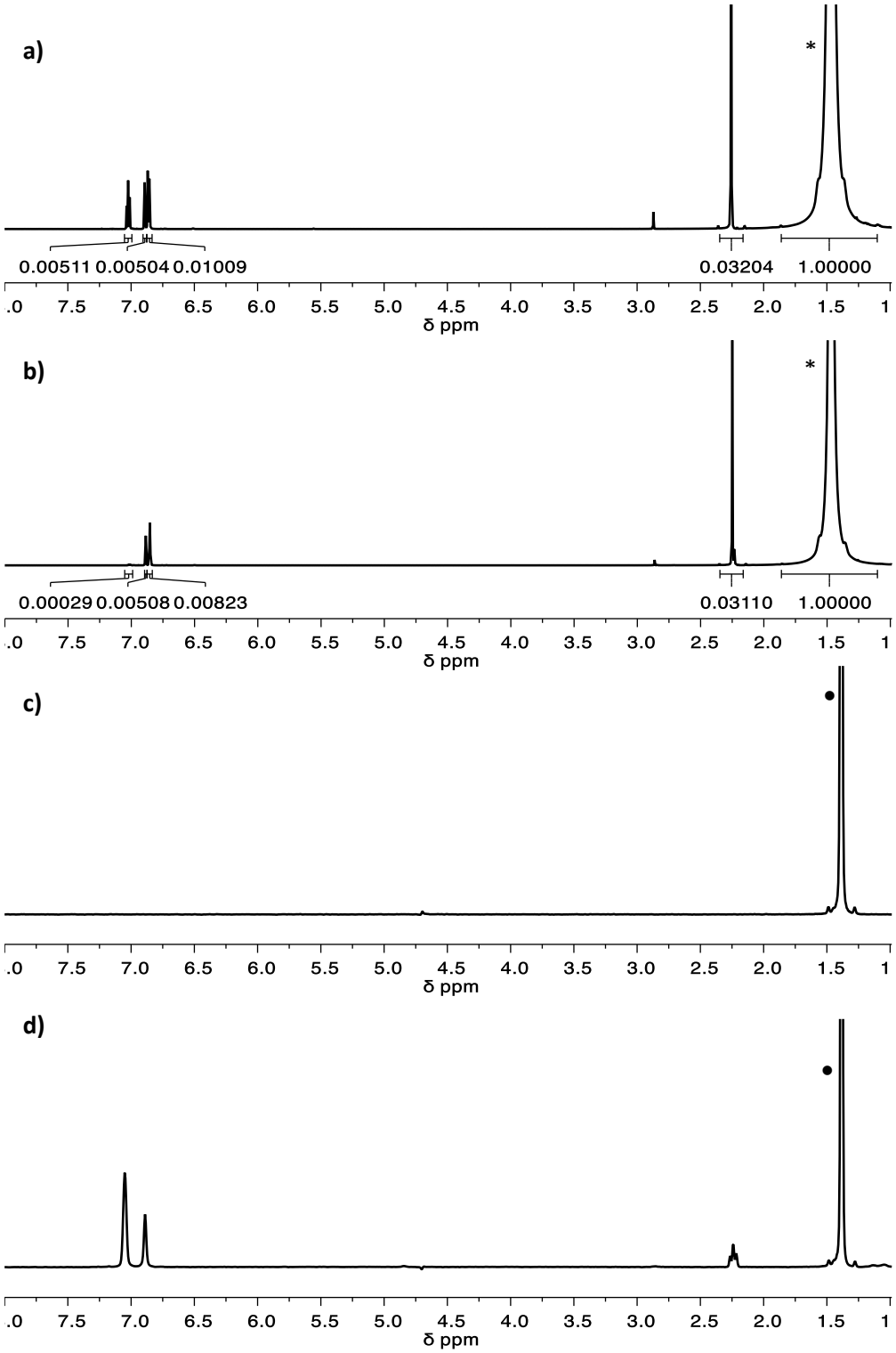


Figure S24. ^{1}H NMR (600 MHz, C_6H_{12}, spiked with C_6D_{12}) spectra of *m*-xylene (a) before and (b) after deuteration under the conditions outlined for method [3] in Figure 4. ^{2}H NMR (92 MHz, C_6H_{12}, spiked with C_6D_{12}) spectra of *m*-xylene (c) before and (d) after deuteration under the conditions outlined for [3] in Figure 4. Asterisk (*) denotes C_6H_{12} solvent, bullet (•) denotes C_6D_{12} spike.

NMR Spectra of Deuterated Compounds from Neat Reactions

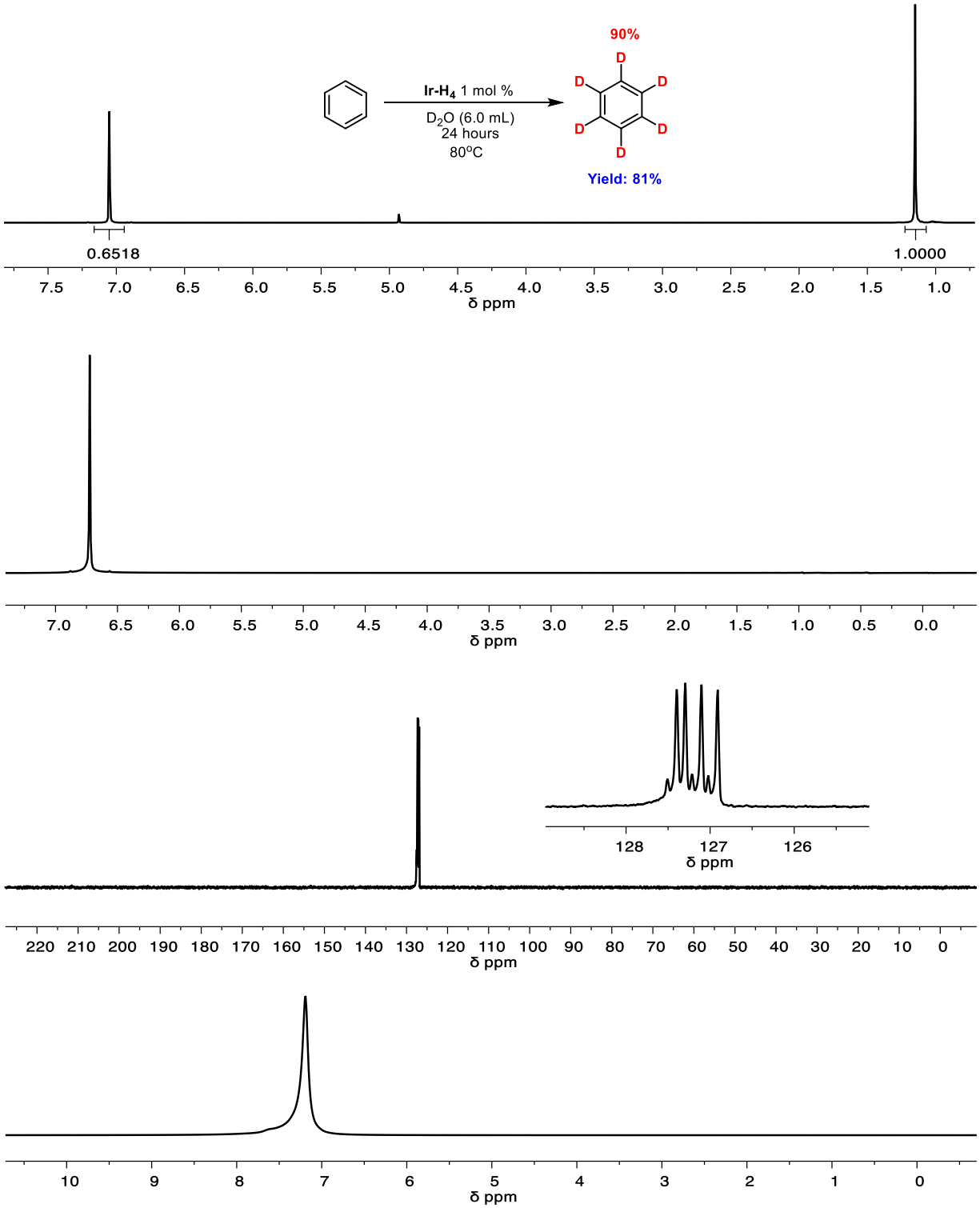


Figure S25. NMR spectra following deuteration of neat benzene using D_2O and **Ir-H₄** (1 mol %). ^{1}H NMR (500 MHz, top) of benzene product (0.0777 g) and C_6H_{12} (0.0061 g, 0.0725 mmol) in 0.6 mL of CD_2Cl_2. ^{1}H NMR (500 MHz, 2nd from top), ^{13}C {^{1}H} NMR (126 MHz, 2nd from bottom) and ^{2}H NMR (77 MHz, bottom) of neat deuterated benzene product.

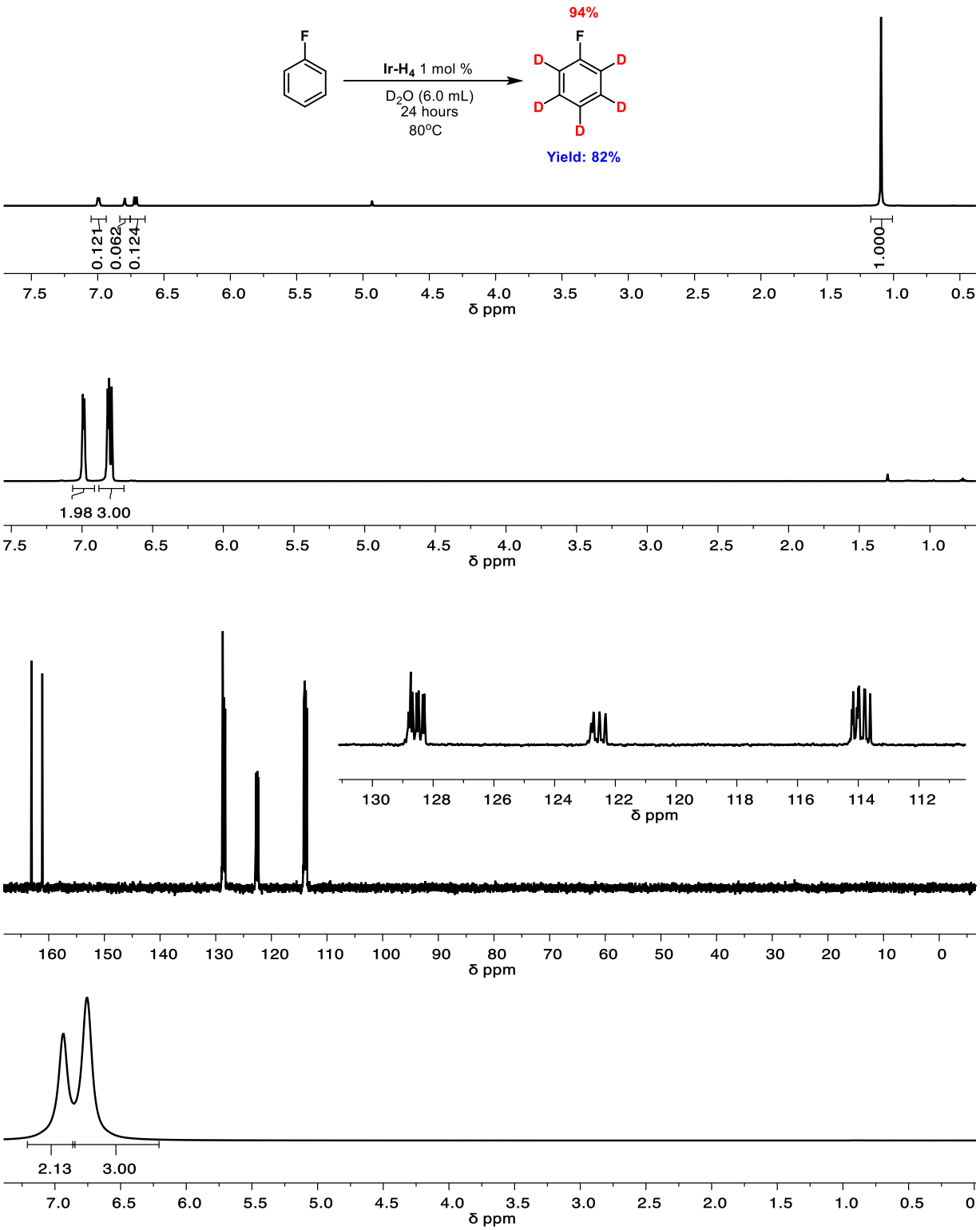


Figure S26. NMR spectra following deuteration of neat fluorobenzene using D_2O and **Ir-H₄** (1 mol %). ^1H NMR (500 MHz, top) of fluorobenzene product (0.0808 g) and C_6H_{12} (0.0058 g, 0.0689 mmol) in 0.6 mL of CD_2Cl_2. ^1H NMR (500 MHz, 2nd from top), ^{13}C {^1H} NMR (126 MHz, 2nd from bottom) and ^2H NMR (77 MHz) of neat deuterated fluorobenzene product.

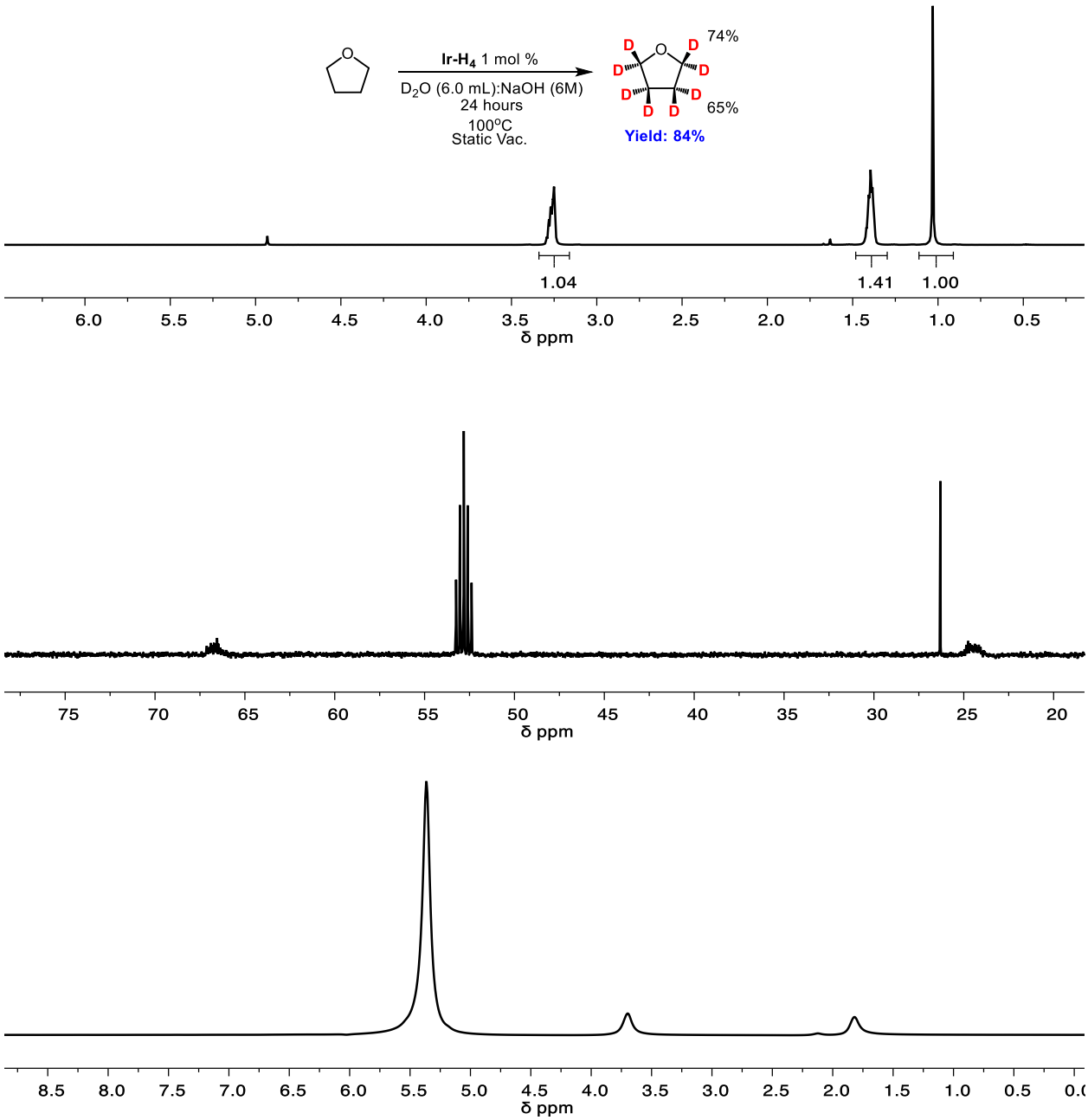


Figure S27. NMR spectra following deuteration of neat THF using a NaOH:D_2O (6 M) solution and **Ir-H4** (1 mol %). ^{1}H NMR (500 MHz, top), ^{13}C {^{1}H} NMR (126 MHz, middle) and ^{2}H NMR (77 MHz, bottom) of THF product (0.0506 g) and C_6H_{12} (0.0049 g, 0.0582 mmol) in 0.6 mL of CD_2Cl_2.

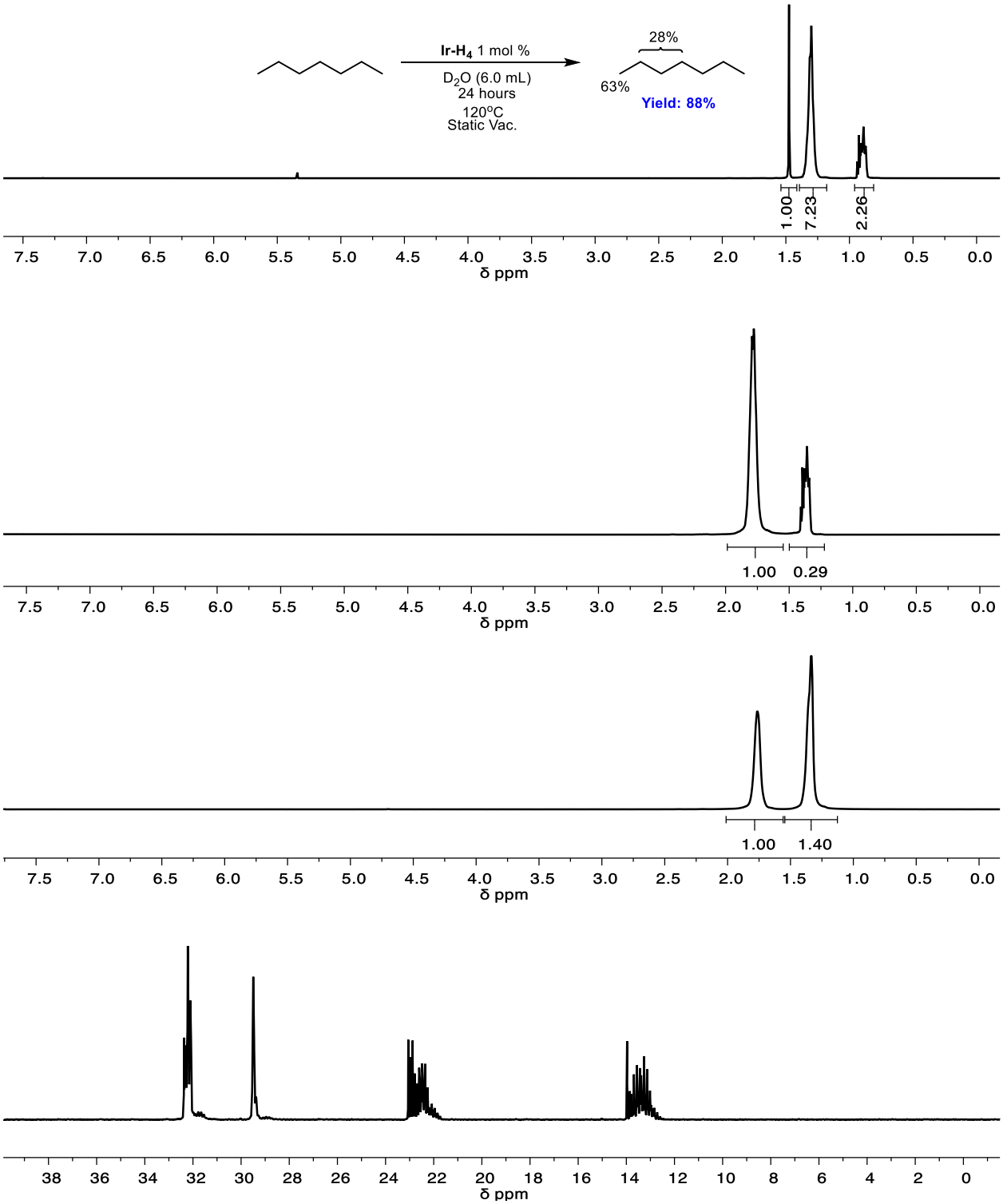


Figure S28. NMR spectra following deuteration of neat *n*-heptane using D_2O and **Ir-H₄** (1 mol %). ^1H NMR (500 MHz, top) of *n*-heptane product (0.0786 g) and C_6H_{12} (0.0051 g, 0.0606 mmol) in 0.6 mL of CD_2Cl_2. ^1H NMR (500 MHz, 2nd from top), ^{13}C {^1H} NMR (126 MHz, 2nd from bottom) and ^2H NMR (77 MHz, bottom) of neat deuterated *n*-heptane product.

Crystallographic Data

Table S3. Crystal Data Collection and Refinement Parameters for **Ir-H$_4$** and **Ir-Ph**.

	Ir-H$_4$	**Ir-Ph**
formula	C32H51N2P2Ir1	C38H55IrN2P2
fw	719.90	793.98
crystal system	triclinic	orthorhombic
space group	P-1	Pbca
a (Å)	10.1782(6)	10.1805(7)
b (Å)	10.3490(5)	22.3462(15)
c (Å)	16.3636(11)	31.760(2)
α (deg)	82.024(3)	90
β (deg)	74.304(4)	90
γ (deg)	82.558(3)	90
V (Å^3)	1635.65(17)	7225.3(9)
Z	2	8
T (K)	173(2)	173(2)
Wavelength (Å)	0.71073	0.71073
ρ_{calcd} (g·cm^{-3})	1.462	1.460
F(000)	732	3232
μ (mm^{-1})	4.201	3.812
crystal size, mm^3	0.2×0.2×0.2	0.1×0.1×0.05
transmission factors	0.5024 − 0.7456	0.5598 − 0.7456
θ range (deg)	2.157 − 24.999	3.321 − 24.999
data/restraints/param	5744/0/348	6342/0/402
GOF	1.025	1.076
R_1 [I > 2σ(I)]	0.0403	0.0335
wR_2 [all data]	0.0922	0.0680
residual density, e/Å^3	1.435 and -1.537	1.013 and -1.287

DFT Calculation Details

The M06 functional[3] was used with the 6-31G**[LANL2DZ for Ir][4] basis set for geometry optimizations in Gaussian 16.[5] Stationary points were verified as either minima or transition-state structures by calculation and visualization of vibrational frequencies. Geometry optimization and single point calculations were done in both the gas phase and benzene solvent using the SMD model.[6] For all ground-state and transition-state structures we calculated all reasonable conformations. The xyz coordinates of the lowest energy conformations are found below. Reported enthalpies and free energies in SMD benzene solvent are at 1 atm and 298 K. Final energies were calculated using M06/Def2-TZVP//M06-L/6-31G**[LANL2DZ for Ir].

Cartesian Coordinates for Structures Calculated using M06 DFT.

92

Gas phase 1-H_4 (tetrahydride)

C	-1.24169	1.03335	0.39215
C	-2.41874	0.36393	0.04091
C	-3.58613	1.04869	-0.29264
C	-3.60524	2.45075	-0.30169
C	-2.41383	3.11897	0.03400
H	-4.46776	0.48724	-0.59069
H	-2.40513	4.20316	0.01291
C	3.60500	2.45112	-0.30159
C	3.58606	1.04907	-0.29241
C	2.41874	0.36418	0.04112
C	1.24158	1.03347	0.39225
C	1.25207	2.43887	0.39113
C	2.41349	3.11921	0.03405
H	4.46779	0.48771	-0.59034
H	2.40465	4.20340	0.01293
C	-1.25234	2.43874	0.39107
C	-0.00018	3.18303	0.85999
C	-0.00003	0.27424	0.77271
N	4.75565	3.15553	-0.62964
N	-4.75590	3.15508	-0.62972
C	-0.00025	4.64565	0.42098
H	0.87308	5.17174	0.82092
H	-0.00023	4.74918	-0.67100
H	-0.87365	5.17166	0.82088
C	-0.00021	3.17236	2.40376
H	-0.89221	3.68681	2.78430
H	-0.00016	2.15306	2.80484
H	0.89170	3.68692	2.78434
C	4.67284	4.57565	-0.86861
H	5.65946	4.95216	-1.15015
H	3.96570	4.83435	-1.67428
H	4.36307	5.11901	0.03497
C	5.90233	2.43101	-1.11728
H	5.70085	1.88094	-2.05255
H	6.72079	3.13071	-1.30445
H	6.25811	1.70404	-0.37337
C	-4.67342	4.57535	-0.86779
H	-3.96641	4.83468	-1.67338
H	-5.66013	4.95184	-1.14902
H	-4.36365	5.11823	0.03608
C	-5.90290	2.43061	-1.11665
H	-6.72133	3.13038	-1.30367

H	-5.70190	1.88031	-2.05190
H	-6.25846	1.70383	-0.37243
P	-2.28717	-1.46018	0.03559
P	2.28736	-1.45995	0.03583
C	-3.27953	-2.04415	-1.42165
C	-3.31540	-3.56837	-1.44304
C	-2.71795	-1.49069	-2.72423
H	-4.30236	-1.65961	-1.28577
H	-3.79971	-3.99426	-0.55604
H	-3.86557	-3.92242	-2.32386
H	-2.29674	-3.97409	-1.49603
H	-2.67506	-0.39546	-2.72171
H	-1.70086	-1.86243	-2.89543
H	-3.34658	-1.80828	-3.56601
C	-3.26054	-2.03812	1.52349
C	-4.76619	-1.82468	1.42032
C	-2.72120	-1.37922	2.78767
H	-3.03923	-3.11643	1.57069
H	-5.22110	-2.35050	0.57319
H	-5.25701	-2.18754	2.33246
H	-5.00239	-0.75571	1.32876
H	-1.64486	-1.54618	2.90355
H	-2.90230	-0.29594	2.76960
H	-3.22947	-1.78764	3.67001
C	3.27994	-2.04385	-1.42129
C	2.71831	-1.49066	-2.72397
C	3.31613	-3.56807	-1.44251
H	4.30268	-1.65909	-1.28539
H	2.67525	-0.39544	-2.72160
H	3.34702	-1.80827	-3.56568
H	1.70128	-1.86259	-2.89516
H	3.80044	-3.99375	-0.55540
H	2.29757	-3.97401	-1.49555
H	3.86646	-3.92211	-2.32322
C	3.26061	-2.03776	1.52386
C	2.72107	-1.37887	2.78795
C	4.76626	-1.82423	1.42084
H	3.03937	-3.11609	1.57107
H	1.64473	-1.54592	2.90371
H	3.22927	-1.78724	3.67036
H	2.90209	-0.29558	2.76988
H	5.22130	-2.35009	0.57381
H	5.00239	-0.75525	1.32923
H	5.25700	-2.18697	2.33307
H	-0.00007	0.17984	1.87127
Ir	0.00011	-1.79652	0.03715
H	0.00005	-2.13013	1.65813
H	0.00014	-0.89276	-1.35211
H	0.00018	-3.39550	0.37417
H	0.00023	-2.79149	-1.25234

92

Gas phase 2-H_4 (dihydrogen dihydride)

C	-1.23497	1.02998	0.44048
C	-2.40021	0.36882	0.03585
C	-3.55504	1.05942	-0.33237
C	-3.57593	2.46044	-0.32074
C	-2.39526	3.12339	0.06131
H	-4.42424	0.50235	-0.67206
H	-2.38402	4.20779	0.05104
C	3.57589	2.46048	-0.32059
C	3.55498	1.05947	-0.33229
C	2.40014	0.36885	0.03590
C	1.23489	1.02999	0.44054
C	1.24710	2.43739	0.44666
C	2.39520	3.12342	0.06145
H	4.42416	0.50240	-0.67201
H	2.38395	4.20781	0.05121
C	-1.24716	2.43738	0.44659
C	-0.00005	3.17551	0.93737
C	-0.00005	0.26564	0.84478
N	4.71646	3.17042	-0.67418
N	-4.71647	3.17034	-0.67443
C	-0.00004	4.64617	0.52647
H	0.87392	5.16359	0.93668
H	0.00002	4.77171	-0.56327
H	-0.87406	5.16357	0.93659
C	-0.00011	3.14068	2.48038
H	-0.89181	3.65036	2.86808
H	-0.00013	2.11624	2.86684
H	0.89155	3.65036	2.86815
C	4.62369	4.59215	-0.89930

H	5.60196	4.97376	-1.20255
H	3.89544	4.85615	-1.68436
H	4.33581	5.12683	0.01652
C	5.84552	2.45278	-1.21024
H	5.61500	1.92046	-2.14919
H	6.66019	3.15398	-1.40848
H	6.22094	1.71114	-0.49085
C	-4.62384	4.59212	-0.89927
H	-3.89547	4.85633	-1.68414
H	-5.60210	4.97366	-1.20266
H	-4.33620	5.12670	0.01669
C	-5.84568	2.45267	-1.21011
H	-6.66034	3.15388	-1.40835
H	-5.61537	1.92016	-2.14901
H	-6.22101	1.71119	-0.49051
P	-2.27389	-1.45459	0.01370
P	2.27402	-1.45458	0.01370
C	-3.21347	-2.01987	-1.48568
C	-3.29676	-3.54190	-1.50341
C	-2.55621	-1.49790	-2.75669
H	-4.22833	-1.59897	-1.41096
H	-3.86004	-3.94714	-0.65399
H	-3.79112	-3.88333	-2.42162
H	-2.28815	-3.97543	-1.47910
H	-2.45587	-0.40620	-2.75102
H	-1.55311	-1.92702	-2.87161
H	-3.15381	-1.78348	-3.63188
C	-3.31291	-2.03617	1.45906
C	-4.80910	-1.78514	1.31389
C	-2.80130	-1.40719	2.75030
H	-3.12414	-3.12137	1.49596
H	-5.24502	-2.27495	0.43583
H	-5.33951	-2.16303	2.19754
H	-5.01739	-0.70887	1.24552
H	-1.73186	-1.58832	2.90485
H	-2.95740	-0.32023	2.74019
H	-3.34423	-1.81519	3.61205
C	3.21367	-2.01981	-1.48566
C	2.55668	-1.49761	-2.75671
C	3.29665	-3.54186	-1.50356
H	4.22860	-1.59911	-1.41082
H	2.45673	-0.40587	-2.75103
H	3.15426	-1.78341	-3.63185
H	1.55345	-1.92641	-2.87172
H	3.85921	-3.94739	-0.65381
H	2.28792	-3.97515	-1.47999
H	3.79159	-3.88326	-2.42146
C	3.31298	-2.03604	1.45914
C	2.80150	-1.40665	2.75021
C	4.80924	-1.78535	1.31393
H	3.12400	-3.12120	1.49631
H	1.73198	-1.58733	2.90476
H	3.34423	-1.81469	3.61206
H	2.95801	-0.31975	2.73989
H	5.24509	-2.27548	0.43602
H	5.01777	-0.70914	1.24529
H	5.33953	-2.16312	2.19769
H	-0.00006	0.20411	1.94781
Ir	-0.00003	-1.81503	0.09973
H	0.00037	-2.39603	1.80896
H	0.00005	-1.06892	-1.31158
H	0.00005	-3.11474	1.31967
H	-0.00048	-3.21833	-0.79848

92

Gas phase 3-H_4 (dihydrogen dihydride)

C	-1.23820	1.01844	0.35969
C	-2.41768	0.35964	0.00649
C	-3.58274	1.04777	-0.32564
C	-3.59747	2.44965	-0.32376
C	-2.40685	3.11035	0.02872
H	-4.46623	0.48997	-0.62506
H	-2.39606	4.19466	0.02440
C	3.59750	2.44965	-0.32355
C	3.58276	1.04778	-0.32545
C	2.41769	0.35963	0.00658
C	1.23820	1.01845	0.35975
C	1.24763	2.42347	0.38048
C	2.40685	3.11036	0.02885
H	4.46628	0.49000	-0.62482
H	2.39608	4.19466	0.02450
C	-1.24765	2.42347	0.38040

C	-0.00004	3.15981	0.86684
C	-0.00001	0.23995	0.73152
N	4.74357	3.16052	-0.65172
N	-4.74351	3.16052	-0.65204
C	-0.00011	4.63187	0.46117
H	0.87332	5.14832	0.87336
H	0.00009	4.76047	-0.62813
H	-0.87381	5.14813	0.87301
C	-0.00016	3.11494	2.41019
H	-0.89216	3.62109	2.80168
H	-0.00024	2.08717	2.78943
H	0.89179	3.62104	2.80185
C	4.65775	4.58396	-0.86797
H	5.64121	4.96537	-1.15387
H	3.94246	4.85396	-1.66255
H	4.35646	5.11363	0.04668
C	5.89157	2.44416	-1.14801
H	5.68735	1.89662	-2.08407
H	6.70505	3.14899	-1.33752
H	6.25563	1.71607	-0.40904
C	-4.65765	4.58393	-0.86845
H	-3.94211	4.85381	-1.66284
H	-5.64103	4.96528	-1.15475
H	-4.35666	5.11377	0.04621
C	-5.89161	2.44412	-1.14801
H	-6.70513	3.14894	-1.33742
H	-5.68760	1.89646	-2.08404
H	-6.25552	1.71612	-0.40887
P	-2.28532	-1.45706	0.03610
P	2.28526	-1.45708	0.03601
C	-3.30493	-2.07106	-1.39290
C	-3.35566	-3.59467	-1.38349
C	-2.77042	-1.54914	-2.71923
H	-4.32335	-1.68014	-1.24342
H	-3.79828	-4.00093	-0.46610
H	-3.94966	-3.96121	-2.23006
H	-2.34618	-4.01505	-1.48314
H	-2.72927	-0.45433	-2.74267
H	-1.75355	-1.91741	-2.89886
H	-3.41408	-1.88812	-3.54136
C	-3.25305	-1.99184	1.54632
C	-4.75814	-1.76977	1.45888
C	-2.68681	-1.31042	2.78655
H	-3.03917	-3.07060	1.61830
H	-5.22971	-2.31545	0.63339
H	-5.23864	-2.10316	2.38773
H	-4.98810	-0.70200	1.34087
H	-1.60883	-1.48465	2.87853
H	-2.86337	-0.22663	2.75088
H	-3.17881	-1.69899	3.68699
C	3.30474	-2.07089	-1.39325
C	2.76993	-1.54892	-2.71943
C	3.35571	-3.59449	-1.38401
H	4.32310	-1.67978	-1.24386
H	2.72806	-0.45412	-2.74256
H	3.41384	-1.88722	-3.54165
H	1.75330	-1.91776	-2.89922
H	3.79992	-4.00076	-0.46741
H	2.34617	-4.01510	-1.48206
H	3.94837	-3.96085	-2.23160
C	3.25324	-1.99204	1.54601
C	2.68707	-1.31087	2.78638
C	4.75829	-1.76965	1.45846
H	3.03955	-3.07086	1.61771
H	1.60910	-1.48511	2.87841
H	3.17919	-1.69943	3.68675
H	2.86356	-0.22706	2.75080
H	5.22994	-2.31491	0.63276
H	4.98798	-0.70178	1.34078
H	5.23894	-2.10322	2.38716
H	-0.00002	0.14612	1.83214
Ir	0.00003	-1.78330	0.03801
H	-0.00021	-2.30567	1.64192
H	0.00003	-1.07105	-1.48470
H	0.00015	-3.53869	-0.09857
H	0.00028	-3.24560	-0.93918

92

Gas phase 4-H_4 (dihydrogen dihydride)

C	-1.24346	1.03232	0.38108
C	-2.43097	0.36116	0.05782
C	-3.60360	1.04731	-0.25434

C	-3.61698	2.44973	-0.28334	**P**	-2.28300	-1.46701	0.05338
C	-2.41884	3.11819	0.02667	**P**	2.28306	-1.46691	0.05365
H	-4.49648	0.48679	-0.51947	**C**	-3.43159	-2.07151	-1.27963
H	-2.40752	4.20228	-0.00382	**C**	-3.49981	-3.59450	-1.24938
C	3.61681	2.44991	-0.28356	**C**	-2.97685	-1.58010	-2.64750
C	3.60353	1.04748	-0.25441	**H**	-4.42900	-1.65615	-1.06832
C	2.43097	0.36128	0.05787	**H**	-3.94818	-3.98070	-0.32651
C	1.24343	1.03240	0.38108	**H**	-4.10104	-3.96415	-2.08969
C	1.25431	2.43780	0.37499	**H**	-2.49200	-4.02190	-1.33783
C	2.41865	3.11831	0.02648	**H**	-2.84939	-0.49128	-2.67816
H	4.49645	0.48701	-0.51951	**H**	-2.02203	-2.04506	-2.92328
H	2.40726	4.20240	-0.00407	**H**	-3.71307	-1.85891	-3.41190
C	-1.25444	2.43773	0.37506	**C**	-3.09564	-2.03455	1.63733
C	-0.00007	3.17886	0.84296	**C**	-4.59325	-1.75833	1.69672
C	0.00000	0.26234	0.72457	**C**	-2.39964	-1.41333	2.84243
N	4.77042	3.15477	-0.60596	**H**	-2.91310	-3.12061	1.64989
N	-4.77068	3.15453	-0.60555	**H**	-5.15799	-2.26295	0.90458
C	-0.00011	4.64469	0.41631	**H**	-4.99864	-2.10173	2.65704
H	0.87364	5.16734	0.82003	**H**	-4.79177	-0.68022	1.62598
H	-0.00018	4.75751	-0.67490	**H**	-1.32800	-1.63809	2.85185
H	-0.87381	5.16733	0.82015	**H**	-2.52205	-0.32136	2.84485
C	-0.00000	3.15142	2.38681	**H**	-2.84028	-1.79955	3.77006
H	-0.89227	3.66077	2.77377	**C**	3.43191	-2.07155	-1.27908
H	0.00005	2.12560	2.77248	**C**	2.97730	-1.58038	-2.64709
H	0.89226	3.66084	2.77370	**C**	3.50024	-3.59451	-1.24858
C	4.68194	4.57059	-0.86757	**H**	4.42926	-1.65608	-1.06768
H	5.67034	4.94954	-1.13963	**H**	2.84979	-0.49157	-2.67793
H	3.98459	4.81388	-1.68684	**H**	3.71360	-1.85929	-3.41137
H	4.35595	5.12440	0.02365	**H**	2.02253	-2.04543	-2.92286
C	5.91560	2.42861	-1.09530	**H**	3.94838	-3.98054	-0.32553
H	5.70794	1.86798	-2.02319	**H**	2.49248	-4.02200	-1.33723
H	6.73017	3.12899	-1.29652	**H**	4.10173	-3.96425	-2.08867
H	6.28054	1.71090	-0.34736	**C**	3.09551	-2.03415	1.63783
C	-4.68244	4.57043	-0.86671	**C**	2.39927	-1.41291	2.84277
H	-3.98535	4.81411	-1.68609	**C**	4.59308	-1.75774	1.69740
H	-5.67097	4.94937	-1.13835	**H**	2.91311	-3.12024	1.65048
H	-4.35628	5.12398	0.02461	**H**	1.32766	-1.63781	2.85207
C	-5.91581	2.42834	-1.09496	**H**	2.83984	-1.79899	3.77050
H	-6.73043	3.12867	-1.29608	**H**	2.52154	-0.32092	2.84511
H	-5.70811	1.86785	-2.02291	**H**	5.15800	-2.26242	0.90543
H	-6.28069	1.71049	-0.34710	**H**	4.79147	-0.67961	1.62651

H	4.99838	-2.10092	2.65785
H	0.00001	0.09933	1.81648
Ir	0.00011	-1.77462	-0.13832
H	0.00001	-2.43019	1.31477
H	-0.00004	-0.78105	-1.65701
H	-0.00006	-3.37117	-0.60797
H	0.00002	-1.60491	-1.91678

92

Gas phase transition state for 1-H_4 to 2-H_4 (tetrahydride to dihydrogen dihydride)

C	-1.23707	1.03184	0.42548
C	-2.40602	0.36806	0.03741
C	-3.56518	1.05671	-0.31935
C	-3.58585	2.45803	-0.31296
C	-2.40150	3.12266	0.05415
H	-4.43822	0.49821	-0.64655
H	-2.39120	4.20700	0.04107
C	3.58583	2.45808	-0.31292
C	3.56518	1.05677	-0.31931
C	2.40602	0.36810	0.03744
C	1.23706	1.03186	0.42550
C	1.24875	2.43862	0.42966
C	2.40145	3.12270	0.05417
H	4.43823	0.49828	-0.64650
H	2.39113	4.20703	0.04109
C	-1.24878	2.43860	0.42964
C	-0.00003	3.17879	0.91329
C	-0.00000	0.27074	0.82372
N	4.73016	3.16623	-0.65690
N	-4.73018	3.16615	-0.65697
C	-0.00003	4.64683	0.49292
H	0.87371	5.16716	0.89973
H	-0.00003	4.76499	-0.59761
H	-0.87379	5.16714	0.89973
C	-0.00003	3.15239	2.45662
H	-0.89180	3.66386	2.84174
H	-0.00003	2.12992	2.84859
H	0.89172	3.66387	2.84175
C	4.64058	4.58744	-0.88693
H	5.62195	4.96748	-1.18192
H	3.92007	4.84954	-1.67968
H	4.34441	5.12495	0.02458
C	5.86483	2.44641	-1.17824
H	5.64394	1.91046	-2.11741
H	6.68148	3.14686	-1.37080
H	6.23284	1.70775	-0.45203
C	-4.64072	4.58740	-0.88672
H	-3.92016	4.84971	-1.67934
H	-5.62210	4.96740	-1.18176
H	-4.34469	5.12479	0.02492
C	-5.86494	2.44632	-1.17809
H	-6.68157	3.14678	-1.37067
H	-5.64417	1.91024	-2.11721
H	-6.23292	1.70776	-0.45175
P	-2.27920	-1.45511	0.01723
P	2.27923	-1.45508	0.01726
C	-3.23081	-2.02324	-1.47314
C	-3.30047	-3.54600	-1.49444
C	-2.60039	-1.48900	-2.75231
H	-4.24865	-1.61328	-1.38024
H	-3.84259	-3.95909	-0.63518
H	-3.81006	-3.88895	-2.40365
H	-2.28842	-3.97181	-1.49239
H	-2.52001	-0.39577	-2.74686
H	-1.59079	-1.89756	-2.88165
H	-3.20549	-1.78510	-3.61882
C	-3.29930	-2.04090	1.47208
C	-4.79794	-1.79650	1.34119
C	-2.77568	-1.41231	2.75852
H	-3.10371	-3.12493	1.50576
H	-5.24114	-2.29017	0.46887
H	-5.31736	-2.17470	2.23110
H	-5.01174	-0.72124	1.27297
H	-1.70405	-1.59292	2.89726
H	-2.93704	-0.32595	2.75298
H	-3.30801	-1.82477	3.62470
C	3.23087	-2.02319	-1.47309
C	2.60046	-1.48895	-2.75228
C	3.30056	-3.54595	-1.49440
H	4.24871	-1.61321	-1.38018
H	2.52006	-0.39572	-2.74683

H	3.20558	-1.78505	-3.61878
H	1.59087	-1.89753	-2.88163
H	3.84267	-3.95903	-0.63513
H	2.28850	-3.97177	-1.49236
H	3.81016	-3.88889	-2.40361
C	3.29933	-2.04086	1.47212
C	2.77568	-1.41227	2.75855
C	4.79796	-1.79644	1.34125
H	3.10375	-3.12489	1.50580
H	1.70405	-1.59290	2.89728
H	3.30800	-1.82473	3.62474
H	2.93703	-0.32591	2.75302
H	5.24118	-2.29011	0.46893
H	5.01175	-0.72118	1.27303
H	5.31737	-2.17463	2.23117
H	-0.00001	0.19844	1.92473
Ir	0.00002	-1.81114	0.08797
H	0.00001	-2.29004	1.71278
H	0.00002	-1.00417	-1.32890
H	0.00002	-3.18108	1.04322
H	0.00004	-3.10497	-0.94290

92

Gas phase transition state for 1-H_4 to 3-H_4 (tetrahydride to dihydrogen dihydride)

C	-1.23886	1.02405	0.37123
C	-2.41731	0.36243	0.01696
C	-3.58311	1.04929	-0.31635
C	-3.59922	2.45119	-0.31764
C	-2.40852	3.11417	0.03054
H	-4.46565	0.49033	-0.61637
H	-2.39833	4.19848	0.02097
C	3.59922	2.45119	-0.31764
C	3.58311	1.04929	-0.31636
C	2.41731	0.36242	0.01696
C	1.23886	1.02404	0.37123
C	1.24897	2.42930	0.38489
C	2.40853	3.11417	0.03053
H	4.46565	0.49033	-0.61638
H	2.39834	4.19848	0.02097
C	-1.24897	2.42931	0.38489
C	0.00000	3.16803	0.86628
C	0.00000	0.25101	0.74557
N	4.74650	3.16014	-0.64662
N	-4.74650	3.16015	-0.64661
C	0.00000	4.63740	0.45083
H	0.87353	5.15661	0.85933
H	0.00000	4.75870	-0.63932
H	-0.87352	5.15661	0.85933
C	0.00000	3.13316	2.40981
H	-0.89196	3.64179	2.79818
H	0.00000	2.10782	2.79535
H	0.89197	3.64179	2.79817
C	4.66131	4.58254	-0.87003
H	5.64544	4.96241	-1.15569
H	3.94770	4.84891	-1.66738
H	4.35827	5.11662	0.04145
C	5.89391	2.44127	-1.14058
H	5.69027	1.89285	-2.07630
H	6.70887	3.14450	-1.32970
H	6.25566	1.71356	-0.40014
C	-4.66130	4.58254	-0.87004
H	-3.94769	4.84890	-1.66739
H	-5.64544	4.96242	-1.15570
H	-4.35825	5.11663	0.04143
C	-5.89390	2.44127	-1.14060
H	-6.70887	3.14450	-1.32972
H	-5.69025	1.89287	-2.07632
H	-6.25566	1.71356	-0.40017
P	-2.28616	-1.45642	0.03645
P	2.28616	-1.45642	0.03645
C	-3.29498	-2.06284	-1.40214
C	-3.34205	-3.58668	-1.40062
C	-2.74964	-1.53300	-2.72108
H	-4.31487	-1.67334	-1.25894
H	-3.79997	-3.99785	-0.49298
H	-3.92081	-3.95010	-2.25898
H	-2.32955	-4.00328	-1.48334
H	-2.70678	-0.43806	-2.73747
H	-1.73276	-1.90334	-2.89629
H	-3.38802	-1.86557	-3.54984
C	-3.25617	-2.00467	1.53930

C	-4.76131	-1.78455	1.44595
C	-2.69857	-1.33041	2.78729
H	-3.04037	-3.08343	1.60345
H	-5.22741	-2.32339	0.61298
H	-5.24588	-2.12741	2.36916
H	-4.99249	-0.71613	1.33660
H	-1.62118	-1.50304	2.88713
H	-2.87588	-0.24667	2.75689
H	-3.19649	-1.72486	3.68186
C	3.29498	-2.06284	-1.40215
C	2.74963	-1.53300	-2.72108
C	3.34204	-3.58669	-1.40062
H	4.31487	-1.67335	-1.25894
H	2.70677	-0.43806	-2.73748
H	3.38801	-1.86557	-3.54984
H	1.73275	-1.90335	-2.89629
H	3.79997	-3.99785	-0.49299
H	2.32955	-4.00329	-1.48334
H	3.92080	-3.95011	-2.25899
C	3.25617	-2.00467	1.53930
C	2.69857	-1.33041	2.78729
C	4.76131	-1.78455	1.44594
H	3.04037	-3.08343	1.60344
H	1.62119	-1.50305	2.88713
H	3.19649	-1.72486	3.68186
H	2.87588	-0.24667	2.75689
H	5.22740	-2.32339	0.61298
H	4.99249	-0.71613	1.33659
H	5.24588	-2.12741	2.36916
H	0.00000	0.15682	1.84555
Ir	-0.00000	-1.79084	0.03811
H	-0.00000	-2.26085	1.64954
H	-0.00000	-1.01992	-1.44981
H	-0.00000	-3.47139	0.00733
H	-0.00000	-3.10751	-1.00036

92

Gas phase transition state for 1-H_4 to 4-H_4 (tetrahydride to dihydrogen dihydride)

C	-1.24382	1.03397	0.36514
C	-2.43084	0.36209	0.04737
C	-3.60566	1.04614	-0.26021
C	-3.62109	2.44858	-0.28673
C	-2.42230	3.11806	0.01828
H	-4.49810	0.48446	-0.52423
H	-2.41293	4.20216	-0.01087
C	3.62104	2.44865	-0.28670
C	3.60564	1.04622	-0.26016
C	2.43084	0.36214	0.04742
C	1.24380	1.03399	0.36516
C	1.25497	2.43905	0.36003
C	2.42223	3.11811	0.01830
H	4.49810	0.48455	-0.52416
H	2.41283	4.20220	-0.01087
C	-1.25503	2.43903	0.36001
C	-0.00004	3.18288	0.82218
C	-0.00001	0.26788	0.71467
N	4.77711	3.15216	-0.60111
N	-4.77717	3.15206	-0.60115
C	-0.00005	4.64538	0.38356
H	0.87337	5.17164	0.78309
H	-0.00005	4.74883	-0.70850
H	-0.87349	5.17163	0.78309
C	-0.00005	3.16779	2.36624
H	-0.89230	3.68019	2.74912
H	-0.00004	2.14541	2.76084
H	0.89219	3.68021	2.74912
C	4.69398	4.56915	-0.85777
H	5.68439	4.94599	-1.12529
H	4.00041	4.81700	-1.67874
H	4.36633	5.12114	0.03409
C	5.92802	2.42507	-1.07503
H	5.73215	1.86423	-2.00527
H	6.74565	3.12473	-1.26596
H	6.28252	1.70728	-0.32193
C	-4.69413	4.56908	-0.85764
H	-4.00054	4.81707	-1.67853
H	-5.68456	4.94587	-1.12519
H	-4.36658	5.12101	0.03431
C	-5.92816	2.42495	-1.07484
H	-6.74580	3.12461	-1.26571
H	-5.73243	1.86404	-2.00506

H	-6.28257	1.70722	-0.32163
P	-2.28708	-1.46456	0.05200
P	2.28713	-1.46451	0.05205
C	-3.40073	-2.07016	-1.30804
C	-3.44463	-3.59430	-1.29801
C	-2.94367	-1.54898	-2.66396
H	-4.40731	-1.67522	-1.10101
H	-3.87868	-3.99988	-0.37645
H	-4.04681	-3.96213	-2.13838
H	-2.43168	-4.00559	-1.39941
H	-2.84521	-0.45717	-2.67806
H	-1.97310	-1.98048	-2.93707
H	-3.66512	-1.83773	-3.43874
C	-3.13432	-2.02590	1.62040
C	-4.63969	-1.78802	1.63479
C	-2.48859	-1.36827	2.83452
H	-2.92395	-3.10650	1.65547
H	-5.17026	-2.32116	0.83775
H	-5.06121	-2.12532	2.59030
H	-4.86444	-0.71682	1.54059
H	-1.41090	-1.55991	2.87413
H	-2.64582	-0.28095	2.81960
H	-2.94069	-1.75756	3.75525
C	3.40082	-2.07011	-1.30794
C	2.94381	-1.54894	-2.66388
C	3.44475	-3.59425	-1.29790
H	4.40740	-1.67516	-1.10088
H	2.84535	-0.45713	-2.67800
H	3.66528	-1.83770	-3.43864
H	1.97324	-1.98044	-2.93700
H	3.87877	-3.99983	-0.37633
H	2.43180	-4.00555	-1.39932
H	4.04694	-3.96208	-2.13826
C	3.13434	-2.02583	1.62049
C	2.48855	-1.36820	2.83458
C	4.63970	-1.78792	1.63492
H	2.92398	-3.10643	1.65556
H	1.41087	-1.55987	2.87417
H	2.94065	-1.75748	3.75533
H	2.64576	-0.28088	2.81966
H	5.17030	-2.32105	0.83790
H	4.86443	-0.71671	1.54071
H	5.06119	-2.12518	2.59044
H	-0.00002	0.12272	1.80898
Ir	0.00003	-1.78408	-0.09631
H	0.00002	-2.31118	1.44416
H	0.00004	-0.91003	-1.55406
H	-0.00002	-3.42772	-0.30719
H	0.00006	-1.99699	-1.74780

92

Gas phase transition state 3-H_4 to Ir-H_2 (H_2 loss)

C	-1.24502	1.04420	0.24318
C	-2.43349	0.36131	-0.03337
C	-3.60630	1.03696	-0.35456
C	-3.62128	2.43910	-0.41933
C	-2.42786	3.11720	-0.11640
H	-4.50404	0.46986	-0.58588
H	-2.42586	4.20097	-0.14455
C	3.62132	2.43905	-0.41935
C	3.60632	1.03691	-0.35457
C	2.43350	0.36127	-0.03336
C	1.24505	1.04418	0.24318
C	1.25253	2.44639	0.21738
C	2.42791	3.11716	-0.11643
H	4.50405	0.46979	-0.58589
H	2.42592	4.20094	-0.14458
C	-1.25248	2.44641	0.21739
C	0.00003	3.20341	0.65984
C	0.00001	0.28184	0.60579
N	4.77346	3.12836	-0.77188
N	-4.77341	3.12843	-0.77184
C	0.00004	4.65219	0.17640
H	0.87285	5.19119	0.55943
H	0.00003	4.72065	-0.91815
H	-0.87277	5.19120	0.55944
C	0.00004	3.23355	2.20374
H	-0.89211	3.75651	2.57213
H	0.00003	2.22325	2.62933
H	0.89219	3.75650	2.57212
C	4.80334	4.56491	-0.64451

H	5.78017	4.93538	-0.96545
H	4.04910	5.03702	-1.28818
H	4.62798	4.91101	0.38846
C	6.02368	2.40984	-0.82265
H	6.01530	1.64386	-1.61037
H	6.83268	3.10629	-1.05626
H	6.26744	1.90787	0.12970
C	-4.80326	4.56499	-0.64448
H	-4.04903	5.03708	-1.28817
H	-5.78010	4.93547	-0.96542
H	-4.62789	4.91109	0.38847
C	-6.02364	2.40993	-0.82264
H	-6.83264	3.10639	-1.05624
H	-6.01527	1.64397	-1.61038
H	-6.26742	1.90794	0.12970
P	-2.28146	-1.46097	0.05124
P	2.28144	-1.46100	0.05126
C	-3.31849	-2.11191	-1.34827
C	-3.45790	-3.62652	-1.24424
C	-2.71134	-1.70339	-2.68421
H	-4.31556	-1.65345	-1.25450
H	-3.99161	-3.94050	-0.33964
H	-4.01122	-4.01614	-2.10806
H	-2.47179	-4.10909	-1.23548
H	-2.60285	-0.61610	-2.76928
H	-1.71250	-2.14179	-2.80409
H	-3.34400	-2.05281	-3.51036
C	-3.21403	-1.95579	1.59078
C	-4.69573	-1.60530	1.59504
C	-2.50949	-1.36916	2.80790
H	-3.08709	-3.05000	1.61732
H	-5.24509	-2.05375	0.75826
H	-5.16402	-1.95976	2.52242
H	-4.83850	-0.51695	1.55221
H	-1.45400	-1.66733	2.83020
H	-2.56316	-0.27116	2.80003
H	-2.98876	-1.71809	3.73128
C	3.31848	-2.11196	-1.34823
C	2.71140	-1.70339	-2.68418
C	3.45781	-3.62659	-1.24423
H	4.31558	-1.65356	-1.25442
H	2.60297	-0.61609	-2.76924
H	3.34407	-2.05283	-3.51031
H	1.71255	-2.14173	-2.80411
H	3.99146	-3.94063	-0.33962
H	2.47168	-4.10910	-1.23553
H	4.01115	-4.01621	-2.10804
C	3.21399	-1.95580	1.59082
C	2.50939	-1.36920	2.80793
C	4.69567	-1.60524	1.59514
H	3.08710	-3.05001	1.61735
H	1.45391	-1.66741	2.83020
H	2.98865	-1.71812	3.73132
H	2.56303	-0.27120	2.80007
H	5.24509	-2.05363	0.75837
H	4.83839	-0.51688	1.55234
H	5.16395	-1.95970	2.52253
H	0.00001	0.13523	1.70404
Ir	-0.00002	-1.74541	0.02634
H	-0.00004	-3.06733	1.15502
H	-0.00000	-0.89044	-1.37013
H	-0.00007	-4.11750	-1.05290
H	0.00025	-4.16128	-1.80345

90

Gas phase Ir-H_2

C	-1.24853	1.03124	0.37094
C	-2.43781	0.36080	0.05781
C	-3.61271	1.04789	-0.24292
C	-3.62836	2.45011	-0.26048
C	-2.42661	3.11725	0.03774
H	-4.50509	0.48799	-0.51046
H	-2.41795	4.20155	0.01579
C	3.62834	2.45014	-0.26048
C	3.61270	1.04792	-0.24292
C	2.43780	0.36083	0.05782
C	1.24851	1.03125	0.37094
C	1.25676	2.43649	0.36734
C	2.42658	3.11727	0.03775
H	4.50508	0.48804	-0.51046
H	2.41789	4.20157	0.01580
C	-1.25679	2.43648	0.36734

C	-0.00002	3.17927	0.82700
C	-0.00000	0.25998	0.69315
N	4.78726	3.15664	-0.55916
N	-4.78728	3.15663	-0.55916
C	-0.00001	4.64175	0.38785
H	0.87318	5.16862	0.78695
H	-0.00002	4.74441	-0.70429
H	-0.87318	5.16864	0.78698
C	-0.00002	3.16330	2.37080
H	-0.89249	3.67466	2.75466
H	-0.00002	2.14000	2.76279
H	0.89246	3.67466	2.75466
C	4.70272	4.57149	-0.82676
H	5.69413	4.94867	-1.09025
H	4.01464	4.81111	-1.65471
H	4.36718	5.13010	0.05815
C	5.94930	2.43171	-1.00777
H	5.78005	1.87916	-1.94825
H	6.77355	3.13135	-1.16843
H	6.27990	1.70655	-0.25076
C	-4.70269	4.57147	-0.82674
H	-4.01460	4.81108	-1.65469
H	-5.69409	4.94870	-1.09022
H	-4.36712	5.13005	0.05819
C	-5.94936	2.43174	-1.00774
H	-6.77358	3.13142	-1.16840
H	-5.78014	1.87917	-1.94821
H	-6.27998	1.70660	-0.25071
P	-2.27998	-1.46633	0.01466
P	2.27999	-1.46631	0.01467
Ir	0.00001	-1.79972	0.06350
C	-3.22644	-1.99363	-1.49460
C	-3.31664	-3.51332	-1.56002
C	-2.55179	-1.42610	-2.73785
H	-4.24127	-1.57291	-1.41370
H	-3.89165	-3.93847	-0.72871
H	-3.80427	-3.82476	-2.49246
H	-2.31396	-3.96011	-1.53942
H	-2.49843	-0.33174	-2.70974
H	-1.52575	-1.80794	-2.82401
H	-3.10449	-1.71994	-3.63950
C	-3.27218	-2.11333	1.45662
C	-4.74609	-1.73329	1.45450
C	-2.59409	-1.67786	2.75055
H	-3.17102	-3.20636	1.36351
H	-5.27126	-2.06663	0.55098
H	-5.25442	-2.18570	2.31594
H	-4.86638	-0.64502	1.53692
H	-1.54734	-2.00608	2.78114
H	-2.61020	-0.58347	2.84934
H	-3.11648	-2.09837	3.61925
C	3.22646	-1.99361	-1.49458
C	2.55179	-1.42610	-2.73784
C	3.31669	-3.51329	-1.55999
H	4.24129	-1.57286	-1.41369
H	2.49841	-0.33174	-2.70974
H	3.10451	-1.71993	-3.63949
H	1.52577	-1.80796	-2.82400
H	3.89171	-3.93842	-0.72867
H	2.31401	-3.96010	-1.53939
H	3.80433	-3.82473	-2.49242
C	3.27219	-2.11331	1.45663
C	2.59409	-1.67785	2.75056
C	4.74610	-1.73326	1.45453
H	3.17103	-3.20634	1.36352
H	1.54734	-2.00607	2.78115
H	3.11647	-2.09836	3.61927
H	2.61019	-0.58345	2.84936
H	5.27128	-2.06659	0.55100
H	4.86638	-0.64498	1.53696
H	5.25443	-2.18567	2.31597
H	0.00001	-2.90232	-1.09225
H	-0.00000	0.05330	1.78687
H	0.00001	-3.38601	0.36535

90

Gas phase Ir-H_3

C	1.23487	1.02696	-0.02216
C	2.46612	0.33542	-0.04615
C	3.67791	0.99084	-0.12353
C	3.72211	2.40203	-0.14089
C	2.49924	3.08897	-0.09665

H	4.59835	0.41601	-0.18094	**Ir**	-0.00000	-1.74700	-0.01833
H	2.51023	4.17532	-0.10363	**H**	-0.00000	-3.42084	-0.23064
C	-3.72208	2.40206	-0.14104	**H**	0.00003	-1.96368	-1.65718
C	-3.67789	0.99087	-0.12369	**H**	-0.00004	-2.41283	1.49866
C	-2.46611	0.33544	-0.04629	**C**	3.11834	-1.98012	1.64687
C	-1.23485	1.02698	-0.02225	**C**	2.55950	-1.15611	2.80183
C	-1.26914	2.43200	-0.05459	**C**	4.64084	-1.93027	1.64588
C	-2.49921	3.08898	-0.09674	**H**	2.78570	-3.02252	1.77294
H	-4.59833	0.41604	-0.18109	**H**	1.46379	-1.16907	2.80974
H	-2.51020	4.17534	-0.10367	**H**	2.91898	-1.55671	3.75801
C	1.26917	2.43198	-0.05449	**H**	2.89201	-0.11199	2.73121
C	0.00003	3.27517	-0.03219	**H**	5.09522	-2.55577	0.86924
C	0.00001	0.24000	0.01675	**H**	5.00364	-0.90143	1.51635
N	-4.92518	3.07251	-0.19866	**H**	5.02140	-2.28195	2.61371
N	4.92520	3.07248	-0.19844	**C**	3.36603	-2.15588	-1.29823
C	-0.00001	4.11806	1.25695	**C**	2.94435	-1.60724	-2.65459
H	-0.88569	4.76152	1.31028	**C**	3.31257	-3.67933	-1.28369
H	-0.00007	3.46647	2.13868	**H**	4.39196	-1.81924	-1.08003
H	0.88571	4.76147	1.31036	**H**	2.99458	-0.51276	-2.69029
C	0.00012	4.20047	-1.26292	**H**	3.59946	-2.00535	-3.44012
H	0.88283	4.84890	-1.27569	**H**	1.91352	-1.90369	-2.88303
H	0.00006	3.60910	-2.18578	**H**	3.66054	-4.10652	-0.33504
H	-0.88243	4.84910	-1.27570	**H**	2.28172	-4.02046	-1.44251
C	-4.94754	4.51428	-0.15329	**H**	3.93952	-4.08972	-2.08550
H	-5.98031	4.86330	-0.22193	**C**	-3.11843	-1.98005	1.64673
H	-4.51615	4.91157	0.77916	**C**	-4.64094	-1.93025	1.64561
H	-4.39223	4.95420	-0.99408	**C**	-2.55971	-1.15596	2.80169
C	-6.16212	2.33138	-0.12975	**H**	-2.78577	-3.02244	1.77286
H	-6.23720	1.73036	0.79061	**H**	-5.09523	-2.55576	0.86893
H	-7.00288	3.02848	-0.14366	**H**	-5.02157	-2.28192	2.61341
H	-6.28127	1.65128	-0.98552	**H**	-5.00375	-0.90141	1.51602
C	4.94757	4.51426	-0.15370	**H**	-1.46401	-1.16890	2.80969
H	4.51600	4.91193	0.77850	**H**	-2.89223	-0.11186	2.73098
H	5.98035	4.86325	-0.22225	**H**	-2.91927	-1.55652	3.75786
H	4.39241	4.95386	-0.99477	**C**	-3.36600	-2.15586	-1.29836
C	6.16216	2.33133	-0.13004	**C**	-3.31257	-3.67931	-1.28379
H	7.00291	3.02845	-0.14377	**C**	-2.94426	-1.60726	-2.65471
H	6.23737	1.72998	0.79008	**H**	-4.39193	-1.81921	-1.08019
H	6.28121	1.65155	-0.98608	**H**	-3.66058	-4.10648	-0.33513
P	2.27499	-1.49006	0.05012	**H**	-3.93950	-4.08971	-2.08560
P	-2.27499	-1.49004	0.05002	**H**	-2.28172	-4.02046	-1.44256

H	-2.99448	-0.51278	-2.69044
H	-1.91344	-1.90373	-2.88312
H	-3.59937	-2.00537	-3.44025

88

Gas phase Ir-H

C	-1.23364	1.01904	0.00789
C	-2.46653	0.32728	-0.03336
C	-3.67574	0.98508	-0.13287
C	-3.71943	2.39582	-0.14463
C	-2.49675	3.08301	-0.08161
H	-4.59560	0.41135	-0.20459
H	-2.50805	4.16930	-0.08328
C	3.71943	2.39583	-0.14463
C	3.67573	0.98509	-0.13287
C	2.46652	0.32728	-0.03335
C	1.23363	1.01904	0.00789
C	1.26846	2.42569	-0.02842
C	2.49674	3.08301	-0.08161
H	4.59560	0.41136	-0.20459
H	2.50804	4.16931	-0.08328
C	-1.26847	2.42569	-0.02843
C	-0.00000	3.26814	0.01336
C	-0.00000	0.22901	0.06696
N	4.92049	3.06752	-0.21368
N	-4.92050	3.06751	-0.21368
C	0.00001	4.22833	-1.19010
H	0.88165	4.87793	-1.18483
H	-0.00000	3.66414	-2.12979
H	-0.88162	4.87795	-1.18483
C	-0.00000	4.07372	1.32650
H	-0.88657	4.71446	1.39770
H	-0.00001	3.39643	2.18874
H	0.88658	4.71445	1.39771
C	4.94355	4.50925	-0.16017
H	5.97561	4.85846	-0.23762
H	4.37944	4.95447	-0.99223
H	4.52244	4.90069	0.77929
C	6.15913	2.32668	-0.16901
H	6.26433	1.65150	-1.03028
H	6.99908	3.02447	-0.19262
H	6.24900	1.72051	0.74645
C	-4.94357	4.50924	-0.16017
H	-4.37947	4.95446	-0.99223
H	-5.97563	4.85844	-0.23762
H	-4.52246	4.90067	0.77929
C	-6.15913	2.32665	-0.16900
H	-6.99909	3.02443	-0.19262
H	-6.26433	1.65147	-1.03026
H	-6.24899	1.72049	0.74646
P	-2.26390	-1.50120	0.03639
P	2.26390	-1.50120	0.03639
Ir	0.00000	-1.73757	0.00958
C	-3.30301	-2.12982	-1.37097
C	-3.39404	-3.64992	-1.31237
C	-2.67255	-1.67230	-2.68105
H	-4.31046	-1.69305	-1.27911
H	-3.93846	-4.00647	-0.42955
H	-3.91350	-4.03393	-2.19972
H	-2.38753	-4.08841	-1.28841
H	-2.60861	-0.57940	-2.74643
H	-1.65268	-2.07147	-2.76750
H	-3.25959	-2.03291	-3.53574
C	-3.15263	-2.04494	1.58504
C	-4.65420	-1.79785	1.63087
C	-2.45955	-1.43057	2.79582
H	-2.96128	-3.13018	1.59259
H	-5.18502	-2.21460	0.76617
H	-5.08273	-2.25561	2.53218
H	-4.87181	-0.72259	1.68190
H	-1.38483	-1.64834	2.78911
H	-2.57939	-0.33835	2.79946
H	-2.89488	-1.81827	3.72592
C	3.30301	-2.12982	-1.37097
C	2.67254	-1.67232	-2.68105
C	3.39406	-3.64991	-1.31236
H	4.31045	-1.69303	-1.27912
H	2.60858	-0.57942	-2.74644
H	3.25958	-2.03292	-3.53574
H	1.65267	-2.07150	-2.76750
H	3.93849	-4.00645	-0.42954
H	2.38755	-4.08842	-1.28839

H	3.91351	-4.03392	-2.19971
C	3.15263	-2.04494	1.58504
C	2.45958	-1.43054	2.79582
C	4.65421	-1.79789	1.63085
H	2.96126	-3.13017	1.59260
H	1.38486	-1.64828	2.78912
H	2.89490	-1.81824	3.72592
H	2.57945	-0.33833	2.79945
H	5.18501	-2.21466	0.76615
H	4.87184	-0.72262	1.68188
H	5.08273	-2.25565	2.53216
H	0.00000	-3.42805	-0.33673

88

Gas phase Ir-[]

C	-1.24092	0.98324	0.36662
C	-2.42348	0.32047	0.02637
C	-3.58436	1.01142	-0.31109
C	-3.59972	2.41378	-0.30848
C	-2.40870	3.07532	0.04070
H	-4.46880	0.45394	-0.60798
H	-2.39939	4.15961	0.03997
C	3.59967	2.41257	-0.31164
C	3.58406	1.01018	-0.31373
C	2.42319	0.31967	0.02459
C	1.24104	0.98285	0.36554
C	1.24730	2.38799	0.38207
C	2.40922	3.07461	0.03868
H	4.46833	0.45250	-0.61080
H	2.40045	4.15892	0.03810
C	-1.24672	2.38836	0.38323
C	0.00062	3.12615	0.86501
C	0.00010	0.19992	0.72661
N	4.74590	3.12118	-0.63597
N	-4.74646	3.12309	-0.63101
C	0.00064	4.59705	0.45499
H	0.87429	5.11469	0.86498
H	0.00015	4.72220	-0.63468
H	-0.87248	5.11495	0.86579
C	0.00135	3.08420	2.40846
H	-0.89055	3.59040	2.80013
H	0.00142	2.05616	2.78717
H	0.89376	3.59018	2.79925
C	4.67654	4.55052	-0.81166
H	5.66179	4.92779	-1.09652
H	3.95911	4.84889	-1.59360
H	4.38718	5.06032	0.11864
C	5.91010	2.40505	-1.09275
H	5.73081	1.84391	-2.02533
H	6.72327	3.11217	-1.27436
H	6.26078	1.68843	-0.33569
C	-4.67294	4.55093	-0.81826
H	-3.95787	4.84138	-1.60544
H	-5.65836	4.92932	-1.10115
H	-4.37816	5.06635	0.10704
C	-5.90769	2.40719	-1.09607
H	-6.72193	3.11372	-1.27538
H	-5.72477	1.85169	-2.03143
H	-6.25886	1.68581	-0.34401
P	-2.26958	-1.49915	0.01485
P	2.26887	-1.49991	0.01390
Ir	-0.00040	-1.77580	0.11189
C	-3.20506	-2.04593	-1.49966
C	-3.24722	-3.56812	-1.55912
C	-2.54122	-1.46934	-2.74376
H	-4.23354	-1.65886	-1.42625
H	-3.77508	-4.01169	-0.70615
H	-3.75350	-3.90328	-2.47337
H	-2.22795	-3.97893	-1.57530
H	-2.54296	-0.37353	-2.73686
H	-1.49425	-1.79716	-2.80109
H	-3.06248	-1.80885	-3.64850
C	-3.31996	-2.09271	1.44651
C	-4.79903	-1.73859	1.38480
C	-2.68817	-1.59369	2.74097
H	-3.20508	-3.18826	1.40843
H	-5.29297	-2.12380	0.48422
H	-5.32556	-2.15787	2.25238
H	-4.94016	-0.64987	1.41255
H	-1.62964	-1.87939	2.79790
H	-2.74561	-0.49790	2.80356
H	-3.21312	-2.00515	3.61263

C	3.20370	-2.04763	-1.50066
C	2.53943	-1.47167	-2.74482
C	3.24571	-3.56985	-1.55932
H	4.23224	-1.66060	-1.42785
H	2.54094	-0.37585	-2.73836
H	3.06053	-1.81143	-3.64956
H	1.49252	-1.79972	-2.80176
H	3.77408	-4.01301	-0.70644
H	2.22641	-3.98062	-1.57462
H	3.75137	-3.90556	-2.47371
C	3.31971	-2.09302	1.44544
C	2.68842	-1.59348	2.73995
C	4.79878	-1.73901	1.38306
H	3.20475	-3.18858	1.40781
H	1.62991	-1.87912	2.79740
H	3.21370	-2.00460	3.61157
H	2.74591	-0.49766	2.80208
H	5.29239	-2.12461	0.48246
H	4.93999	-0.65028	1.41030
H	5.32559	-2.15797	2.25064
H	0.00047	0.04300	1.82780

88

Gas Phase transition state for Ir-H to Ir-[] (1,2-hydride shift)

C	-1.23410	0.99536	0.14137
C	-2.46024	0.31793	-0.03171
C	-3.64355	0.99346	-0.30158
C	-3.66620	2.39477	-0.36826
C	-2.45483	3.07129	-0.12710
H	-4.55239	0.42519	-0.47916
H	-2.46094	4.15588	-0.13209
C	3.66620	2.39477	-0.36827
C	3.64355	0.99346	-0.30160
C	2.46024	0.31792	-0.03173
C	1.23410	0.99536	0.14136
C	1.25702	2.41299	0.11832
C	2.45483	3.07129	-0.12710
H	4.55239	0.42519	-0.47919
H	2.46095	4.15588	-0.13209
C	-1.25701	2.41300	0.11832
C	0.00000	3.17726	0.52669
C	0.00000	0.26253	0.31731
N	4.84094	3.08696	-0.65449
N	-4.84093	3.08697	-0.65448
C	0.00001	4.61317	0.00465
H	0.87162	5.16509	0.37124
H	0.00000	4.64891	-1.09144
H	-0.87160	5.16509	0.37124
C	0.00001	3.23678	2.07173
H	-0.89325	3.76457	2.43099
H	0.00001	2.22836	2.50193
H	0.89326	3.76457	2.43099
C	4.87318	4.51615	-0.46111
H	5.86540	4.89308	-0.72288
H	4.15199	5.02090	-1.11718
H	4.65248	4.81979	0.57725
C	6.08913	2.36648	-0.60247
H	6.12979	1.58272	-1.37120
H	6.91432	3.05545	-0.80043
H	6.26942	1.88478	0.37549
C	-4.87317	4.51616	-0.46113
H	-4.15197	5.02090	-1.11720
H	-5.86539	4.89309	-0.72291
H	-4.65247	4.81981	0.57723
C	-6.08913	2.36649	-0.60246
H	-6.91431	3.05546	-0.80042
H	-6.12979	1.58272	-1.37118
H	-6.26941	1.88480	0.37550
P	-2.29872	-1.49655	0.03106
P	2.29872	-1.49656	0.03102
Ir	0.00000	-1.73455	0.22319
C	-3.11286	-2.07606	-1.53880
C	-3.19850	-3.59627	-1.57859
C	-2.34639	-1.53825	-2.74051
H	-4.12950	-1.65163	-1.54855
H	-3.80054	-4.01034	-0.76067
H	-3.65008	-3.92787	-2.52242
H	-2.19377	-4.03603	-1.51496
H	-2.29095	-0.44386	-2.73475
H	-1.31956	-1.92806	-2.74306
H	-2.83146	-1.85310	-3.67328

C	-3.41023	-2.09647	1.40599
C	-4.89618	-1.80414	1.23932
C	-2.90077	-1.54856	2.73492
H	-3.25388	-3.18791	1.39576
H	-5.30555	-2.16800	0.28923
H	-5.46332	-2.28477	2.04699
H	-5.08856	-0.72546	1.30539
H	-1.86381	-1.84541	2.92373
H	-2.94090	-0.45072	2.74166
H	-3.52478	-1.91202	3.56138
C	3.11282	-2.07605	-1.53886
C	2.34634	-1.53821	-2.74055
C	3.19844	-3.59625	-1.57867
H	4.12947	-1.65163	-1.54862
H	2.29092	-0.44382	-2.73478
H	2.83139	-1.85306	-3.67333
H	1.31950	-1.92799	-2.74308
H	3.80049	-4.01034	-0.76077
H	2.19371	-4.03601	-1.51503
H	3.65001	-3.92784	-2.52251
C	3.41025	-2.09650	1.40593
C	2.90082	-1.54860	2.73487
C	4.89620	-1.80418	1.23923
H	3.25389	-3.18793	1.39568
H	1.86386	-1.84545	2.92370
H	3.52484	-1.91208	3.56132
H	2.94096	-0.45077	2.74163
H	5.30555	-2.16803	0.28913
H	5.08859	-0.72550	1.30532
H	5.46335	-2.28483	2.04689
H	0.00001	-0.96441	1.64268

92

Benzene solvent 1-H_4 (tetrahydride)

C	-1.24276	1.03696	0.37256
C	-2.42299	0.36505	0.03438
C	-3.59429	1.04723	-0.29146
C	-3.61585	2.45048	-0.30456
C	-2.42038	3.12059	0.01725
H	-4.47955	0.48431	-0.57580
H	-2.41379	4.20467	-0.00746
C	3.61590	2.45049	-0.30432
C	3.59432	1.04725	-0.29130
C	2.42301	0.36506	0.03448
C	1.24276	1.03696	0.37262
C	1.25419	2.44269	0.36522
C	2.42041	3.12058	0.01740
H	4.47956	0.48431	-0.57568
H	2.41379	4.20467	-0.00730
C	-1.25418	2.44269	0.36514
C	-0.00001	3.19361	0.82105
C	-0.00001	0.28113	0.75670
N	4.76824	3.15081	-0.62256
N	-4.76812	3.15079	-0.62294
C	0.00003	4.64885	0.35765
H	0.87237	5.18401	0.74783
H	0.00005	4.73672	-0.73596
H	-0.87230	5.18405	0.74781
C	-0.00005	3.20638	2.36429
H	-0.89090	3.72678	2.74027
H	-0.00009	2.19374	2.78367
H	0.89080	3.72674	2.74032
C	4.70602	4.57938	-0.81517
H	5.70053	4.95236	-1.07236
H	4.01535	4.87438	-1.62235
H	4.39211	5.09844	0.10151
C	5.92276	2.42812	-1.09619
H	5.73117	1.87563	-2.03154
H	6.73993	3.12978	-1.28143
H	6.27891	1.70499	-0.34826
C	-4.70611	4.57947	-0.81474
H	-4.01533	4.87499	-1.62162
H	-5.70063	4.95242	-1.07195
H	-4.39247	5.09811	0.10227
C	-5.92282	2.42810	-1.09610
H	-6.73979	3.12985	-1.28186
H	-5.73131	1.87502	-2.03111
H	-6.27918	1.70547	-0.34777
P	-2.29539	-1.46020	0.03718
P	2.29540	-1.46019	0.03721
C	-3.28382	-2.04713	-1.42151
C	-3.33888	-3.56999	-1.43611

C	-2.71420	-1.50883	-2.72611
H	-4.30206	-1.64943	-1.29185
H	-3.83090	-3.98856	-0.54975
H	-3.89236	-3.92027	-2.31684
H	-2.32708	-3.99353	-1.48771
H	-2.64326	-0.41471	-2.72941
H	-1.70901	-1.90761	-2.90836
H	-3.35566	-1.80942	-3.56488
C	-3.26662	-2.03811	1.52636
C	-4.77257	-1.83191	1.42245
C	-2.73464	-1.37827	2.79226
H	-3.04132	-3.11564	1.57418
H	-5.22660	-2.35438	0.57270
H	-5.26173	-2.20542	2.33166
H	-5.01834	-0.76428	1.34043
H	-1.65747	-1.53661	2.91635
H	-2.92569	-0.29647	2.78255
H	-3.24106	-1.79490	3.67229
C	3.28384	-2.04707	-1.42149
C	2.71431	-1.50861	-2.72607
C	3.33879	-3.56993	-1.43623
H	4.30210	-1.64945	-1.29175
H	2.64344	-0.41448	-2.72927
H	3.35580	-1.80915	-3.56484
H	1.70911	-1.90731	-2.90840
H	3.83070	-3.98863	-0.54987
H	2.32696	-3.99339	-1.48795
H	3.89232	-3.92017	-2.31694
C	3.26660	-2.03817	1.52638
C	2.73455	-1.37843	2.79231
C	4.77255	-1.83191	1.42255
H	3.04134	-3.11572	1.57411
H	1.65738	-1.53681	2.91633
H	3.24093	-1.79512	3.67233
H	2.92557	-0.29663	2.78268
H	5.22664	-2.35428	0.57278
H	5.01828	-0.76425	1.34063
H	5.26169	-2.20546	2.33175
H	-0.00003	0.19710	1.85578
Ir	0.00001	-1.79700	0.04144
H	-0.00003	-2.09551	1.66801
H	0.00001	-0.89865	-1.34794
H	0.00010	-3.39959	0.38328
H	0.00003	-2.77526	-1.25976

92

Benzene solvent 2-H_4 (dihydride dihydrogen)

C	-1.23676	1.03239	0.42229
C	-2.40726	0.36969	0.03333
C	-3.56636	1.05895	-0.32392
C	-3.58760	2.46131	-0.31808
C	-2.40161	3.12512	0.04909
H	-4.44110	0.50072	-0.64727
H	-2.39001	4.20943	0.03383
C	3.58694	2.46196	-0.31831
C	3.56606	1.05961	-0.32381
C	2.40711	0.37014	0.03355
C	1.23642	1.03262	0.42235
C	1.24868	2.44019	0.42562
C	2.40083	3.12556	0.04885
H	4.44097	0.50151	-0.64692
H	2.38904	4.20986	0.03340
C	-1.24931	2.43993	0.42568
C	-0.00042	3.18220	0.90823
C	-0.00012	0.26806	0.82271
N	4.72891	3.16901	-0.66450
N	-4.72978	3.16823	-0.66397
C	-0.00082	4.65009	0.48692
H	0.87183	5.17309	0.89342
H	-0.00058	4.77223	-0.60340
H	-0.87410	5.17243	0.89294
C	-0.00041	3.15874	2.45111
H	-0.89118	3.67098	2.83842
H	-0.00016	2.13771	2.84823
H	0.89011	3.67142	2.83841
C	4.65255	4.59760	-0.85259
H	5.63930	4.97806	-1.12876
H	3.94277	4.89140	-1.64380
H	4.35508	5.11108	0.07229
C	5.85752	2.45471	-1.20854
H	5.62228	1.92533	-2.14745

H	6.66838	3.15857	-1.41265
H	6.24416	1.71296	-0.49506
C	-4.65344	4.59677	-0.85252
H	-3.94404	4.89034	-1.64417
H	-5.64032	4.97720	-1.12826
H	-4.35550	5.11046	0.07208
C	-5.85818	2.45386	-1.20836
H	-6.66939	3.15755	-1.41174
H	-5.62296	1.92527	-2.14773
H	-6.24435	1.71146	-0.49533
P	-2.28260	-1.45519	0.01513
P	2.28311	-1.45478	0.01531
C	-3.24195	-2.02154	-1.47192
C	-3.35837	-3.54075	-1.47617
C	-2.58807	-1.52366	-2.75351
H	-4.24788	-1.58109	-1.39243
H	-3.92857	-3.92780	-0.62274
H	-3.86440	-3.87905	-2.38968
H	-2.36239	-4.00306	-1.45421
H	-2.45679	-0.43488	-2.75858
H	-1.59925	-1.98018	-2.88659
H	-3.20610	-1.79396	-3.61979
C	-3.29998	-2.03813	1.47499
C	-4.79752	-1.78929	1.34833
C	-2.77666	-1.41315	2.76248
H	-3.10941	-3.12317	1.50804
H	-5.24495	-2.27254	0.47221
H	-5.31696	-2.17726	2.23460
H	-5.01269	-0.71348	1.29327
H	-1.70560	-1.59285	2.91083
H	-2.93849	-0.32683	2.76508
H	-3.30916	-1.82853	3.62769
C	3.24268	-2.02092	-1.47172
C	2.58891	-1.52316	-2.75340
C	3.35926	-3.54016	-1.47590
H	4.24852	-1.58033	-1.39215
H	2.45753	-0.43441	-2.75854
H	3.20710	-1.79347	-3.61956
H	1.60018	-1.97985	-2.88662
H	3.92939	-3.92710	-0.62238
H	2.36331	-4.00253	-1.45401
H	3.86544	-3.87843	-2.38933
C	3.30047	-2.03751	1.47530
C	2.77692	-1.41240	2.76259
C	4.79803	-1.78862	1.34877
H	3.10993	-3.12255	1.50846
H	1.70582	-1.59203	2.91072
H	3.30922	-1.82772	3.62795
H	2.93881	-0.32609	2.76508
H	5.24559	-2.27205	0.47281
H	5.01321	-0.71282	1.29354
H	5.31738	-2.17641	2.23517
H	-0.00014	0.20709	1.92576
Ir	0.00017	-1.81282	0.08082
H	0.00054	-2.39007	1.80048
H	0.00040	-1.05735	-1.32454
H	-0.00017	-3.10720	1.32233
H	0.00066	-3.22657	-0.81428

92

Benzene solvent 3-H_4 (dihydride-dihydrogen)

C	-1.23908	1.01993	0.35216
C	-2.42137	0.36128	0.00429
C	-3.58730	1.04924	-0.32585
C	-3.60181	2.45236	-0.32824
C	-2.40843	3.11258	0.01954
H	-4.47419	0.49209	-0.61640
H	-2.39652	4.19681	0.01135
C	3.60187	2.45227	-0.32825
C	3.58732	1.04915	-0.32586
C	2.42137	0.36121	0.00428
C	1.23911	1.01988	0.35216
C	1.24847	2.42540	0.37009
C	2.40850	3.11251	0.01953
H	4.47420	0.49198	-0.61641
H	2.39658	4.19674	0.01137
C	-1.24840	2.42545	0.37010
C	0.00007	3.16512	0.85188
C	0.00000	0.24171	0.72639
N	4.74614	3.16107	-0.65685
N	-4.74606	3.16119	-0.65685

C	0.00020	4.63531	0.43890
H	0.87296	5.15578	0.84807
H	0.00007	4.76325	-0.65070
H	-0.87230	5.15602	0.84831
C	0.00010	3.12925	2.39500
H	-0.89072	3.63800	2.78662
H	0.00003	2.10459	2.78403
H	0.89101	3.63786	2.78658
C	4.67382	4.59110	-0.83507
H	5.66293	4.97177	-1.10186
H	3.97063	4.89019	-1.62988
H	4.36972	5.09948	0.09073
C	5.89283	2.44859	-1.16431
H	5.68134	1.90268	-2.09917
H	6.70125	3.15651	-1.36353
H	6.27139	1.72141	-0.43152
C	-4.67369	4.59122	-0.83506
H	-3.97047	4.89029	-1.62984
H	-5.66278	4.97193	-1.10188
H	-4.36960	5.09959	0.09075
C	-5.89279	2.44875	-1.16427
H	-6.70117	3.15670	-1.36351
H	-5.68133	1.90280	-2.09912
H	-6.27137	1.72161	-0.43145
P	-2.29363	-1.45639	0.03881
P	2.29359	-1.45646	0.03882
C	-3.31606	-2.07992	-1.38386
C	-3.38191	-3.60215	-1.35676
C	-2.78047	-1.58167	-2.71808
H	-4.33032	-1.67729	-1.24005
H	-3.84126	-3.99549	-0.44186
H	-3.97016	-3.97218	-2.20633
H	-2.37711	-4.03836	-1.43948
H	-2.69821	-0.48905	-2.75118
H	-1.78293	-1.99078	-2.91856
H	-3.44867	-1.89804	-3.53003
C	-3.25401	-1.98861	1.55468
C	-4.75894	-1.76870	1.47171
C	-2.68914	-1.30682	2.79419
H	-3.03962	-3.06724	1.62666
H	-5.23393	-2.30915	0.64469
H	-5.23637	-2.11114	2.39933
H	-4.99460	-0.70105	1.36388
H	-1.61059	-1.47577	2.89083
H	-2.87075	-0.22348	2.76579
H	-3.17807	-1.69985	3.69487
C	3.31600	-2.08003	-1.38385
C	2.78048	-1.58170	-2.71806
C	3.38172	-3.60227	-1.35679
H	4.33029	-1.67749	-1.24001
H	2.69832	-0.48907	-2.75113
H	3.44867	-1.89811	-3.53001
H	1.78290	-1.99072	-2.91857
H	3.84102	-3.99568	-0.44190
H	2.37688	-4.03839	-1.43955
H	3.96996	-3.97233	-2.20635
C	3.25393	-1.98868	1.55471
C	2.68905	-1.30686	2.79419
C	4.75887	-1.76877	1.47176
H	3.03953	-3.06730	1.62670
H	1.61049	-1.47581	2.89081
H	3.17796	-1.69988	3.69489
H	2.87066	-0.22353	2.76579
H	5.23387	-2.30923	0.64477
H	4.99454	-0.70112	1.36392
H	5.23628	-2.11120	2.39940
H	0.00000	0.15243	1.82717
Ir	-0.00003	-1.78156	0.03145
H	-0.00004	-2.32636	1.63176
H	-0.00001	-1.05611	-1.48517
H	-0.00004	-3.55442	-0.15690
H	-0.00006	-3.23457	-0.97433

92

Benzene solvent 4-H_4 (dihydride dihydrogen)

C	-1.24412	1.03728	0.34910
C	-2.43453	0.36290	0.04271
C	-3.61259	1.04508	-0.25834
C	-3.63068	2.44859	-0.28980
C	-2.42813	3.11990	0.00110
H	-4.50856	0.48218	-0.50739

H	-2.42114	4.20391	-0.03180	**C**	-3.51973	-3.59309	-1.25030
C	3.63036	2.44887	-0.29028	**C**	-2.94370	-1.60327	-2.65920
C	3.61248	1.04535	-0.25844	**H**	-4.41557	-1.63994	-1.10033
C	2.43454	0.36310	0.04285	**H**	-3.98209	-3.96585	-0.32859
C	1.24404	1.03739	0.34914	**H**	-4.12385	-3.95660	-2.09175
C	1.25646	2.44311	0.33461	**H**	-2.52291	-4.04719	-1.33179
C	2.42778	3.12009	0.00068	**H**	-2.79068	-0.51782	-2.70172
H	4.50850	0.48250	-0.50744	**H**	-1.99893	-2.09222	-2.92910
H	2.42067	4.20409	-0.03242	**H**	-3.68173	-1.86907	-3.42706
C	-1.25668	2.44301	0.33475	**C**	-3.12387	-2.02722	1.63065
C	-0.00012	3.19392	0.78399	**C**	-4.62432	-1.76627	1.66788
C	-0.00001	0.26984	0.69914	**C**	-2.45326	-1.39613	2.84413
N	4.78776	3.14867	-0.59482	**H**	-2.93261	-3.11183	1.65194
N	-4.78824	3.14828	-0.59394	**H**	-5.17430	-2.26948	0.86435
C	-0.00021	4.64915	0.32120	**H**	-5.04023	-2.12373	2.61899
H	0.87221	5.18462	0.71085	**H**	-4.83737	-0.69019	1.60657
H	-0.00031	4.73737	-0.77252	**H**	-1.37861	-1.60709	2.87449
H	-0.87258	5.18457	0.71101	**H**	-2.59067	-0.30597	2.84984
C	-0.00000	3.20234	2.32754	**H**	-2.90132	-1.78961	3.76565
H	-0.89115	3.72055	2.70606	**C**	3.42277	-2.07304	-1.29133
H	0.00013	2.18642	2.74015	**C**	2.94467	-1.60377	-2.65835
H	0.89111	3.72072	2.70592	**C**	3.52045	-3.59318	-1.24878
C	4.72523	4.57478	-0.80332	**H**	4.41612	-1.63993	-1.09906
H	5.72339	4.94817	-1.04548	**H**	2.79169	-0.51833	-2.70123
H	4.04855	4.86013	-1.62594	**H**	3.68286	-1.86982	-3.42596
H	4.39302	5.10204	0.10216	**H**	1.99994	-2.09278	-2.92831
C	5.94895	2.42362	-1.04783	**H**	3.98254	-3.96569	-0.32682
H	5.76746	1.85829	-1.97764	**H**	2.52370	-4.04738	-1.33048
H	6.76565	3.12541	-1.23489	**H**	4.12488	-3.95686	-2.08993
H	6.30071	1.71147	-0.28760	**C**	3.12368	-2.02650	1.63164
C	-4.72604	4.57446	-0.80215	**C**	2.45258	-1.39533	2.84482
H	-4.04959	4.86011	-1.62485	**C**	4.62405	-1.76518	1.66924
H	-5.72432	4.94770	-1.04400	**H**	2.93268	-3.11115	1.65311
H	-4.39372	5.10159	0.10337	**H**	1.37797	-1.60653	2.87491
C	-5.94945	2.42312	-1.04671	**H**	2.90046	-1.78855	3.76653
H	-6.76636	3.12479	-1.23330	**H**	2.58976	-0.30514	2.85038
H	-5.76818	1.85805	-1.97673	**H**	5.17439	-2.26851	0.86604
H	-6.30077	1.71071	-0.28652	**H**	4.83685	-0.68907	1.60764
P	-2.29148	-1.46604	0.05492	**H**	5.03977	-2.12223	2.62059
P	2.29165	-1.46587	0.05551	**H**	-0.00005	0.12803	1.79452
C	-3.42213	-2.07294	-1.29243	**Ir**	0.00015	-1.78177	-0.11328

H	0.00002	-2.36458	1.37188
H	0.00026	-0.82469	-1.65335
H	0.00011	-3.40310	-0.53781
H	0.00033	-1.64640	-1.90481

92

Benzene solvent transition state for 1-H_4 to 2-H_4 (tetrahydride to dihydrogen dihydride)

C	-1.23874	1.03449	0.40631
C	-2.41220	0.36856	0.03325
C	-3.57545	1.05524	-0.31402
C	-3.59732	2.45788	-0.31293
C	-2.40812	3.12391	0.03939
H	-4.45323	0.49526	-0.62590
H	-2.39837	4.20812	0.02138
C	3.59732	2.45787	-0.31296
C	3.57545	1.05523	-0.31404
C	2.41220	0.36856	0.03324
C	1.23874	1.03449	0.40631
C	1.25085	2.44142	0.40594
C	2.40813	3.12391	0.03938
H	4.45322	0.49526	-0.62592
H	2.39838	4.20812	0.02137
C	-1.25085	2.44142	0.40595
C	0.00000	3.18708	0.87872
C	0.00000	0.27560	0.80481
N	4.74320	3.16225	-0.64888
N	-4.74321	3.16226	-0.64884
C	0.00000	4.65009	0.44056
H	0.87272	5.17781	0.84044
H	0.00000	4.75846	-0.65121
H	-0.87271	5.17782	0.84045
C	0.00001	3.17854	2.42183
H	-0.89068	3.69444	2.80436
H	0.00001	2.16120	2.82869
H	0.89070	3.69444	2.80436
C	4.67351	4.59160	-0.83354
H	5.66380	4.96935	-1.10036
H	3.97176	4.88962	-1.63021
H	4.36968	5.10386	0.09005
C	5.88046	2.44532	-1.17102
H	5.65929	1.90947	-2.10957
H	6.69344	3.14856	-1.36850
H	6.25751	1.70871	-0.44703
C	-4.67350	4.59161	-0.83355
H	-3.97180	4.88959	-1.63028
H	-5.66380	4.96937	-1.10031
H	-4.36960	5.10388	0.09001
C	-5.88042	2.44533	-1.17109
H	-6.69341	3.14856	-1.36857
H	-5.65919	1.90955	-2.10966
H	-6.25750	1.70867	-0.44717
P	-2.28889	-1.45605	0.01866
P	2.28889	-1.45605	0.01865
C	-3.24847	-2.02675	-1.46576
C	-3.34138	-3.54765	-1.47812
C	-2.61985	-1.50891	-2.75167
H	-4.26013	-1.60285	-1.37100
H	-3.88846	-3.94942	-0.61652
H	-3.85951	-3.88752	-2.38414
H	-2.33857	-3.99532	-1.47872
H	-2.51427	-0.41748	-2.75337
H	-1.62200	-1.94015	-2.89864
H	-3.24203	-1.79028	-3.61143
C	-3.29629	-2.04328	1.48133
C	-4.79598	-1.80481	1.35961
C	-2.77062	-1.41584	2.76649
H	-3.09674	-3.12666	1.51347
H	-5.24448	-2.29451	0.48760
H	-5.30845	-2.19310	2.24968
H	-5.01905	-0.73070	1.30209
H	-1.69745	-1.59022	2.90529
H	-2.94154	-0.33082	2.77198
H	-3.29551	-1.83726	3.63335
C	3.24845	-2.02675	-1.46578
C	2.61983	-1.50892	-2.75168
C	3.34137	-3.54765	-1.47813
H	4.26012	-1.60285	-1.37102
H	2.51424	-0.41749	-2.75338
H	3.24200	-1.79030	-3.61144

H	1.62198	-1.94017	-2.89864
H	3.88846	-3.94942	-0.61654
H	2.33856	-3.99533	-1.47872
H	3.85949	-3.88753	-2.38415
C	3.29630	-2.04328	1.48132
C	2.77063	-1.41584	2.76648
C	4.79598	-1.80481	1.35959
H	3.09675	-3.12666	1.51345
H	1.69746	-1.59023	2.90528
H	3.29552	-1.83727	3.63333
H	2.94154	-0.33083	2.77197
H	5.24448	-2.29451	0.48758
H	5.01905	-0.73070	1.30207
H	5.30846	-2.19311	2.24965
H	0.00000	0.21052	1.90599
Ir	-0.00000	-1.80849	0.08141
H	-0.00000	-2.24196	1.70852
H	-0.00000	-0.99179	-1.33368
H	-0.00000	-3.17022	1.04841
H	-0.00001	-3.10220	-0.95602

92

Benzene solvent transition state for 1-H_4 to 3-H_4 (tetrahydride to dihydrogen dihydride)

C	-1.23995	1.02817	0.35594
C	-2.42124	0.36423	0.01186
C	-3.59020	1.04910	-0.31566
C	-3.60855	2.45218	-0.32061
C	-2.41415	3.11686	0.01563
H	-4.47609	0.48916	-0.60391
H	-2.40522	4.20110	0.00191
C	3.60861	2.45213	-0.32055
C	3.59022	1.04904	-0.31567
C	2.42124	0.36420	0.01183
C	1.23997	1.02816	0.35594
C	1.25090	2.43394	0.36329
C	2.41422	3.11683	0.01569
H	4.47610	0.48909	-0.60394
H	2.40531	4.20106	0.00200
C	-1.25086	2.43396	0.36327
C	0.00002	3.17889	0.83346
C	0.00000	0.25873	0.73501
N	4.75715	3.15724	-0.64199
N	-4.75706	3.15732	-0.64213
C	0.00004	4.64249	0.39739
H	0.87253	5.16991	0.79792
H	0.00005	4.75193	-0.69426
H	-0.87246	5.16992	0.79790
C	0.00001	3.16497	2.37681
H	-0.89084	3.67897	2.76146
H	-0.00001	2.14559	2.77942
H	0.89087	3.67895	2.76147
C	4.69097	4.58730	-0.82169
H	5.68299	4.96434	-1.08268
H	3.99396	4.88807	-1.62125
H	4.38265	5.09773	0.10169
C	5.90872	2.44054	-1.13164
H	5.70873	1.89249	-2.06779
H	6.72172	3.14571	-1.32180
H	6.27517	1.71439	-0.39158
C	-4.69079	4.58735	-0.82201
H	-3.99367	4.88797	-1.62153
H	-5.68276	4.96440	-1.08320
H	-4.38257	5.09792	0.10132
C	-5.90873	2.44062	-1.13152
H	-6.72170	3.14582	-1.32172
H	-5.70888	1.89240	-2.06761
H	-6.27515	1.71462	-0.39131
P	-2.29453	-1.45614	0.03768
P	2.29450	-1.45617	0.03762
C	-3.29651	-2.06843	-1.40302
C	-3.35477	-3.59116	-1.39313
C	-2.74657	-1.55244	-2.72476
H	-4.31381	-1.67068	-1.26698
H	-3.82555	-3.99627	-0.48919
H	-3.92907	-3.95432	-2.25510
H	-2.34622	-4.02031	-1.46520
H	-2.67203	-0.45890	-2.74556
H	-1.74436	-1.95393	-2.91693
H	-3.40241	-1.86436	-3.54833
C	-3.26585	-2.00492	1.53950

C	-4.77142	-1.79474	1.44126
C	-2.72074	-1.32760	2.79031
H	-3.04492	-3.08258	1.60529
H	-5.23306	-2.33097	0.60413
H	-5.25652	-2.14922	2.36029
H	-5.01362	-0.72785	1.34084
H	-1.64263	-1.48927	2.90229
H	-2.90876	-0.24538	2.76615
H	-3.21922	-1.72945	3.68176
C	3.29643	-2.06846	-1.40311
C	2.74647	-1.55243	-2.72483
C	3.35466	-3.59119	-1.39325
H	4.31374	-1.67072	-1.26708
H	2.67195	-0.45889	-2.74561
H	3.40228	-1.86434	-3.54842
H	1.74426	-1.95390	-2.91699
H	3.82545	-3.99632	-0.48933
H	2.34610	-4.02031	-1.46531
H	3.92894	-3.95434	-2.25524
C	3.26584	-2.00500	1.53941
C	2.72078	-1.32767	2.79025
C	4.77142	-1.79486	1.44114
H	3.04488	-3.08265	1.60519
H	1.64267	-1.48931	2.90224
H	3.21927	-1.72956	3.68168
H	2.90885	-0.24546	2.76610
H	5.23302	-2.33110	0.60399
H	5.01365	-0.72798	1.34072
H	5.25653	-2.14938	2.36015
H	0.00001	0.17599	1.83556
Ir	-0.00002	-1.79166	0.04480
H	0.00000	-2.23911	1.66310
H	-0.00003	-1.02049	-1.44177
H	-0.00004	-3.47205	0.03011
H	-0.00004	-3.10242	-0.99396

92

Benzene solvent transition state for 1-H_4 to 4-H_4 (tetrahydride to dihydrogen dihydride)

C	-1.24475	1.03827	0.34417
C	-2.43440	0.36385	0.03949
C	-3.61328	1.04471	-0.26040
C	-3.63229	2.44821	-0.29051
C	-2.42968	3.11980	-0.00093
H	-4.50849	0.48128	-0.51089
H	-2.42358	4.20376	-0.03362
C	3.63229	2.44820	-0.29052
C	3.61328	1.04471	-0.26041
C	2.43439	0.36384	0.03948
C	1.24475	1.03827	0.34417
C	1.25701	2.44372	0.33023
C	2.42968	3.11980	-0.00093
H	4.50849	0.48128	-0.51090
H	2.42358	4.20376	-0.03363
C	-1.25701	2.44372	0.33024
C	0.00000	3.19663	0.77521
C	0.00000	0.27554	0.70058
N	4.79038	3.14727	-0.59246
N	-4.79038	3.14727	-0.59245
C	0.00000	4.64879	0.30246
H	0.87217	5.18703	0.68862
H	0.00000	4.72907	-0.79182
H	-0.87216	5.18703	0.68862
C	0.00000	3.21541	2.31864
H	-0.89109	3.73632	2.69350
H	0.00000	2.20263	2.73876
H	0.89110	3.73632	2.69350
C	4.72895	4.57320	-0.80303
H	5.72714	4.94527	-1.04691
H	4.05187	4.85726	-1.62564
H	4.39787	5.10245	0.10176
C	5.95437	2.42126	-1.03661
H	5.77928	1.85554	-1.96741
H	6.77291	3.12237	-1.21806
H	6.29989	1.70935	-0.27320
C	-4.72894	4.57320	-0.80304
H	-4.05187	4.85725	-1.62566
H	-5.72713	4.94527	-1.04691
H	-4.39785	5.10246	0.10174
C	-5.95436	2.42127	-1.03663
H	-6.77290	3.12238	-1.21809

H	-5.77925	1.85557	-1.96744
H	-6.29989	1.70934	-0.27325
P	-2.29578	-1.46364	0.05339
P	2.29578	-1.46364	0.05339
C	-3.38866	-2.07002	-1.32282
C	-3.45696	-3.59223	-1.30443
C	-2.90646	-1.56652	-2.67597
H	-4.39268	-1.66028	-1.13505
H	-3.90594	-3.98831	-0.38570
H	-4.05876	-3.95412	-2.14811
H	-2.45256	-4.02634	-1.39768
H	-2.78267	-0.47709	-2.69932
H	-1.94468	-2.02177	-2.94304
H	-3.62866	-1.84127	-3.45567
C	-3.16013	-2.02671	1.61146
C	-4.66738	-1.80493	1.60549
C	-2.53938	-1.36377	2.83474
H	-2.94099	-3.10556	1.65159
H	-5.18312	-2.33379	0.79578
H	-5.09821	-2.16026	2.55068
H	-4.90674	-0.73575	1.52409
H	-1.45999	-1.54306	2.89431
H	-2.70974	-0.27835	2.82554
H	-2.99904	-1.76205	3.74838
C	3.38866	-2.07002	-1.32283
C	2.90645	-1.56653	-2.67597
C	3.45695	-3.59224	-1.30443
H	4.39267	-1.66028	-1.13506
H	2.78266	-0.47709	-2.69932
H	3.62865	-1.84128	-3.45567
H	1.94467	-2.02178	-2.94305
H	3.90594	-3.98831	-0.38570
H	2.45256	-4.02635	-1.39768
H	4.05876	-3.95412	-2.14811
C	3.16013	-2.02671	1.61146
C	2.53938	-1.36378	2.83473
C	4.66738	-1.80493	1.60548
H	2.94099	-3.10557	1.65158
H	1.45999	-1.54307	2.89430
H	2.99904	-1.76205	3.74837
H	2.70974	-0.27836	2.82554
H	5.18312	-2.33379	0.79577
H	4.90674	-0.73575	1.52409
H	5.09821	-2.16026	2.55067
H	0.00000	0.14718	1.79710
Ir	-0.00000	-1.78635	-0.07457
H	-0.00000	-2.26123	1.48512
H	-0.00000	-0.93274	-1.53523
H	0.00000	-3.44057	-0.24031
H	-0.00000	-2.03683	-1.71815

92

Benzene solvent transition state 3-H_4 to Ir-H_2 (H_2 loss)

C	-1.24490	1.04292	0.25320
C	-2.43568	0.36254	-0.02255
C	-3.60914	1.03829	-0.34345
C	-3.62302	2.44111	-0.41407
C	-2.42743	3.11737	-0.11073
H	-4.50736	0.47128	-0.57297
H	-2.42486	4.20113	-0.13973
C	3.62300	2.44114	-0.41407
C	3.60913	1.03832	-0.34345
C	2.43568	0.36256	-0.02255
C	1.24489	1.04293	0.25319
C	1.25228	2.44611	0.22373
C	2.42740	3.11739	-0.11075
H	4.50736	0.47131	-0.57297
H	2.42482	4.20115	-0.13975
C	-1.25230	2.44610	0.22374
C	-0.00001	3.20665	0.66198
C	-0.00000	0.27993	0.61958
N	4.77050	3.13088	-0.77249
N	-4.77053	3.13084	-0.77248
C	-0.00002	4.65204	0.16866
H	0.87176	5.19558	0.54780
H	-0.00002	4.71639	-0.92643
H	-0.87181	5.19557	0.54780
C	-0.00001	3.24733	2.20505
H	-0.89098	3.77358	2.57250
H	-0.00001	2.24105	2.64101
H	0.89096	3.77358	2.57250

C	4.79862	4.56925	-0.65484
H	5.76896	4.93975	-0.99491
H	4.03411	5.03667	-1.28948
H	4.64267	4.92267	0.37866
C	6.02503	2.41805	-0.82124
H	6.01566	1.63899	-1.59584
H	6.82852	3.11432	-1.07430
H	6.28151	1.93582	0.13767
C	-4.79868	4.56921	-0.65478
H	-4.03418	5.03667	-1.28940
H	-5.76903	4.93970	-0.99485
H	-4.64274	4.92260	0.37872
C	-6.02505	2.41799	-0.82126
H	-6.82855	3.11424	-1.07435
H	-6.01564	1.63893	-1.59586
H	-6.28155	1.93576	0.13765
P	-2.29196	-1.45961	0.05512
P	2.29198	-1.45960	0.05513
C	-3.30917	-2.10335	-1.36307
C	-3.44677	-3.61856	-1.27022
C	-2.69859	-1.68378	-2.69354
H	-4.30781	-1.64803	-1.27431
H	-3.99944	-3.94035	-0.37957
H	-3.98226	-4.00484	-2.14718
H	-2.46174	-4.10374	-1.24327
H	-2.57378	-0.59703	-2.76687
H	-1.70966	-2.13797	-2.83413
H	-3.34186	-2.00838	-3.52208
C	-3.24623	-1.96816	1.57779
C	-4.73216	-1.63956	1.55463
C	-2.58026	-1.37706	2.81351
H	-3.10713	-3.06087	1.60426
H	-5.26008	-2.08311	0.70170
H	-5.21344	-2.01669	2.46675
H	-4.89483	-0.55336	1.52842
H	-1.52229	-1.66127	2.86942
H	-2.64709	-0.27990	2.81386
H	-3.07861	-1.73755	3.72272
C	3.30919	-2.10333	-1.36306
C	2.69858	-1.68381	-2.69354
C	3.44684	-3.61854	-1.27019
H	4.30781	-1.64798	-1.27432
H	2.57373	-0.59706	-2.76687
H	3.34186	-2.00839	-3.52208
H	1.70967	-2.13804	-2.83411
H	3.99962	-3.94028	-0.37958
H	2.46183	-4.10375	-1.24311
H	3.98226	-4.00483	-2.14718
C	3.24627	-1.96815	1.57778
C	2.58025	-1.37715	2.81353
C	4.73217	-1.63946	1.55465
H	3.10724	-3.06086	1.60421
H	1.52231	-1.66145	2.86944
H	3.07864	-1.73762	3.72273
H	2.64698	-0.27998	2.81391
H	5.26012	-2.08292	0.70168
H	4.89477	-0.55324	1.52850
H	5.21348	-2.01661	2.46674
H	0.00000	0.13562	1.71794
Ir	0.00001	-1.75083	0.04851
H	-0.00003	-3.04213	1.22670
H	0.00002	-0.91374	-1.35907
H	0.00006	-3.66282	-1.64066
H	0.00025	-4.35571	-1.93436

90

Benzene solvent Ir-H_2

C	-1.25081	1.03685	0.35427
C	-2.44541	0.36333	0.06325
C	-3.62613	1.04743	-0.22075
C	-3.64472	2.45091	-0.24482
C	-2.43756	3.11992	0.02991
H	-4.52245	0.48516	-0.46911
H	-2.43186	4.20409	0.00293
C	3.64466	2.45097	-0.24482
C	3.62609	1.04750	-0.22075
C	2.44539	0.36337	0.06326
C	1.25078	1.03687	0.35427
C	1.26022	2.44221	0.34277
C	2.43749	3.11996	0.02990
H	4.52242	0.48523	-0.46910

H	2.43177	4.20413	0.00292
C	-1.26028	2.44219	0.34277
C	-0.00003	3.19456	0.78133
C	-0.00001	0.26745	0.66686
N	4.80737	3.15329	-0.52742
N	-4.80746	3.15318	-0.52741
C	-0.00004	4.64518	0.30329
H	0.87174	5.18558	0.68707
H	-0.00005	4.72080	-0.79133
H	-0.87180	5.18559	0.68709
C	-0.00003	3.21648	2.32450
H	-0.89141	3.73705	2.69940
H	-0.00003	2.20327	2.74362
H	0.89136	3.73704	2.69939
C	4.73823	4.57410	-0.76901
H	5.73734	4.94888	-1.00509
H	4.07120	4.83613	-1.60722
H	4.38999	5.11926	0.11959
C	5.97563	2.42826	-0.96187
H	5.81624	1.87511	-1.90335
H	6.80059	3.12823	-1.11780
H	6.30329	1.70527	-0.20125
C	-4.73841	4.57400	-0.76896
H	-4.07137	4.83610	-1.60715
H	-5.73754	4.94871	-1.00506
H	-4.39024	5.11916	0.11966
C	-5.97568	2.42808	-0.96184
H	-6.80068	3.12800	-1.11778
H	-5.81626	1.87493	-1.90332
H	-6.30329	1.70507	-0.20122
P	-2.28970	-1.46556	0.01295
P	2.28971	-1.46553	0.01298
Ir	0.00001	-1.80117	0.07703
C	-3.22267	-1.97937	-1.51022
C	-3.31961	-3.49724	-1.59159
C	-2.54416	-1.40293	-2.74613
H	-4.23611	-1.55556	-1.43105
H	-3.90122	-3.93069	-0.76908
H	-3.80520	-3.79705	-2.52939
H	-2.32105	-3.95373	-1.57216
H	-2.47467	-0.30944	-2.70683
H	-1.52448	-1.79740	-2.84903
H	-3.10533	-1.67378	-3.65017
C	-3.29086	-2.13415	1.43885
C	-4.76640	-1.76289	1.43418
C	-2.62627	-1.72416	2.74718
H	-3.18510	-3.22493	1.32659
H	-5.28426	-2.07237	0.51790
H	-5.27937	-2.24661	2.27619
H	-4.89957	-0.67918	1.55125
H	-1.57824	-2.04902	2.78377
H	-2.65014	-0.63332	2.87852
H	-3.15184	-2.17050	3.60141
C	3.22272	-1.97934	-1.51016
C	2.54426	-1.40289	-2.74609
C	3.31968	-3.49721	-1.59153
H	4.23617	-1.55553	-1.43096
H	2.47475	-0.30940	-2.70678
H	3.10547	-1.67373	-3.65012
H	1.52459	-1.79737	-2.84904
H	3.90129	-3.93066	-0.76902
H	2.32111	-3.95370	-1.57210
H	3.80526	-3.79702	-2.52934
C	3.29086	-2.13408	1.43891
C	2.62648	-1.72371	2.74722
C	4.76647	-1.76313	1.43403
H	3.18486	-3.22485	1.32684
H	1.57838	-2.04834	2.78397
H	3.15204	-2.17003	3.60148
H	2.65061	-0.63286	2.87837
H	5.28418	-2.07287	0.51775
H	4.89989	-0.67943	1.55090
H	5.27943	-2.24682	2.27607
H	0.00002	-2.81661	-1.14227
H	-0.00001	0.04781	1.76039
H	0.00002	-3.39755	0.37736

90

Benzene solvent Ir-H_3

C	1.23369	1.02842	-0.03079
C	2.46607	0.33594	-0.04123
C	3.67810	0.99071	-0.10672

C	3.72301	2.40366	-0.13008	**P**	2.28406	-1.49116	0.05292
C	2.49743	3.09179	-0.09995	**P**	-2.28407	-1.49116	0.05277
H	4.59967	0.41639	-0.14658	**Ir**	-0.00000	-1.74762	0.02118
H	2.50926	4.17780	-0.11099	**H**	0.00000	-3.44690	-0.01900
C	-3.72301	2.40366	-0.13019	**H**	0.00005	-2.06025	-1.61420
C	-3.67809	0.99071	-0.10687	**H**	-0.00005	-2.17081	1.63203
C	-2.46607	0.33594	-0.04136	**C**	3.16851	-2.00047	1.62320
C	-1.23369	1.02842	-0.03086	**C**	2.70248	-1.13965	2.79140
C	-1.26881	2.43547	-0.06456	**C**	4.68988	-2.03337	1.56331
C	-2.49743	3.09179	-0.09998	**H**	2.78916	-3.02306	1.77638
H	-4.59966	0.41638	-0.14673	**H**	1.60917	-1.08013	2.84148
H	-2.50926	4.17780	-0.11098	**H**	3.06350	-1.56263	3.73764
C	1.26881	2.43547	-0.06452	**H**	3.09979	-0.11895	2.71199
C	0.00000	3.27819	-0.04193	**H**	5.08152	-2.69392	0.78165
C	0.00000	0.24562	-0.00089	**H**	5.10981	-1.03003	1.40786
N	-4.92131	3.07258	-0.17934	**H**	5.08605	-2.39587	2.52132
N	4.92131	3.07258	-0.17917	**C**	3.34428	-2.13901	-1.32984
C	-0.00001	4.11430	1.25154	**C**	2.92247	-1.55557	-2.67043
H	-0.88504	4.75873	1.30773	**C**	3.27513	-3.66079	-1.35134
H	-0.00002	3.46341	2.13424	**H**	4.37554	-1.81945	-1.11223
H	0.88502	4.75873	1.30775	**H**	3.00236	-0.46226	-2.69211
C	0.00002	4.21271	-1.26471	**H**	3.55937	-1.95669	-3.46995
H	0.88175	4.86296	-1.27248	**H**	1.88269	-1.82024	-2.89911
H	0.00002	3.63354	-2.19582	**H**	3.59077	-4.11575	-0.40401
H	-0.88172	4.86297	-1.27249	**H**	2.24771	-3.99157	-1.54864
C	-4.94617	4.51584	-0.12094	**H**	3.92074	-4.06016	-2.14442
H	-5.98093	4.86187	-0.16742	**C**	-3.16861	-2.00050	1.62298
H	-4.50302	4.90265	0.80956	**C**	-4.68998	-2.03337	1.56302
H	-4.40765	4.96775	-0.96618	**C**	-2.70261	-1.13975	2.79124
C	-6.16316	2.33359	-0.14617	**H**	-2.78930	-3.02311	1.77614
H	-6.27007	1.73685	0.77337	**H**	-5.08160	-2.69387	0.78130
H	-7.00039	3.03352	-0.18782	**H**	-5.08620	-2.39592	2.52099
H	-6.25788	1.65348	-1.00445	**H**	-5.10988	-1.03001	1.40760
C	4.94613	4.51587	-0.12169	**H**	-1.60930	-1.08027	2.84137
H	4.50276	4.90324	0.80846	**H**	-3.09989	-0.11904	2.71186
H	5.98090	4.86189	-0.16811	**H**	-3.06369	-1.56277	3.73745
H	4.40779	4.96727	-0.96733	**C**	-3.34418	-2.13898	-1.33008
C	6.16317	2.33361	-0.14634	**C**	-3.27506	-3.66076	-1.35160
H	7.00039	3.03359	-0.18754	**C**	-2.92226	-1.55552	-2.67063
H	6.27003	1.73645	0.77292	**H**	-4.37545	-1.81940	-1.11255
H	6.25800	1.65390	-1.00494	**H**	-3.59077	-4.11573	-0.40429

H	-3.92062	-4.06010	-2.14473
H	-2.24763	-3.99154	-1.54883
H	-3.00216	-0.46221	-2.69231
H	-1.88247	-1.82018	-2.89923
H	-3.55910	-1.95664	-3.47021

88

Benzene solvent Ir-H

C	-1.23337	1.01936	0.00838
C	-2.47001	0.33150	-0.00676
C	-3.68073	0.99093	-0.06727
C	-3.72251	2.40319	-0.08299
C	-2.49492	3.08708	-0.05343
H	-4.60372	0.41997	-0.11603
H	-2.50378	4.17319	-0.06364
C	3.72259	2.40310	-0.08296
C	3.68077	0.99084	-0.06727
C	2.47003	0.33144	-0.00678
C	1.23341	1.01933	0.00837
C	1.26807	2.42751	-0.01818
C	2.49501	3.08703	-0.05340
H	4.60375	0.41986	-0.11605
H	2.50390	4.17313	-0.06359
C	-1.26800	2.42754	-0.01818
C	0.00005	3.27057	0.00221
C	0.00001	0.22695	0.02015
N	4.91885	3.07689	-0.12732
N	-4.91876	3.07700	-0.12737
C	0.00005	4.19970	-1.22497
H	0.88193	4.84978	-1.23647
H	0.00006	3.61560	-2.15312
H	-0.88186	4.84976	-1.23649
C	0.00005	4.11261	1.29175
H	-0.88485	4.75741	1.34566
H	0.00005	3.46540	2.17716
H	0.88497	4.75740	1.34566
C	4.93607	4.52046	-0.17046
H	5.96976	4.86894	-0.22267
H	4.40737	4.91184	-1.05222
H	4.47785	4.96718	0.72468
C	6.16349	2.34267	-0.12574
H	6.27073	1.70181	-1.01355
H	6.99816	3.04700	-0.12313
H	6.26429	1.70553	0.76589
C	-4.93594	4.52057	-0.17061
H	-4.40722	4.91187	-1.05240
H	-5.96962	4.86908	-0.22286
H	-4.47772	4.96735	0.72449
C	-6.16341	2.34282	-0.12580
H	-6.99807	3.04716	-0.12317
H	-6.27067	1.70196	-1.01362
H	-6.26422	1.70567	0.76583
P	-2.27308	-1.49717	0.03031
P	2.27306	-1.49722	0.03026
Ir	-0.00001	-1.73858	0.01758
C	-3.28993	-2.08547	-1.41274
C	-3.40345	-3.60414	-1.39599
C	-2.63612	-1.60284	-2.70131
H	-4.29326	-1.63863	-1.32611
H	-3.96174	-3.97856	-0.52938
H	-3.92057	-3.95705	-2.29805
H	-2.40702	-4.06565	-1.37652
H	-2.56058	-0.50917	-2.74241
H	-1.61807	-2.00777	-2.78826
H	-3.21375	-1.93526	-3.57414
C	-3.18226	-2.09690	1.54550
C	-4.68236	-1.84484	1.59102
C	-2.49660	-1.54711	2.78982
H	-2.99742	-3.18272	1.50576
H	-5.20747	-2.19949	0.69551
H	-5.12317	-2.36248	2.45365
H	-4.89980	-0.77560	1.71519
H	-1.42371	-1.77721	2.78697
H	-2.60489	-0.45516	2.85036
H	-2.94331	-1.97576	3.69668
C	3.28984	-2.08551	-1.41285
C	2.63611	-1.60267	-2.70138
C	3.40314	-3.60420	-1.39625
H	4.29322	-1.63882	-1.32617
H	2.56071	-0.50899	-2.74236
H	3.21370	-1.93507	-3.57423
H	1.61800	-2.00747	-2.78838

H	3.96136	-3.97880	-0.52967
H	2.40664	-4.06557	-1.37685
H	3.92023	-3.95709	-2.29835
C	3.18225	-2.09702	1.54542
C	2.49650	-1.54742	2.78977
C	4.68234	-1.84484	1.59106
H	2.99750	-3.18286	1.50557
H	1.42363	-1.77760	2.78684
H	2.94319	-1.97615	3.69661
H	2.60472	-0.45548	2.85045
H	5.20754	-2.19936	0.69555
H	4.89967	-0.77560	1.71534
H	5.12314	-2.36252	2.45366
H	-0.00003	-3.48924	0.01426

88

Benzene solvent Ir-[]

C	-1.24090	0.98612	0.35576
C	-2.42653	0.32395	0.02238
C	-3.59064	1.01410	-0.30717
C	-3.60716	2.41755	-0.30488
C	-2.41286	3.07863	0.03777
H	-4.47780	0.45637	-0.59567
H	-2.40359	4.16293	0.03631
C	3.60757	2.41722	-0.30421
C	3.59084	1.01378	-0.30684
C	2.42658	0.32372	0.02242
C	1.24102	0.98600	0.35582
C	1.24869	2.39145	0.37473
C	2.41330	3.07842	0.03839
H	4.47795	0.45600	-0.59534
H	2.40421	4.16271	0.03714
C	-1.24840	2.39157	0.37447
C	0.00013	3.13237	0.85198
C	0.00002	0.19948	0.71384
N	4.75499	3.12527	-0.62099
N	-4.75444	3.12571	-0.62199
C	0.00025	4.60139	0.43463
H	0.87270	5.12357	0.84205
H	0.00041	4.72547	-0.65544
H	-0.87227	5.12364	0.84181
C	-0.00008	3.09873	2.39518
H	-0.89115	3.60717	2.78671
H	-0.00022	2.07333	2.78265
H	0.89097	3.60702	2.78696
C	4.68999	4.55716	-0.78474
H	5.68145	4.93608	-1.04517
H	3.99069	4.86691	-1.57880
H	4.38474	5.05831	0.14485
C	5.91010	2.41272	-1.10862
H	5.71410	1.86656	-2.04660
H	6.72167	3.12057	-1.29489
H	6.27595	1.68533	-0.36944
C	-4.68899	4.55748	-0.78673
H	-3.98947	4.86648	-1.58088
H	-5.68029	4.93650	-1.04759
H	-4.38375	5.05917	0.14257
C	-5.90956	2.41323	-1.10971
H	-6.72118	3.12109	-1.29573
H	-5.71365	1.86722	-2.04780
H	-6.27532	1.68573	-0.37061
P	-2.27216	-1.49624	0.01329
P	2.27192	-1.49645	0.01259
Ir	-0.00012	-1.77820	0.09413
C	-3.23055	-2.05125	-1.48531
C	-3.28472	-3.57301	-1.53243
C	-2.58249	-1.49093	-2.74382
H	-4.25490	-1.65616	-1.40232
H	-3.81168	-4.00805	-0.67433
H	-3.79972	-3.91237	-2.44076
H	-2.27021	-3.99652	-1.55236
H	-2.56402	-0.39482	-2.74511
H	-1.54280	-1.83655	-2.82687
H	-3.12738	-1.82282	-3.63788
C	-3.30616	-2.09229	1.45797
C	-4.78380	-1.73235	1.41821
C	-2.65799	-1.60891	2.74948
H	-3.19869	-3.18829	1.41062
H	-5.29334	-2.10903	0.52260
H	-5.30125	-2.15781	2.28887
H	-4.92476	-0.64388	1.45751
H	-1.59897	-1.89698	2.79287

H	-2.71249	-0.51423	2.83133
H	-3.17102	-2.03141	3.62355
C	3.22947	-2.05071	-1.48685
C	2.58093	-1.48944	-2.74468
C	3.28331	-3.57245	-1.53499
H	4.25393	-1.65588	-1.40410
H	2.56284	-0.39332	-2.74531
H	3.12524	-1.82098	-3.63922
H	1.54107	-1.83463	-2.82737
H	3.81041	-4.00818	-0.67732
H	2.26870	-3.99573	-1.55492
H	3.79799	-3.91133	-2.44368
C	3.30651	-2.09357	1.45640
C	2.65915	-1.61074	2.74850
C	4.78427	-1.73413	1.41611
H	3.19866	-3.18951	1.40846
H	1.60003	-1.89841	2.79220
H	3.17240	-2.03399	3.62208
H	2.71413	-0.51614	2.83101
H	5.29317	-2.11025	0.51991
H	4.92563	-0.64574	1.45626
H	5.30204	-2.16052	2.28612
H	0.00004	0.05901	1.81717

88

Benzene solvent transition state Ir-H to Ir-[] (1,2-hydride shift)

C	-1.23592	0.99140	0.22266
C	-2.46558	0.32245	0.03277
C	-3.65171	1.00730	-0.20689
C	-3.67647	2.41038	-0.21711
C	-2.45757	3.07643	0.02160
H	-4.55973	0.44424	-0.40466
H	-2.46157	4.16130	0.03556
C	3.67647	2.41038	-0.21710
C	3.65171	1.00730	-0.20689
C	2.46558	0.32245	0.03277
C	1.23592	0.99140	0.22266
C	1.25965	2.41013	0.24542
C	2.45757	3.07643	0.02161
H	4.55973	0.44423	-0.40466
H	2.46157	4.16130	0.03557
C	-1.25965	2.41013	0.24542
C	0.00000	3.16549	0.66631
C	0.00000	0.25057	0.35424
N	4.85705	3.11760	-0.42596
N	-4.85704	3.11761	-0.42597
C	0.00000	4.61145	0.17288
H	0.87077	5.15853	0.54896
H	0.00000	4.67158	-0.92256
H	-0.87076	5.15853	0.54896
C	0.00000	3.19455	2.21148
H	-0.89247	3.71467	2.58471
H	-0.00000	2.17831	2.62410
H	0.89247	3.71467	2.58471
C	4.78851	4.53201	-0.70309
H	5.79691	4.91323	-0.88428
H	4.16999	4.77114	-1.58496
H	4.38271	5.09129	0.15132
C	6.03273	2.39431	-0.84089
H	5.90321	1.86554	-1.80182
H	6.86883	3.09056	-0.94817
H	6.32767	1.64934	-0.08803
C	-4.78851	4.53201	-0.70311
H	-4.16998	4.77113	-1.58498
H	-5.79690	4.91323	-0.88431
H	-4.38270	5.09130	0.15130
C	-6.03273	2.39431	-0.84089
H	-6.86883	3.09057	-0.94817
H	-5.90321	1.86554	-1.80182
H	-6.32766	1.64935	-0.08803
P	-2.30490	-1.49243	0.02144
P	2.30490	-1.49244	0.02143
Ir	-0.00000	-1.74200	0.19099
C	-3.12193	-2.02020	-1.56617
C	-3.19356	-3.53840	-1.66192
C	-2.37175	-1.43198	-2.75356
H	-4.14298	-1.60734	-1.55521
H	-3.79089	-3.99000	-0.86042
H	-3.64411	-3.84064	-2.61646
H	-2.18607	-3.97603	-1.61750
H	-2.32884	-0.33739	-2.71420

H	-1.33937	-1.80696	-2.78267	**H**	2.86089	-1.71887	-3.69374
H	-2.86090	-1.71888	-3.69373	**H**	1.33936	-1.80695	-2.78267
C	-3.40556	-2.15905	1.37495	**H**	3.79089	-3.99000	-0.86043
C	-4.89182	-1.85775	1.23584	**H**	2.18606	-3.97603	-1.61751
C	-2.88559	-1.68467	2.72720	**H**	3.64410	-3.84063	-2.61647
H	-3.25279	-3.24897	1.30671	**C**	3.40556	-2.15906	1.37494
H	-5.31048	-2.16651	0.27028	**C**	2.88559	-1.68469	2.72719
H	-5.45379	-2.38635	2.01730	**C**	4.89182	-1.85776	1.23583
H	-5.08782	-0.78589	1.36820	**H**	3.25278	-3.24898	1.30670
H	-1.85082	-2.00045	2.89959	**H**	1.85082	-2.00046	2.89959
H	-2.91481	-0.58854	2.79664	**H**	3.50809	-2.08617	3.53758
H	-3.50808	-2.08615	3.53759	**H**	2.91482	-0.58855	2.79664
C	3.12193	-2.02020	-1.56618	**H**	5.31048	-2.16651	0.27027
C	2.37174	-1.43197	-2.75356	**H**	5.08782	-0.78590	1.36819
C	3.19355	-3.53840	-1.66193	**H**	5.45379	-2.38636	2.01728
H	4.14297	-1.60734	-1.55522	**H**	0.00000	-0.98923	1.62420
H	2.32883	-0.33738	-2.71420				

References

(1) Hebden, T. J.; Goldberg, K. I.; Heinekey, D. M.; Zhang, X.; Emge, T. J.; Goldman, A. S.; Krogh-Jespersen, K. *Inorg. Chem.* **2010**, *49*, 1733-1742.

(2) Polukeev, A. V.; Marcos, R.; Ahlquist, M. S. G.; Wendt, O. F. *Organometallics* **2016**, *35*, 2600-2608.

(3) Zhao, Y.; Truhlar, D. G. *Theoretical Chemistry Accounts* **2008**, *120*, 215-241.

(4) Hay, P. J.; Wadt, W. R. *The Journal of Chemical Physics* **1985**, *82*, 270-283.

(5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Wallingford, CT, **2016**.

(6) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *The Journal of Physical Chemistry B* **2009**, *113*, 6378-6396.