Electronic Supplementary Material (ESI) for Chemical Science.

A Versatile Strategy for the Formation of Hydride-Bridged Actinide-Iridium Multimetallics

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Supporting Information

Experimental Procedures

General considerations: Unless otherwise noted, all reactions were performed using standard Schlenk line techniques under an atmosphere of nitrogen or argon, or in an MBraun inert atmosphere glove box under an atmosphere of nitrogen. Glassware and Celite® were stored in an oven at ca. 150 °C for at least 3 h prior to use. Molecular sieves (4 Å) were activated by heating to 200 °C overnight under vacuum prior to storage in a glovebox. NMR spectra were recorded on Bruker AV-600 and AVB-400 spectrometers. ^{1}H chemical shifts are given relative to residual solvent peaks and are recorded in units of parts per million (ppm). FT-IR samples were prepared as Nujol mulls pressed between KBr plates or as solutions in C_6D_6 between KBr plates, with data collected with a Nicolet iS10 FT-IR spectrometer. Melting points were determined using sealed capillaries prepared under nitrogen on an OptiMelt automated melting point system. Elemental analyses were determined at the Microanalytical Facility at the College of Chemistry, University of California, Berkeley.

Materials: Toluene, *n*-hexane, and THF were purified by passage through columns of activated alumina and degassed by sparging with nitrogen. Deuterated solvents were degassed with three freeze-pump-thaw cycles and stored over molecular sieves. Benzylpotassium,[1] $IrCp^*H_4$,[2] $UI_3(1,4\text{-dioxane})_{1.5}$,[3] UCl_4,[4] and $ThCl_4(DME)_2$[5] were synthesized according to literature procedures. All other chemicals were purchased from commercial sources and used as received.

U{(μ-H)$_3$IrCp*}$_4$ (1): $IrCp^*H_4$ (68.7 mg, 0.207 mmol, 4.0 equiv.) and benzyl potassium (28.5 mg, 0.219 mmol, 4.2 equiv.) were added to a 20 mL scintillation vial with THF (2 mL) to generate a solution of K[$IrCp^*H_3$]. UCl_4 (19.7 mg, 0.052 mmol, 1.0 equiv.) was dissolved in THF (2 mL) and added to the K[$IrCp^*H_3$] solution. The solution quickly turned orange and slightly opaque as KCl precipitated out of solution. After stirring at room temperature for 2.5 h, the solvent was removed *in vacuo*. The crude solid was then triturated with *n*-hexane and the product was extracted with *n*-hexane (5 mL), filtered through Celite, and concentrated (ca. 1.5 mL). The resulting orange solution was cooled to -40 °C overnight, affording thin orange plates (60.8 mg, 75% yield). X-ray quality crystals were grown by recrystallization of **1** in *n*-hexane at -40 °C. Mp ca. 226 °C (decomp.); ^{1}H NMR (400 MHz, C_6D_6): δ 4.98 (s, 60H, CH_3), no hydride resonances were found within the range 200 ppm to -200 ppm; ^{13}C NMR (600 MHz, C_6D_6): δ 113.97 ($C_5(CH_3)_5$), 7.04 ($C_5(CH_3)_5$); IR (Nujol mull on KBr): 2144 (m), 2017 (m), 1951 (s), 1072 (m), 1029 (m), 856 (w), 802 (m), 615 (w), 585 (w), 561 (w), 530 (w); IR (solution in C_6D_6, solvent subtracted): 2979 (w), 2957 (w), 2902 (m), 2850 (w), 1955 (s), 1476 (w), 1381 (m), 1073 (w), 1033 (m) cm^{-1}. Anal. Calcd (%) for $UIr_4C_{40}H_{72}$: C, 30.80; H, 4.65. Found: C, 30.92; H, 4.67.

Th{[(μ-H$_2$)(H)IrCp*]$_2$[(μ-H)$_3$IrCp*]$_2$} (2). $IrCp^*H_4$ (71.1 mg, 0.214 mmol, 4.0 equiv.) and benzyl potassium (28.3 mg, 0.217 mmol, 4.0 equiv.) were added to a 20 mL scintillation vial with THF (2 mL) to generate a solution of K[$IrCp^*H_3$]. $ThCl_4(DME)_2$ (29.8 mg, 0.054 mmol, 1.0 equiv.) was dissolved in THF (2 mL) and added to the K[$IrCp^*H_3$] solution. The solution quickly turned pale yellow and slightly opaque as KCl precipitated out of solution. After stirring at room

temperature for 2 h, the solvent was removed *in vacuo*. The crude solid was then triturated with *n*-hexane and the product was extracted with *n*-hexane (5 mL), filtered through Celite, and concentrated (ca. 1.5 mL). The resulting pale-yellow solution was cooled to -40 °C overnight, affording thin colorless plates (48.7 mg, 58% yield). X-ray quality crystals were grown by recrystallization of **2** in *n*-hexane at -40 °C. Mp ca. 171 °C (decomp.); ^{1}H NMR (600 MHz, C_6D_6): δ 2.08 (s, 60H, CH_3), -11.31 (s, 12H, Th–H–Ir); ^{13}C NMR (600 MHz, C_6D_6): δ 90.45 ($C_5(CH_3)_5$), 11.57 ($C_5(CH_3)_5$); IR (Nujol mull on KBr): 2138 (m), 2026 (m), 1962 (s), 1072 (m), 1029 (m), 860 (w), 810 (m), 616 (w), 565 (w), 531 (w), 501 (w); IR (solution in C_6D_6, solvent subtracted): 2979 (w), 2958 (w), 2902 (m), 2849 (w), 1962 (s), 1475 (w), 1381 (m), 1073 (w), 1033 (m) cm^{-1}. Anal. Calcd (%) for $ThIr_4C_{40}H_{72}$ (**2**): C, 30.92; H, 4.67. Found: C, 30.87; H, 4.59.

{U[(μ$_2$-H$_3$)IrCp*]$_2$[(μ$_3$-H$_2$)IrCp*]}$_2$ (3): *Method A:* $IrCp^*H_4$ (48.0 mg, 0.145 mmol, 6.0 equiv.) and $U(Terph)_3$ (61.3 mg, 0.049 mmol, 2.0 equiv.) (Terph = C_6H_3-2,6-(C_6H_4-4-^{t}Bu)$_2$) were dissolved in separate 20 mL scintillation vials in *n*-hexane (2 mL and 6 mL, respectively). Both solutions were cooled to -40 °C, then the solution of $IrCp^*H_4$ was added to the solution of $U(Terph)_3$. The resulting black-yellow solution afforded black-yellow crystals of **3** (41.9 mg, 70% yield) after 18 h, which were rinsed with 2 × 2 mL *n*-hexane to remove any crystallized Terph–H. X-ray quality crystals were grown in a similar fashion at room temperature. Mp ca. 327 °C (decomp.); ^{1}H NMR (600 MHz, C_6D_6): δ 3.38 (s, 60H, CH_3 ($Cp^*Ir_{terminal}$)), –0.11 (s, 30H, CH_3 ($Cp^*Ir_{bridging}$)); ^{13}C NMR (600 MHz, C_6D_6): δ 112.63 ($U_2Ir(C_5(CH_3)_5)$), 105.44 ($Ir(C_5(CH_3)_5)$), 5.08 ($C_5(CH_3)_5$); IR (Nujol mull on KBr): 1951 (s), 1071 (w), 1031 (m), 793 (w), 628 (w), 585 (w) cm^{-1}. Anal. Calcd (%) for $U_2Ir_6C_{60}H_{106}$ (**3**): C, 29.33; H, 4.35. Found: C, 29.60; H, 4.39.

Method B: $IrCp^*H_4$ (19.9 mg, 0.060 mmol, 6.0 equiv.) and benzyl potassium (8.1 mg, 0.062 mmol, 6.2 equiv.) were added to a 20 mL scintillation vial with THF (2 mL) to generate a solution of $K[IrCp^*H_3]$. $UI_3(THF)_4$ (18.2 mg, 0.020 mmol, 2.0 equiv.) was dissolved in THF (2 mL) and added to the $K[IrCp^*H_3]$ solution. The solution quickly turned cloudy yellow-brown and slightly opaque as KI precipitated out of solution. After stirring at room temperature for 1 h, the solvent was removed *in vacuo*. The crude solid was extracted in toluene, filtered through Celite, and dried *in vacuo*, affording **3** as a yellow-brown powder (17.1 mg, 70% yield). A slight impurity was detectible in the IR spectrum, corresponding to the peak at 2159 cm^{-1}; this peak is detectable but much smaller in the IR spectrum from Method A. ^{1}H NMR (400 MHz, C_6D_6): δ 3.35 (s, 60H, CH_3 ($Cp^*Ir_{terminal}$)), –0.10 (s, 30H, CH_3 ($Cp^*Ir_{bridging}$)); IR (Nujol mull on KBr): 2159 (m), 1956 (s), 1071 (w), 1032 (m), 813 (m), 564 (w) cm^{-1}. Anal. Calcd (%) for $U_2Ir_6C_{60}H_{106}$ (**3**): C, 29.33; H, 4.35. Found: C, 29.49; H, 3.96.

H$_2$ Monitoring in the Synthesis of 3: $IrCp^*H_4$ (13.7 mg) and $U(Terph)_3$ (17.3 mg) were each dissolved in 0.75 mL C_6D_6. The solution of $IrCp^*H_4$ was added to a J. Young NMR tube, followed by a buffer layer of 0.5 mL C_6D_6, with the $U(Terph)_3$ solution layered on top of that. The remaining headspace of the tube was filled with C_6D_6, after which the tube was sealed, inverted 10 times, and then allowed to sit for 20 minutes before the ^{1}H NMR spectrum was measured.

Magnetism measurements: Samples of UIr_4 (7.1 mg) and U_2Ir_6 (5.4 mg) were loaded into 3 mm (O.D.) quartz tubes and sandwiched between two pieces of quartz wool (UIr_4, 4.1 mg; U_2Ir_6, 6.3 mg) by a modified literature procedure.[6–8] Outside the glovebox, a pre-weighed amount of quartz wool, which had previously been leeched with oxalic and hydrochloric acid, was inserted and packed into a quartz tube with quartz rods. Afterwards, the tubes were oven-dried for 24 h at 150 ° C. Inside a glovebox, two 0.075" (O.D.) polyimide liners were placed inside both ends of the tube. A mild vacuum was applied to one end, such that no quartz wool was pushed out; the other end was used to vacuum sample into tube landing onto the quartz wool without touching the sidewalls. The polyimide liners were removed, and a second piece of quartz wool was inserted into the tube on top of the compound. The sample was compressed into a pellet with two quartz rods. The ends of the tube were capped with two 5 mm NMR tube rubber septa. The capped tubes were removed from the glovebox and surveyed for any contamination. The center of the tube was wrapped with a piece of open-cell foam, saturated with liquid nitrogen, and the ends were flame-sealed with a propane/oxygen torch. Variable temperature magnetization data were recorded from 2–300 K at 1, 2, and 4 T with a 7 T Quantum Design MPMS magnetometer utilizing a superconducting quantum interference device (SQUID). Molar susceptibility, χ_m, was calculated using the formula:

$$\chi_m = \frac{MW}{m}\left[\frac{M_{meas} - M_{imp}}{H} - \chi_{QW}\right] - \chi_d$$

Where MW is the molecular weight of the sample; m is the mass of the sample; M_{meas} is the measured magnetization; M_{imp} is the magnetization due to an assumed ferromagnetic impurity; H is the applied field; and χ_{QW} as well as χ_d are the diamagnetic corrections due to the quartz wool and the sample, respectively, calculated from Pascal's constants.[9] The different applied fields were chosen to saturate M_{imp} so that it's field dependence could be treated as a constant. The value of M_{imp} was allowed to vary to minimize the least squares difference of $\chi_m \cdot T$ between the measured fields from 100−300 K.

UV-Vis Spectra

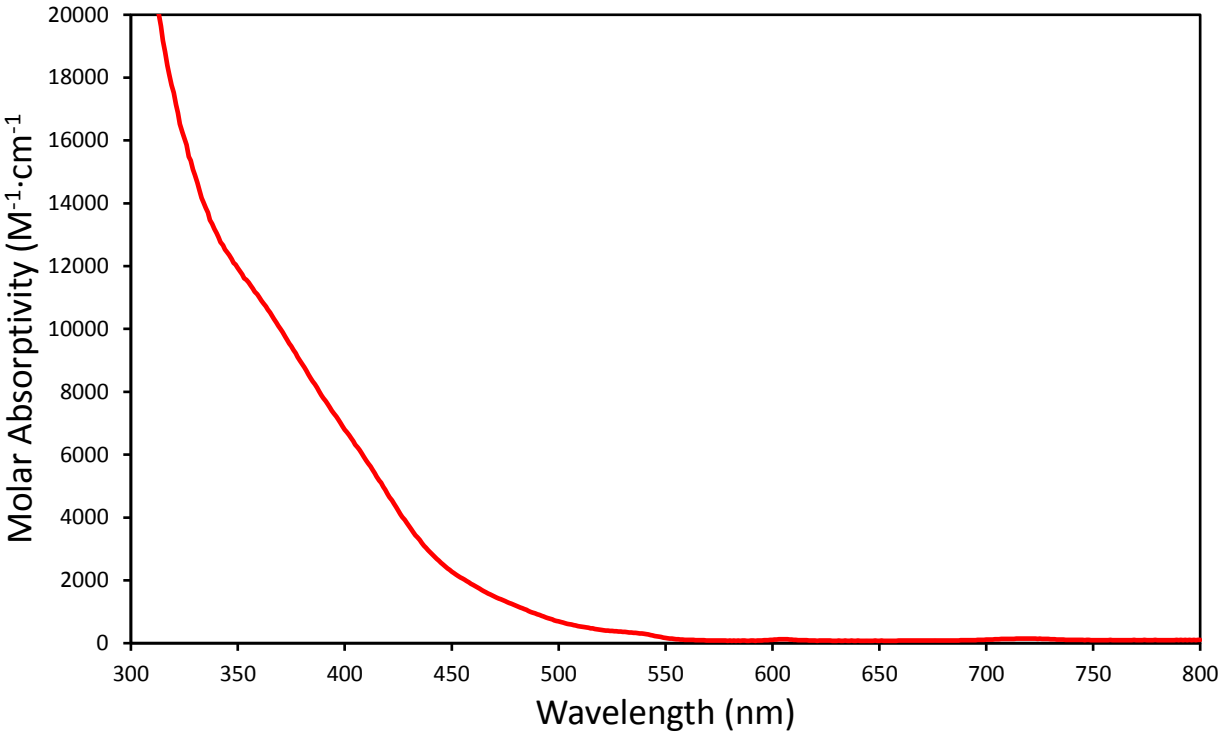


Figure S1. UV-Vis spectrum of **1** in toluene

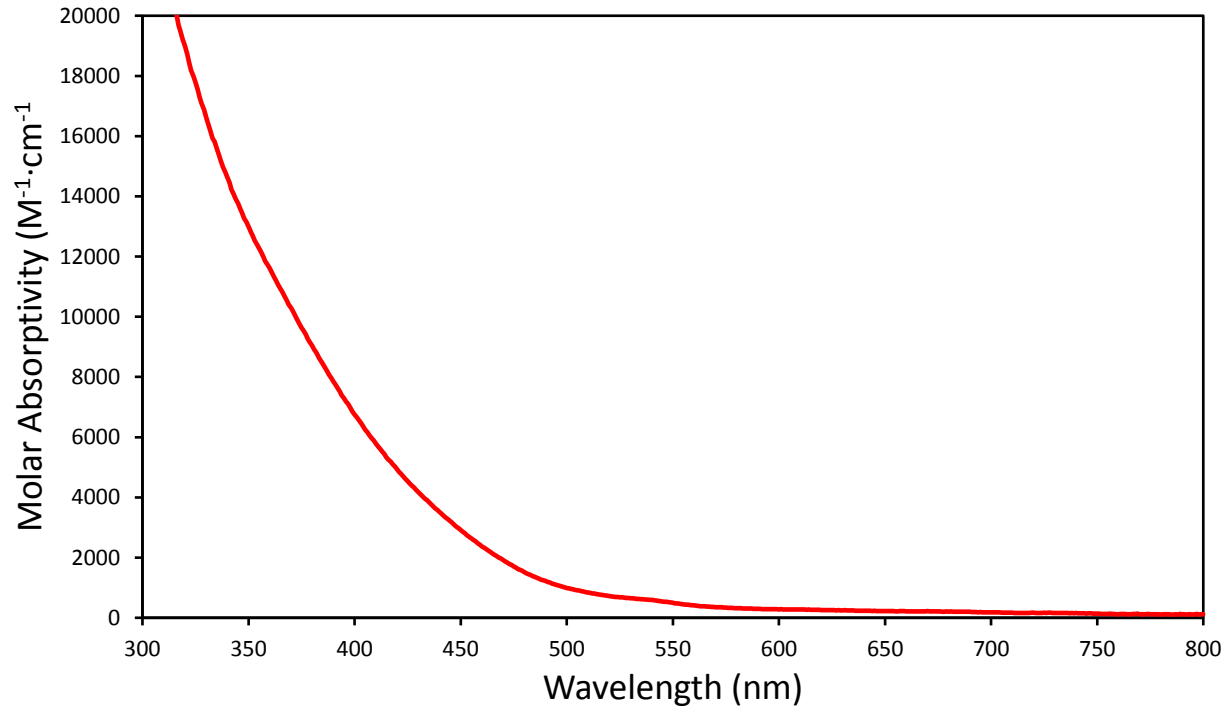


Figure S2. UV-Vis spectrum of **3** in toluene

IR Spectra

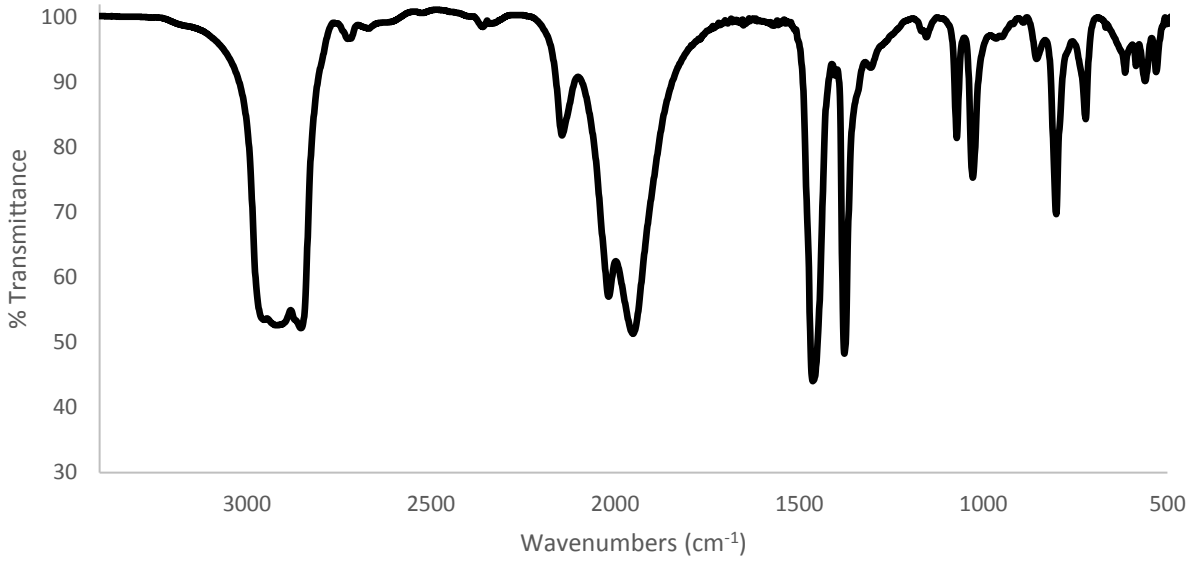


Figure S3. IR spectrum of **1** (Nujol mull)

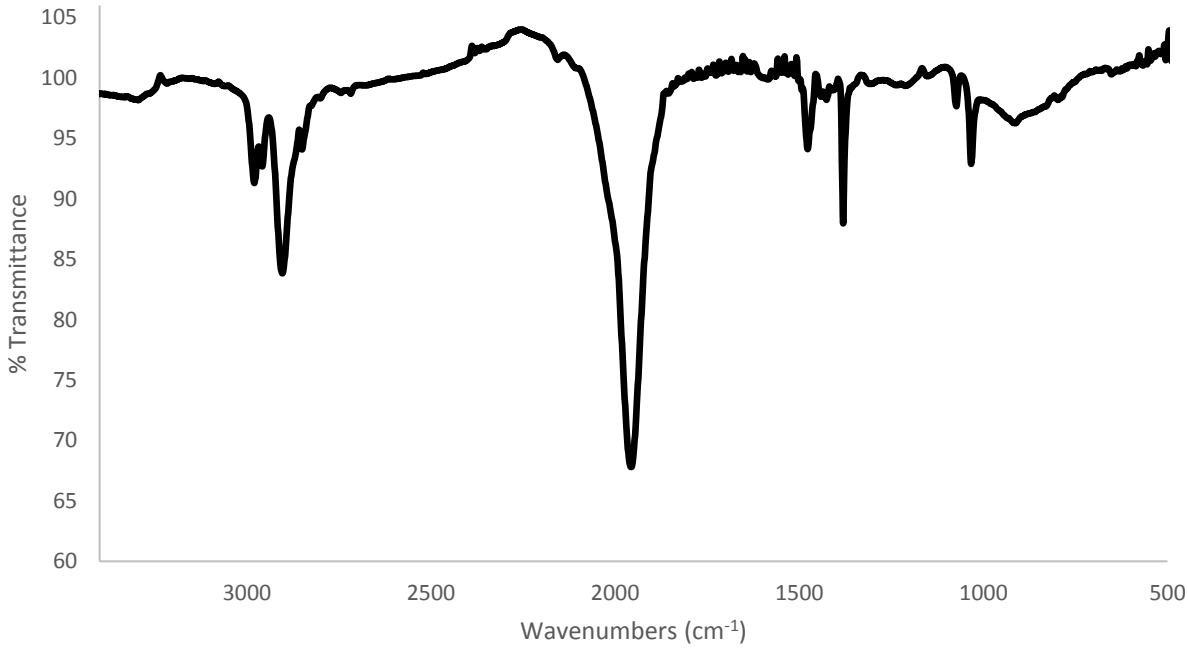


Figure S4. IR spectrum of **1** (in C_6D_6, solvent subtracted)

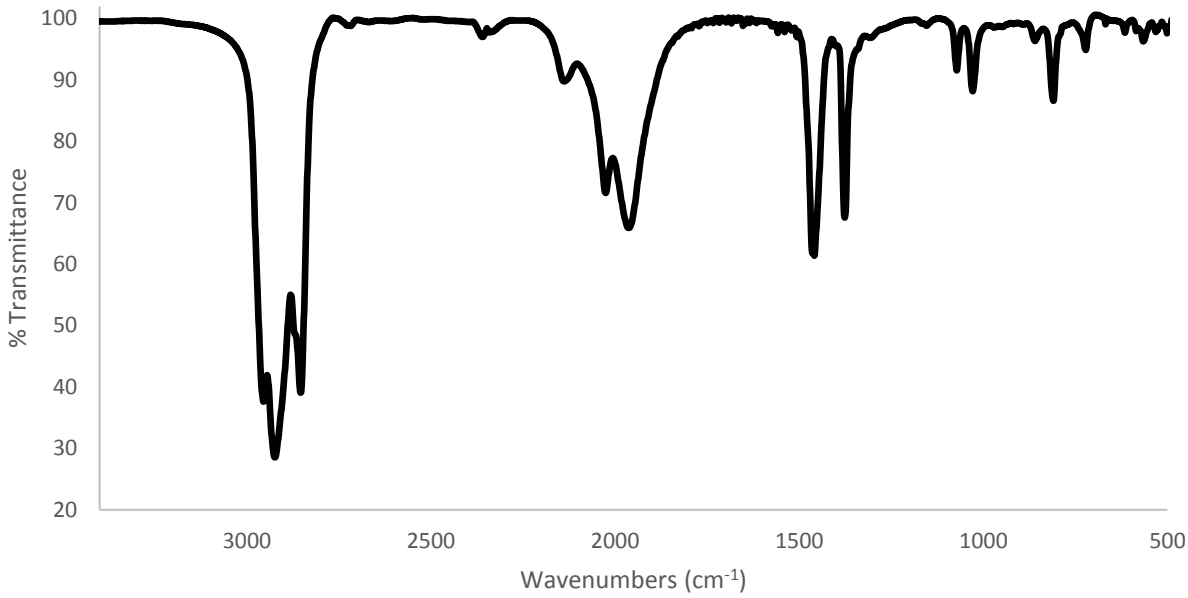


Figure S5. IR spectrum of **2** (Nujol mull)

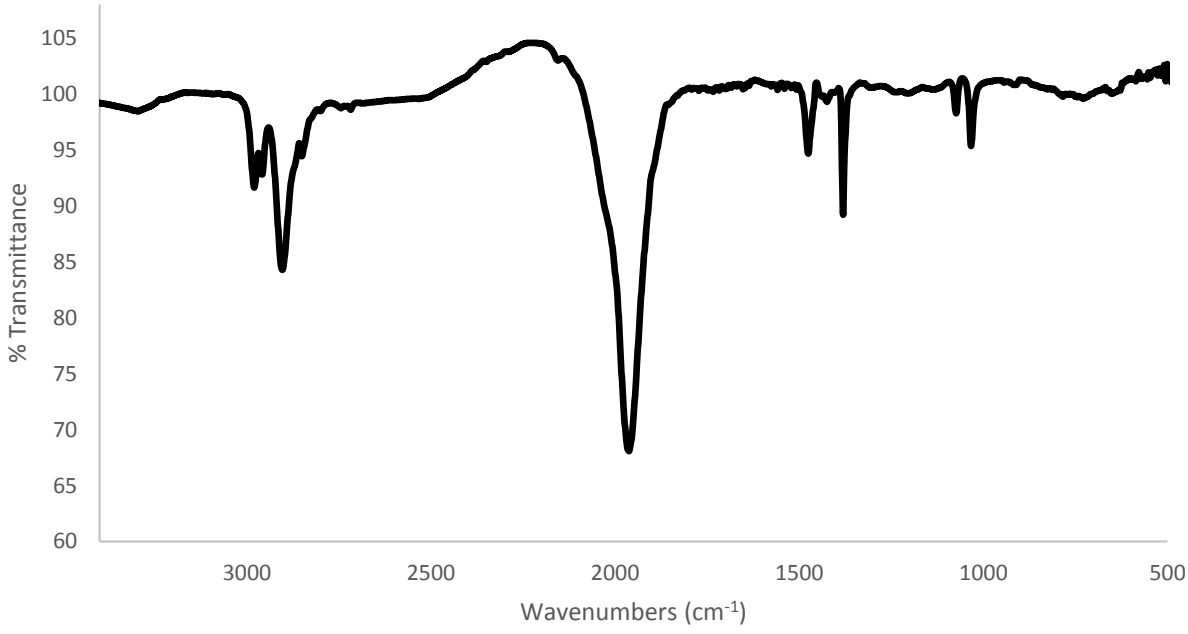


Figure S6. IR spectrum of **2** (in C_6D_6, solvent subtracted)

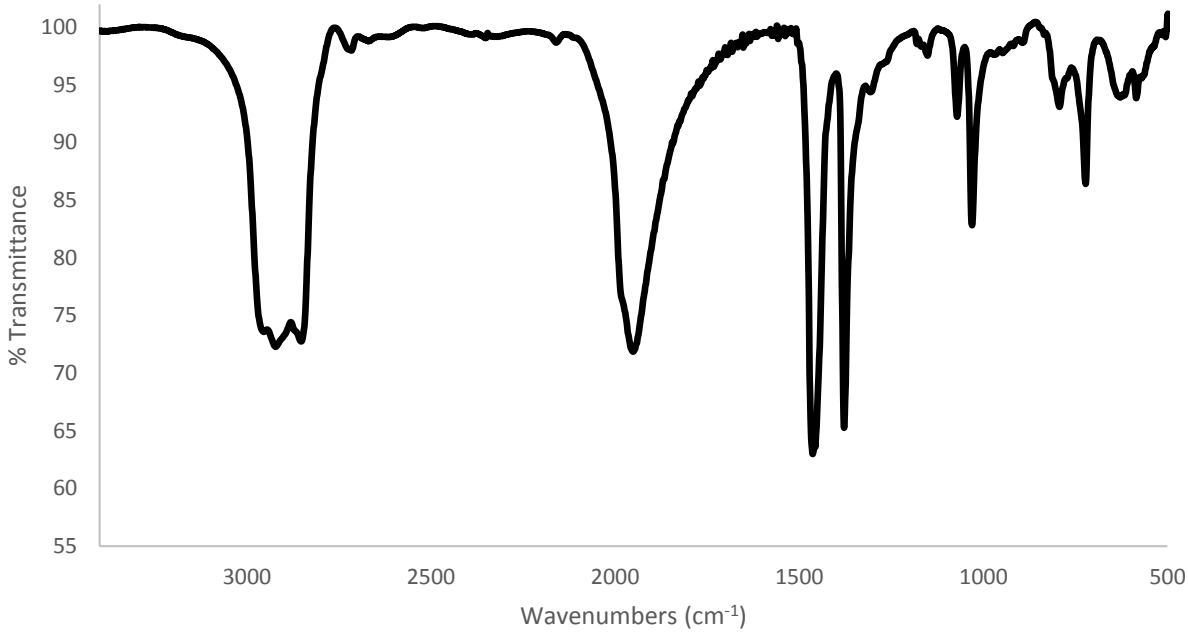


Figure S7. IR spectrum of **3**, synthesized by Method A (Nujol mull)

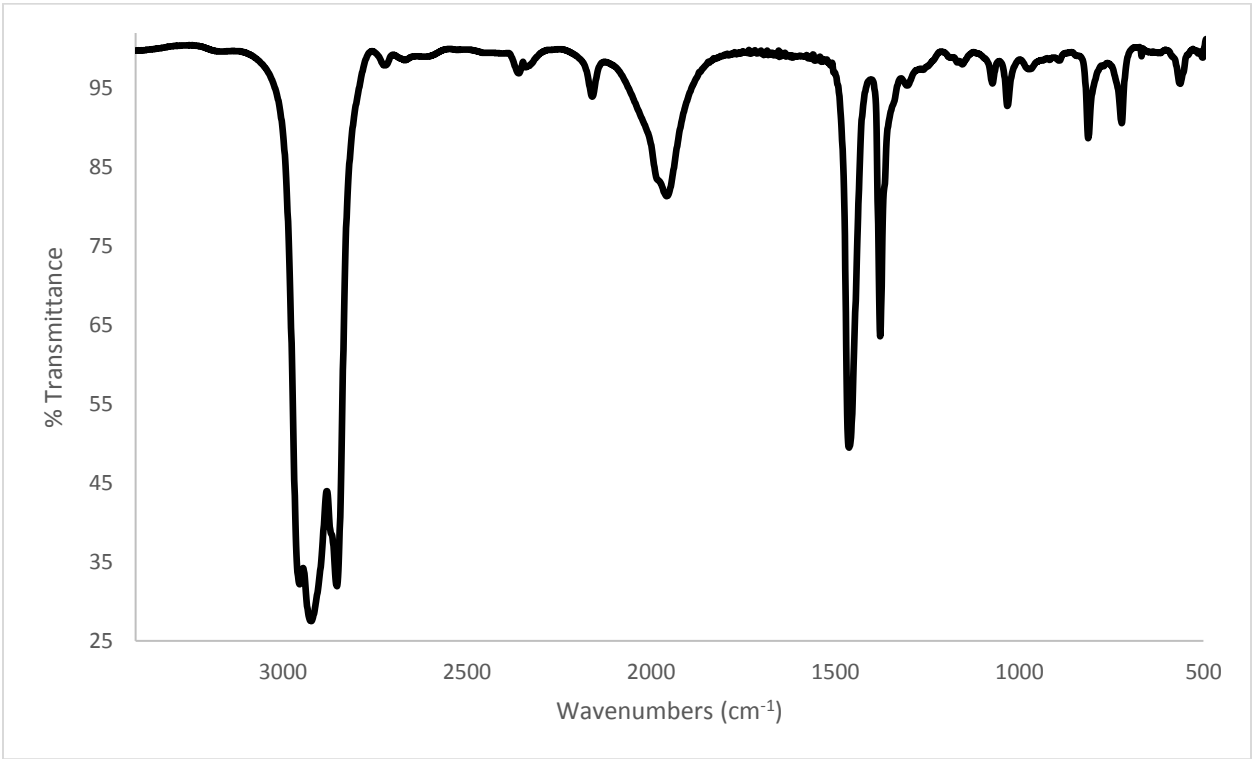


Figure S8. IR spectrum of **3**, synthesized by Method B (Nujol mull)

NMR Spectra

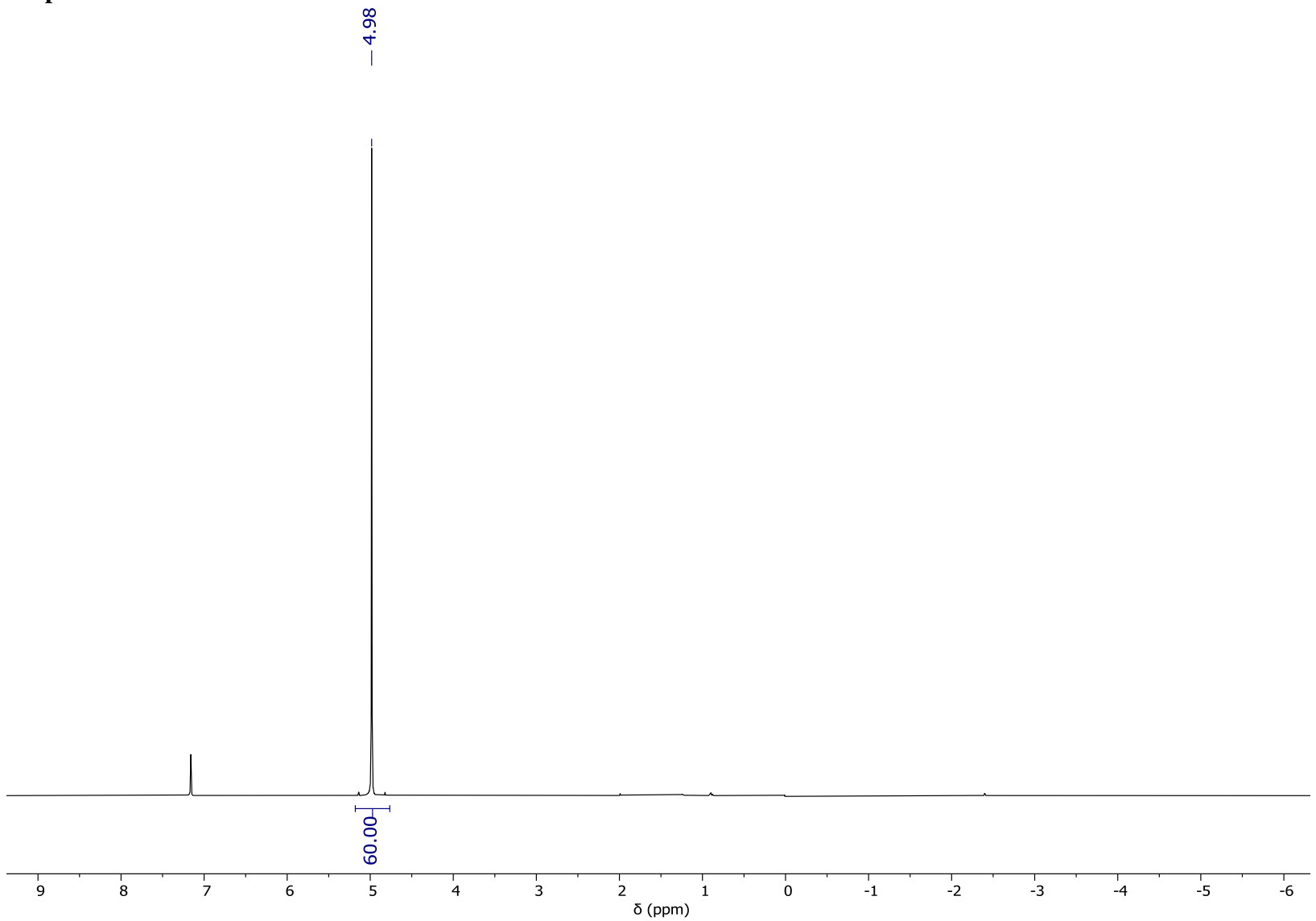


Figure S9. ^{1}H NMR spectrum of **1** in C_6D_6 after initial crystallization from *n*-hexane.

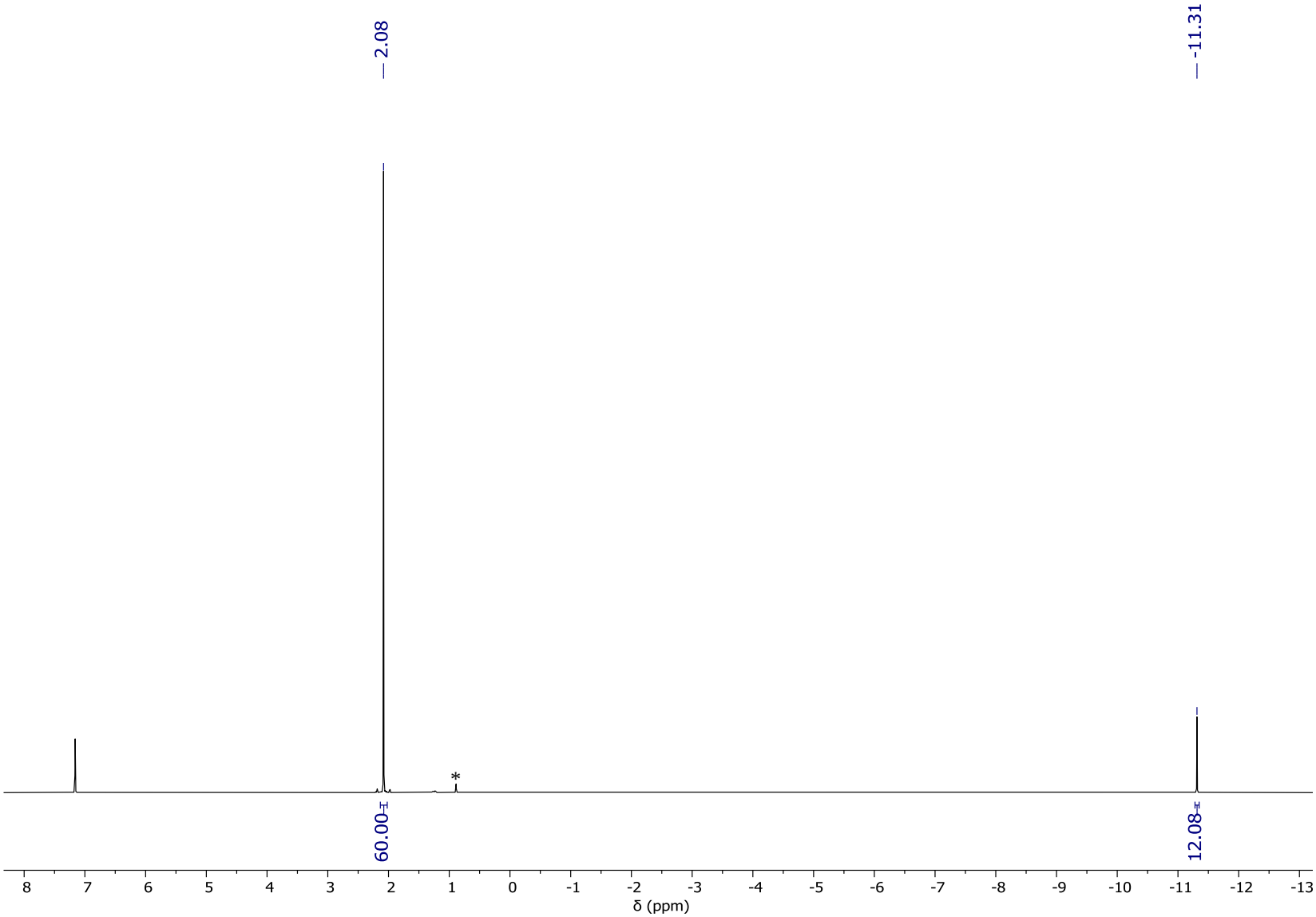


Figure S10. ^{1}H NMR spectrum of **2** in C_6D_6 after initial crystallization from *n*-hexane; * = *n*-hexane.

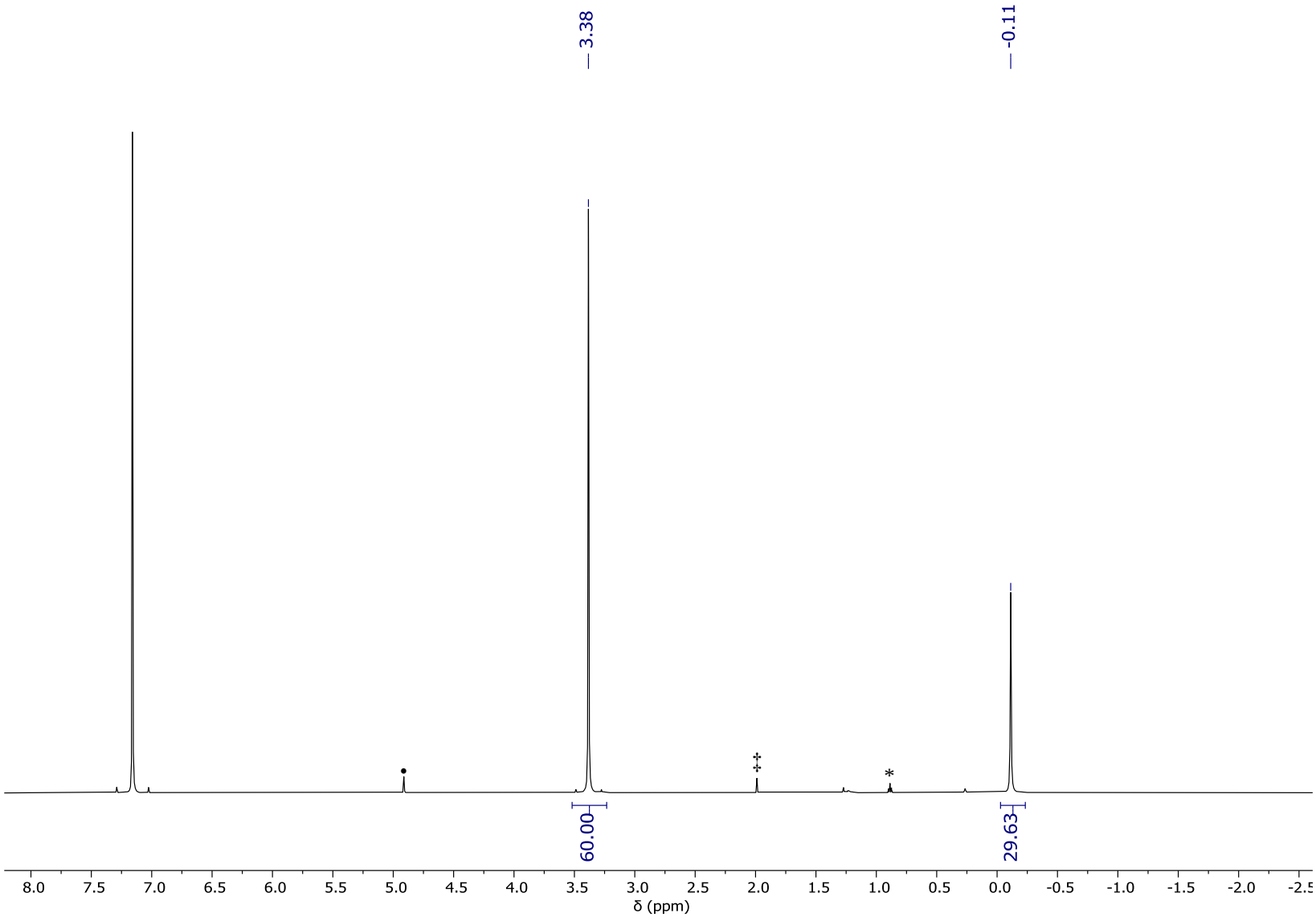


Figure S11. ^{1}H NMR spectrum in C_6D_6 of **3** after crystallization from *n*-hexane; ‡ = $IrCp^*H_4$, * = *n*-hexane, • = impurity of varying concentration, most likely **1** or a similar species formed by the slight decomposition of **3**.

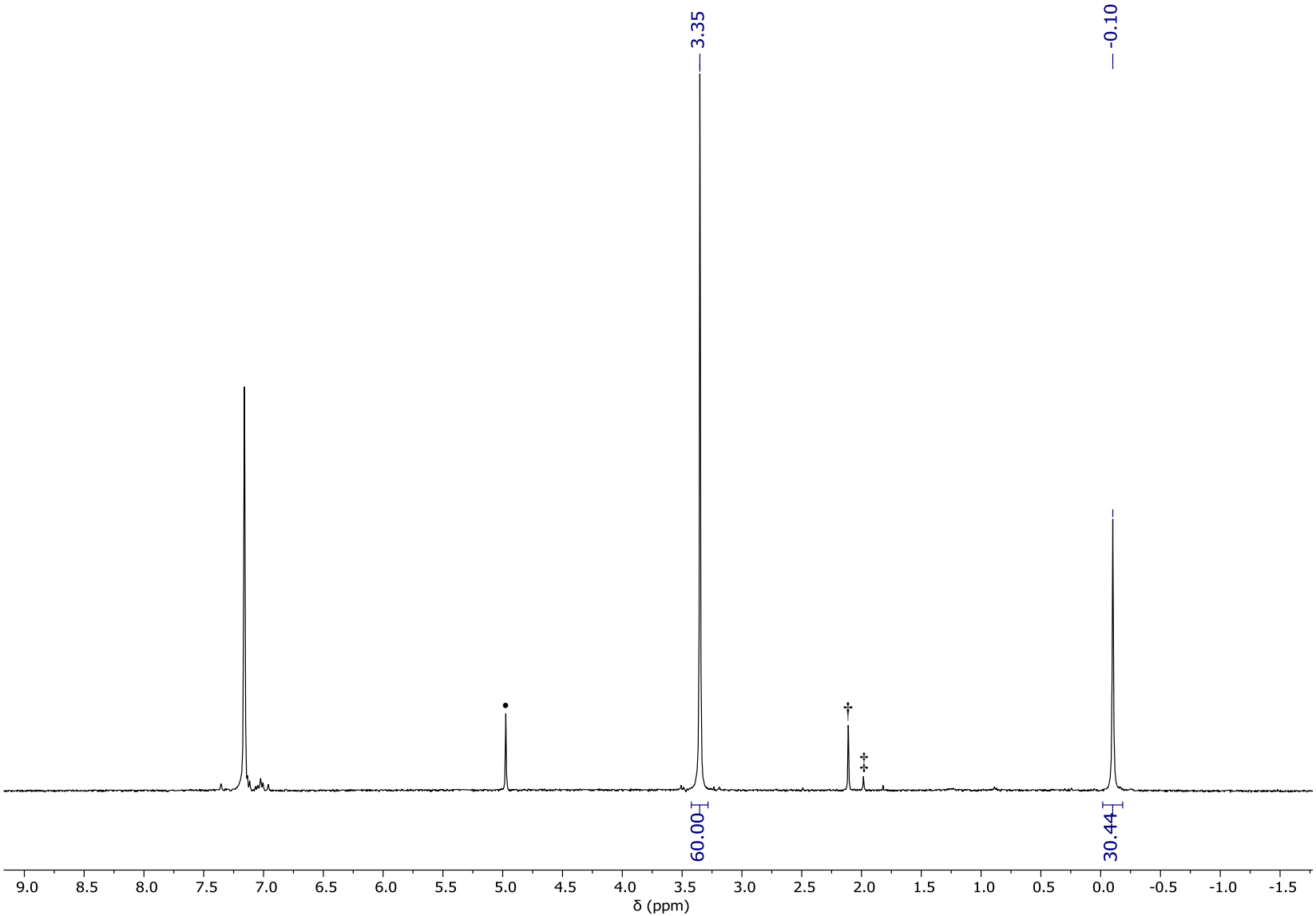


Figure S12. ^{1}H NMR spectrum in C_6D_6 of **3** after extraction from toluene and drying *in vacuo*; † = toluene, ‡ = IrCp*H$_4$, • = impurity of varying concentration, most likely **1** or a similar species formed by the slight decomposition of **3**.

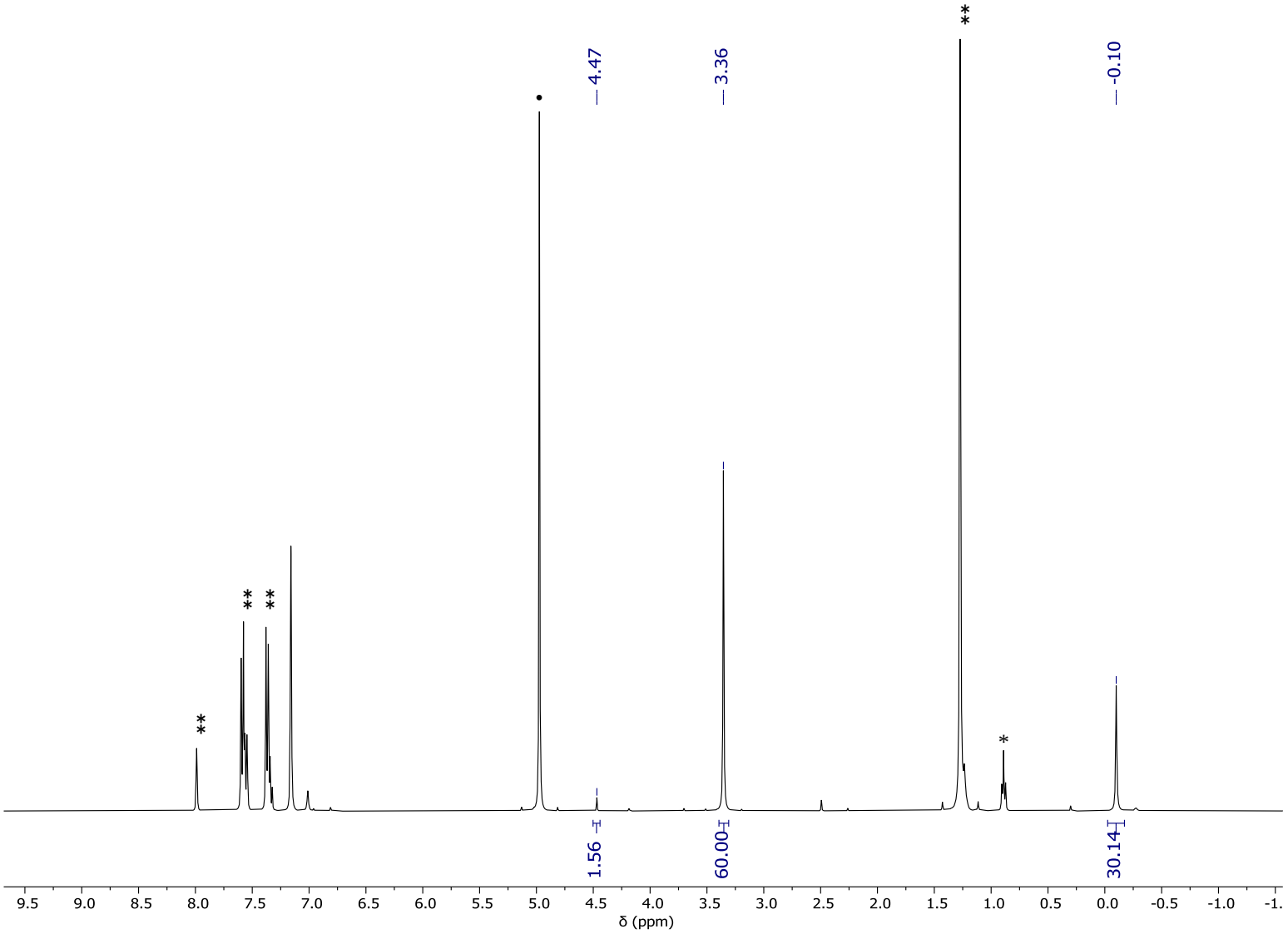


Figure S13. No-headspace ^{1}H NMR spectrum of the synthesis of **3** from Cp*IrH$_4$ and U(Terph)$_3$ in C_6D_6, showing the presence of H_2; * = *n*-hexane, • = impurity of varying concentration, most likely **1** or a similar species formed by the slight decomposition of **3**, ✱ = Terph–H

Table S1. Crystallographic data for U{(μ-H)$_3$IrCp*}$_4$·C$_6$H$_{14}$ (**1**·C$_6$H$_{14}$)

Empirical formula	$C_{46}H_{74}Ir_4U^*$	
Formula weight	1633.88*	
Color, habit	Orange, rod	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 14.8239(6) Å	α = 90°.
	b = 21.1789(6) Å	β = 107.318(5)°.
	c = 17.2427(8) Å	γ = 90°.
Volume	5168.0(4) Å^3	
Z	4	
Density (calculated)	2.100 Mg/m^3	
Absorption coefficient	13.411 mm^{-1}	
F(000)	3000.0	
Crystal size	0.3 × 0.08 × 0.08 mm^3	
Theta range for data collection	3.195 to 29.673°	
Index ranges	$-18 \le h \le 18$, $-26 \le k \le 26$, $-21 \le l \le 21$	
Reflections collected	31322	
Independent reflections	5280 [R_{int} = 0.0472]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.1324	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5280 / 48 / 290	
Goodness-of-fit on F^2	1.389	
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0376, wR$_2$ = 0.0949	
R indices (all data)	R_1 = 0.0400, wR$_2$ = 0.0956	
Largest diff. peak and hole	1.361 and –2.043 e·Å^{-3}	

*The presumed 12 hydrides were not located, hence the reduced empirical formula and formula weight

Table S2. Crystallographic data for Th{[(μ-H_2)(H)IrCp*]$_2$[(μ-H)$_3$IrCp*]$_2$} (**2**)

Empirical formula	$C_{40}H_{60}Ir_4Th$*	
Formula weight	1541.72*	
Color, habit	Colorless, plate	
Temperature	100(2) K	
Wavelength	0.7288 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 13.6424(17) Å	α = 90°.
	b = 19.070(2) Å	β = 102.339(6)°.
	c = 17.520(2) Å	γ = 90°.
Volume	4452.8(10) Å^3	
Z	4	
Density (calculated)	2.300 Mg/m^3	
Absorption coefficient	16.233 mm^{-1}	
F(000)	2792.0	
Crystal size	0.12 × 0.12 × 0.005 mm^3	
Theta range for data collection	3.278 to 27.097°	
Index ranges	$-17 \le h \le 16$, $0 \le k \le 23$, $0 \le l \le 21$	
Reflections collected	9167	
Independent reflections	9167 [R_{int} = 0.0518]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7472 and 0.4006	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9167 / 150 / 427	
Goodness-of-fit on F^2	1.037	
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0625, wR_2 = 0.1430	
R indices (all data)	R_1 = 0.1052, wR_2 = 0.1750	
Largest diff. peak and hole	3.44 and –3.01 e·Å^{-3}	

*The presumed 12 hydrides were not located, hence the reduced empirical formula and formula weight

Table S3. Crystallographic data for $\{U[(\mu_2\text{-}H_3)IrCp^*]_2[(\mu_3\text{-}H_2)IrCp^*]\}_2$ (**3**)

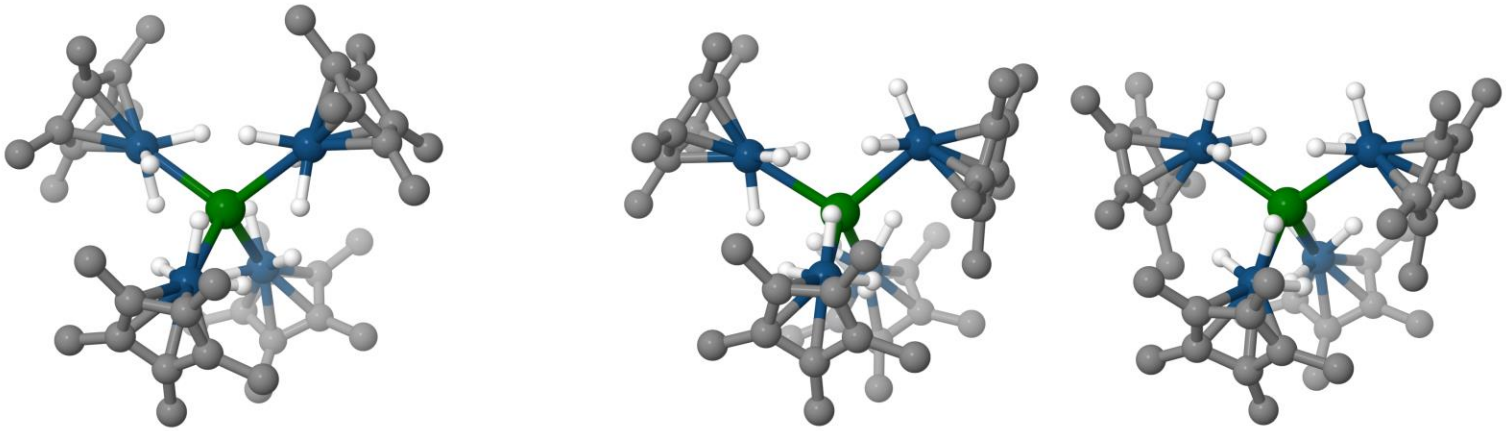
Empirical formula	$C_{60}H_{90}Ir_6U_2$*	
Formula weight	2440.57*	
Color, habit	Black, block	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.0833(2) Å	α = 93.815(1)°.
	b = 15.2848(2) Å	β = 98.607(1)°.
	c = 18.5723(3) Å	γ = 93.365(1)°.
Volume	3375.78(9) Å^3	
Z	2	
Density (calculated)	2.401 Mg/m^3	
Absorption coefficient	16.586 mm^{-1}	
F(000)	2192.0	
Crystal size	0.20 × 0.10 × 0.08 mm^3	
Theta range for data collection	3.007 to 26.370°	
Index ranges	$-15 \le h \le 15$, $-19 \le k \le 18$, $-23 \le l \le 23$	
Reflections collected	69850	
Independent reflections	13763 [R_{int} = 0.0518]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.5156	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13763 / 0 / 643	
Goodness-of-fit on F^2	1.015	
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0243, wR_2 = 0.0579	
R indices (all data)	R_1 = 0.0297, wR_2 = 0.596	
Largest diff. peak and hole	2.723 and –1.262 e·Å^{-3}	

*The presumed 16 hydrides were not located, hence the reduced empirical formula and formula weight

Computational Details

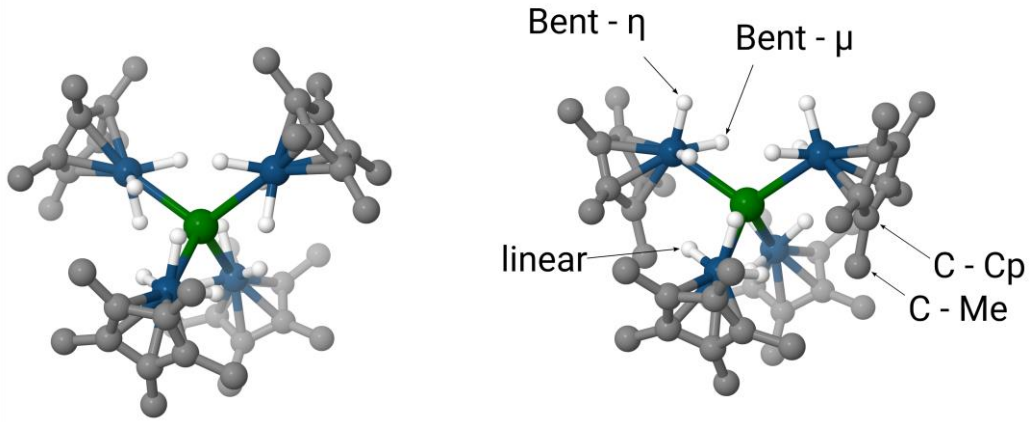
All DFT calculations were carried out with the Gaussian 09 suite of programs.[10] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[11,12] The nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. IRC calculations were performed to confirm the connections of the optimized transition states. Uranium, thorium, and iridium atoms were treated with a small core effective core potential (60 MWB), associated with its adapted basis set[13–15] augmented for iridium atoms with a polarization function ($\zeta f = 0.938$).[16] For the other elements (H, C and N), Pople's double-ζ basis set 6-31G(d,p) was used.[17–19] Dispersion corrections were treated with the D3 version of Grimme's dispersion with Becke-Johnson damping.[20] The electronic charges (at the DFT level) were computed using the natural population analysis (NPA) technique.[21]

Table S4. Calculated and experimental bond distances and angles for **1**



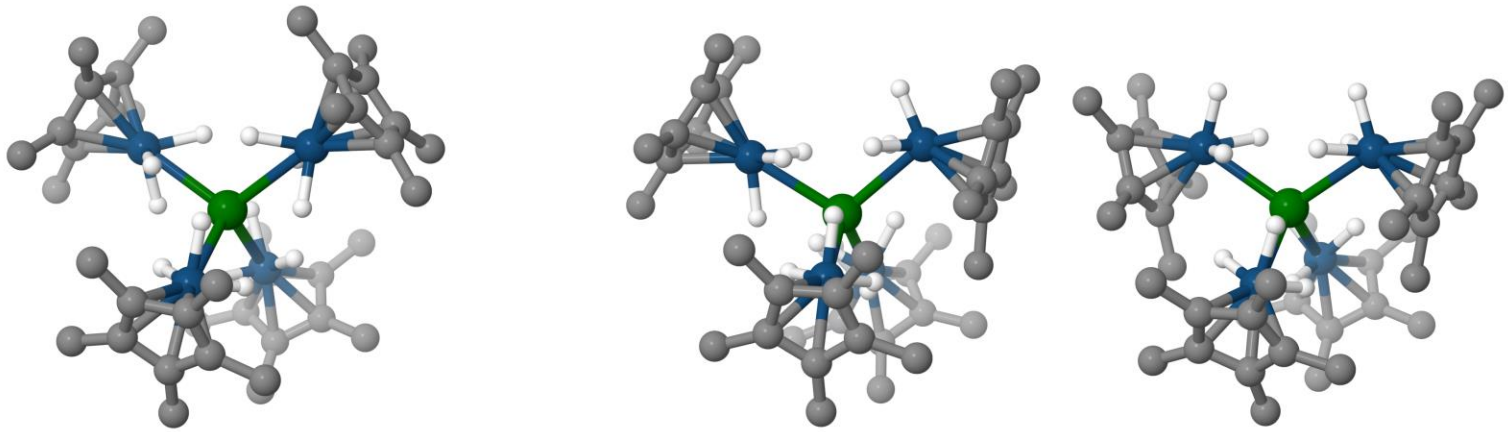
	Linear				Experimental	1-Bent		2-Bent	
Multiplicity	singlet	triplet	triplet (disp)	quintet	–	triplet	triplet (disp)	triplet	triplet (disp)
$\Delta_r G$ (kcal/mol)	30.3	0.0	0.0	41.0	–	10.3	6.8	18.2	4.0
Ir–H dist. (Å)	[1.623–1.629]	[1.625–1.628]	[1.624–1.629]	[1.578–1.655]	–	1.583 [1.618–1.629]	1.584 [1.616–1.629]	[1.581–1.582] [1.615–1.627]	[1.582–1.583] [1.617–1.626]
U–H dist. (Å)	[2.339–2.365]	[2.353–2.467]	[2.326–2.350]	[2.387–2.735]	–	[2.342–2.398] 3.569	[2.319–2.406] 3.641	[2.352–2.390] [3.436–3.487]	[2.325–2.414] [3.607–3.617]
U–Ir dist. (Å)	2.941/2.941 2.940/2.942	2.954/2.956 2.951/2.952	2.905/2.907 2.912/2.913	3.032/3.033 3.056/3.175	2.951/2.959 2.951/2.959	2.921/2.934 2.961/2.964	2.849/2.891 2.920/2.922	2.901/2.903 2.973/2.973	2.828/2.831 2.930/2.932
Ir–U–Ir angle (°)	[108.0–111.5]	[108.8–110.4]	[106.8–111.4]	[109.6–116.7]	[102.8–118.9]	[108.6–110.7]	[106.9–112.8]	[107.1–110.8]	[107.6–113.5]

Table S5. Calculated NBO Wiberg Bond Indices for **1**



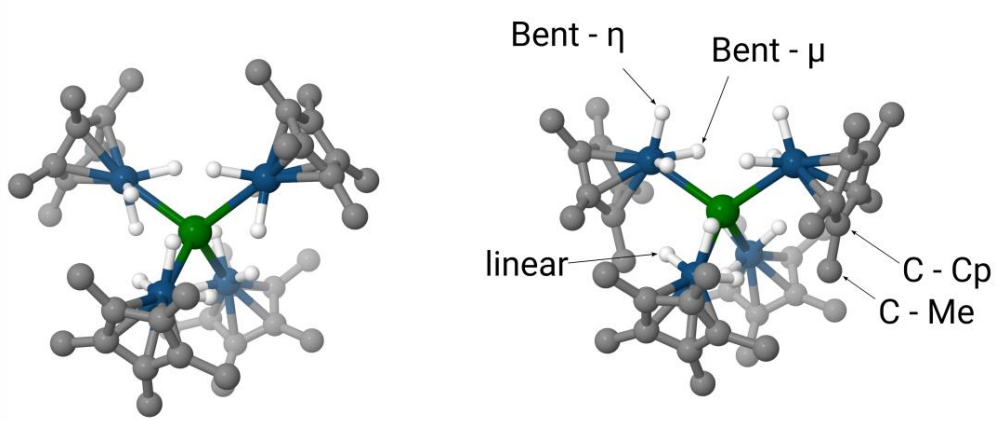
	Linear		2 - Bent	
	With disp	Without disp	With disp	Without disp
U – Ir	[0.96 - 0.98]	[0.94 - 0.95]	0.79 (linear) 0.88 (bent)	0.69 (linear) 0.78 (bent)
Ir – H	0.53	0.55	0.55 (linear) 0.56 (bent – μ) 0.70 (bent - η)	0.57 (linear) 0.56 (bent – μ) 0.70 (bent - η)
U – H	[0.28 – 0.30]	[0.27 - 0.29]	0.27 (linear) 0.25 (bent – μ) 0.04 (bent - η)	0.27 (linear) 0.26 (bent – μ) 0.051 (bent - η)
C(Cp*) – U	–	–	0.08 (C – Cp) 0.01 (C – Me)	0.07 (C – Cp) 0.00 (C – Me)

Table S6. Tabulated calculated bond distances/angles for **2**



	Linear		Experimental	1-Bent		2-Bent	
Multiplicity	singlet	singlet (disp)	–	singlet	singlet (disp)	singlet	singlet (disp)
$\Delta_r G$ (kcal/mol)	0.0	0.0	–	8.5	–4.3	16.4	–9.4
Ir–H dist. (Å)	[1.624–1.625]	[1.623–1.625]	–	1.583 [1.618–1.629]	1.584 [1.616–1.629]	[1.581–1.582] [1.615–1.627]	[1.582–1.583] [1.617–1.626]
Th–H dist. (Å)	[2.426–2.440]	[2.404–2.420]	–	[2.342–2.398] 3.569	[2.319–2.406] 3.641	[2.352–2.390] [3.436–3.487]	[2.325–2.414] [3.607–3.617]
Th–Ir dist. (Å)	3.022/3.022 3.022/3.022	2.978/2.978 2.979/2.979	2.964/2.983 3.010/3.015	2.984/3.005 3.024/3.036	2.916/2.964 2.985/2.988	2.964/2.970 3.036/3.047	2.899/2.902 2.995/2.999
Ir–Th–Ir angle (°)	[109.0–110.1]	[108.8–110.3]	[107.5–113.0]	[107.9–111.3]	[107.6–112.8]	[108.3–111.1]	[107.5–114.4]

Table S7. Calculated NBO Wiberg Bond Indexes for **2**



	Linear		2 - Bent	
	With disp	Without disp	With disp	Without disp
Th – Ir	0.65	0.63	0.63 (linear) 0.65 (Bent)	0.60 (linear) 0.69 (Bent)
Ir – H	0.56	0.57	0.57 (linear) 0.58 (Bent – μ) 0.70 (Bent - η)	0.59 (linear) 0.59 (Bent – μ) 0.70 (Bent - η)
Th – H	0.27	0.26	0.25 (linear) 0.24 (Bent – μ) 0.05 (Bent - η)	0.24 (linear) 0.24 (Bent – μ) 0.05 (Bent - η)
C(Cp*) – Th	–	–	0.10 (C – Cp) 0.04 (C – Me)	0.08 (C – Cp) 0.00 (C – Me)

Figure S14. Renderings of the calculated HOMOs (**2**) or SOMOs (**1**) and LUMO (c) of linear and bent structures of **1** and **2** (isovalue = 0.03)

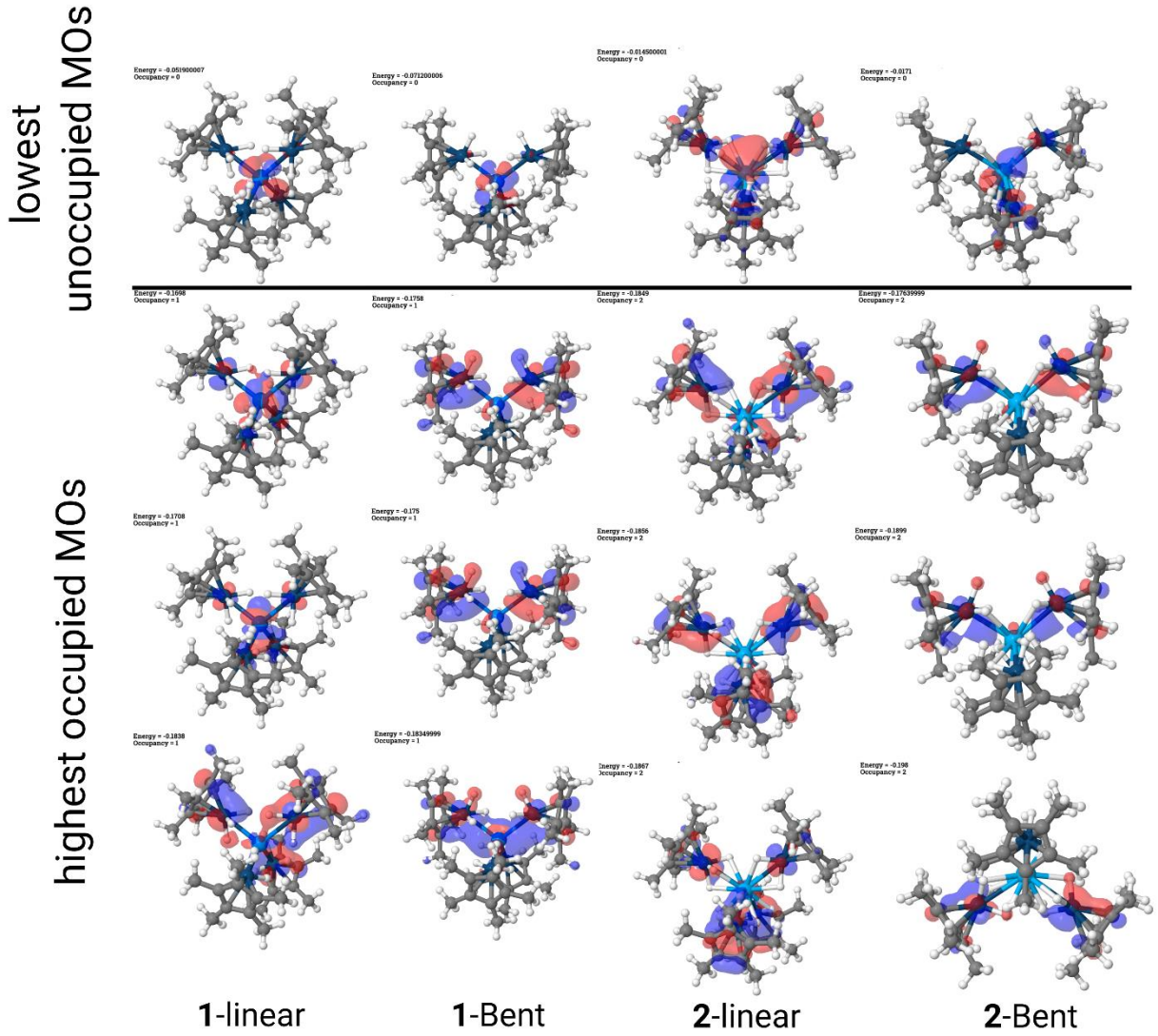


Table S8. U/Th and Ir contributions to the calculated HOMOs or SOMOs and LUMO of linear **1** and **2**. For sake of clarity, only the contributions higher than 0.05 are depicted on this table.

	SOMO-1	SOMO	LUMO		HOMO-1	HOMO	LUMO
U				Th			
5S	-0.02602	0.00031	-0.06169	19PX	-0.00983	-0.00496	0.15726
7S	0.05018	-0.00046	0.11564	19PY	-0.00382	-0.00502	0.28804
9S	-0.00398	0.00073	0.13518	19PZ	-0.00100	0.01422	-0.28669
10S	-0.01538	-0.00084	-0.27810	23D 0	-0.00499	0.00160	0.08906
19PY	0.05177	-0.00307	-0.02755	23D+1	0.00062	0.00227	0.06664
23D 0	-0.05017	-0.00147	0.01106	23D-2	-0.00052	-0.00528	-0.12398
25F 0	-0.00620	-0.11845	-0.00308	24D 0	0.00875	-0.00337	0.17613
25F+1	-0.00409	-0.19062	-0.01142	24D+1	0.00986	-0.00318	0.13394
25F-1	0.37190	-0.00035	0.15941	24D-1	0.00559	0.00806	-0.09313
25F+2	-0.01135	0.25566	-0.01178	24D+2	-0.00524	-0.00033	-0.07914
25F-2	-0.01542	0.01256	0.30710	24D-2	0.00027	0.00596	-0.23796
25F+3	-0.01408	0.21882	0.01216	25F+1	-0.00286	-0.01492	0.08928
25F-3	0.19425	0.02119	-0.27323	25F-1	-0.02126	0.00715	-0.05482
26F 0	-0.00546	-0.10353	-0.00276	26F-3	0.01752	-0.00417	-0.05552
26F+1	-0.00360	-0.16737	-0.01012	27F+1	-0.00263	-0.01399	0.05568
26F-1	0.32708	-0.00030	0.14089	Ir			
26F+2	-0.00999	0.22504	-0.01045	6S	0.00154	-0.00052	0.59538
26F-2	-0.01348	0.01104	0.27192	8PX	-0.04861	-0.05338	0.00607
26F+3	-0.01237	0.19243	0.01079	8PY	0.03359	0.08735	0.00170
26F-3	0.17099	0.01863	-0.24179	8PZ	-0.06883	0.02971	-0.00294
27F 0	-0.00363	-0.06590	-0.00193	10PX	0.05108	0.02696	0.01794

27F+1	-0.00253	-0.11126	-0.00720	10PY	-0.01594	-0.07198	0.06121
27F-1	0.22027	0.00004	0.10267	11PX	-0.00145	-0.00189	0.33522
27F+2	-0.00698	0.15682	-0.00743	11PY	0.00258	0.00350	0.18722
27F-2	-0.00511	0.00790	0.19470	12D 0	0.10653	-0.07212	0.01635
27F+3	-0.00870	0.12850	0.00777	12D+1	-0.01370	-0.21113	-0.09641
27F-3	0.11864	0.01267	-0.17544	12D-1	0.21270	0.18646	-0.05732
28F-1	0.09777	0.00052	0.07186	12D+2	0.04713	0.01644	-0.10350
28F+2	-0.00386	0.08049	-0.00481	12D-2	0.10851	-0.07579	0.06526
28F-2	0.01414	0.00378	0.11663	13D+1	0.00264	-0.08584	-0.04919
4S	0.02235	-0.00220	0.06251	13D-1	0.08722	0.06883	-0.03020
Ir				13D+2	0.02767	0.02084	-0.05952
12D 0	0.09432	-0.02623	0.01985	14D-2	0.00532	0.00673	0.09075
12D+1	0.05627	0.07598	0.00246	Ir			
12D-1	0.03989	-0.15929	0.00590	8PX	-0.06315	0.09228	-0.00405
12D-2	0.08320	-0.05499	-0.06417	10PX	0.05228	-0.06294	0.07285
13D-1	0.01225	-0.05602	0.00742	10PZ	0.00629	0.01551	-0.05273
4S	0.00497	0.01090	0.05741	11PY	-0.00142	-0.00166	-0.12099
Ir				11PZ	0.00124	0.00112	0.12274
5S	0.00325	0.01035	0.08684	12D 0	0.00728	0.02084	0.24999
10PY	0.02145	-0.07226	0.02368	12D+1	0.05657	-0.07790	-0.15368
12D-1	-0.12990	0.09752	-0.03900	12D+2	-0.08119	0.09543	0.11408
12D+2	-0.08886	-0.05755	0.03706	12D-2	-0.15621	0.24178	-0.10986
12D-2	-0.07879	-0.03060	-0.00340	13D 0	0.00539	0.00654	0.13244
Ir				13D+1	0.01277	-0.01799	-0.09025
4S	0.02142	0.00195	0.06105	13D-2	-0.06375	0.09726	-0.06939

5S	0.02217	0.01126	0.08612	14D-2	0.00217	-0.00400	-0.06262
12D 0	0.09478	0.04190	0.01963	Ir			
12D+1	0.06362	-0.06135	0.00264	6S	-0.00086	-0.00162	-0.05074
12D-1	-0.02592	-0.16053	-0.00846	8PX	0.00662	-0.06795	0.00171
12D-2	-0.07971	-0.06508	0.06156	8PY	-0.02785	-0.08636	0.00105
13D-1	-0.00691	-0.05665	-0.00815	8PZ	0.08936	-0.02908	0.00135
Ir				10PX	-0.01708	0.05127	0.00877
4S	0.00517	-0.01006	0.05418	10PY	0.02749	0.06309	0.04448
5S	0.00373	-0.00912	0.08217	10PZ	-0.06388	0.01587	-0.08204
10PY	0.01984	0.07086	0.02284	11PY	0.00011	-0.00431	-0.14276
12D-1	0.13184	0.09599	0.03714	11PZ	0.00543	-0.00220	0.11438
12D+2	-0.10008	0.06361	0.03600	12D 0	0.16916	-0.02649	-0.16340
12D-2	0.06307	-0.03009	0.00448	12D+1	0.13965	0.15425	0.19334
13D-1	0.05617	0.04311	0.01926	12D-1	-0.06388	0.27795	-0.09272
				12D+2	0.03407	-0.05453	-0.16751
				12D-2	-0.15492	0.00947	-0.06573
				13D 0	0.05605	-0.00961	-0.09450
				13D+1	0.06491	0.05702	0.10485
				13D-1	-0.03189	0.10812	-0.06500
				13D+2	0.01073	-0.03721	-0.08837
				13D-2	-0.06177	-0.00154	-0.03615
				Ir			
				5S	-0.00541	0.02821	-0.22680
				6S	0.00013	0.00630	-0.51129
				8PX	0.10954	0.03024	-0.00290

					10PX	-0.08206	-0.01430	0.03619
					10PY	-0.00106	-0.02916	0.07089
					11PX	0.00864	0.00379	-0.17972
					11PY	0.00251	0.00011	0.13058
					11PZ	-0.00033	0.00468	-0.25371
					12D+1	0.09108	0.02313	0.14486
					12D-1	0.04081	-0.02557	0.10218
					12D+2	-0.18147	-0.01911	0.14035
					12D-2	0.24588	0.09257	-0.01328
					13D+1	0.01986	0.00497	0.08227
					13D-1	0.01159	-0.01161	0.06082
					13D+2	-0.07271	-0.01036	0.07590
					13D-2	0.10178	0.03606	-0.00016
					14D-1	0.00874	0.00211	0.09859

Table S9. U/Th, C(Cp) and Ir contributions to the calculated HOMOs or SOMOs and LUMO of bent **1** and **2**. For sake of clarity, only the contributions higher than 0.05 are depicted on this table.

	HOMO-1	HOMO	LUMO		HOMO-1	HOMO	LUMO
U				Th			
4S	-0.10290	0.00008	-0.00278	4S	-0.09269	-0.00019	0.00304
5S	0.14911	0.00017	0.00395	5S	0.13546	0.00037	-0.00348
6S	0.06747	-0.00109	0.00212	6S	0.06012	-0.00019	-0.00560
7S	-0.23710	0.00282	-0.00733	7S	-0.21294	0.00026	0.01693
8S	-0.07471	-0.00494	-0.00006	8S	-0.07906	-0.00141	-0.01678
9S	0.27558	0.02178	-0.00455	9S	0.22743	0.00419	0.00555
10S	-0.09111	-0.00484	-0.00161	10S	-0.13864	-0.00392	0.54834
16PX	-0.00206	0.12766	-0.00169	15PY	-0.05667	-0.00649	-0.02628
16PY	0.06080	0.00992	0.00051	16PX	-0.00437	0.11495	0.00797
16PZ	0.01007	-0.06685	0.00426	16PY	0.08381	0.00963	0.04188
17PX	-0.00242	0.09804	-0.00254	16PZ	0.00792	-0.06146	0.03966
17PY	0.05871	0.00747	-0.00070	17PX	-0.00509	0.13165	0.01050
17PZ	0.00804	-0.05163	0.00269	17PY	0.10256	0.01177	0.04126
23D+1	-0.08901	0.00980	-0.00875	17PZ	0.00886	-0.07046	0.05200
23D-1	-0.01882	-0.06493	0.03133	21D 0	0.01662	0.00278	-0.06700
23D+2	0.05360	-0.01407	0.01431	22D 0	-0.01194	-0.00207	0.05625
23D-2	0.00312	0.12237	-0.06631	23D 0	-0.04623	-0.00740	0.17317
24D+1	-0.06900	0.00624	-0.00095	23D+1	-0.11405	0.01156	0.06041
25F 0	-0.02987	-0.03775	-0.25892	23D-1	-0.00679	-0.06616	0.10138

25F+1	0.09212	0.00234	0.12996	23D+2	0.05979	-0.01673	-0.07795
25F-1	-0.11830	0.00278	0.11279	23D-2	0.01486	0.12438	0.05977
25F-2	-0.20381	0.00720	-0.09002	24D 0	-0.02949	-0.00611	0.25477
25F+3	-0.09877	0.00020	0.30061	24D+1	-0.08645	0.00822	0.10602
25F-3	0.05884	-0.00199	0.04204	24D-1	-0.00850	-0.04042	0.13017
26F 0	-0.02637	-0.03285	-0.22942	24D+2	0.04813	-0.01151	-0.09367
26F+1	0.08109	0.00201	0.11529	24D-2	0.01403	0.08123	0.07359
26F-1	-0.10415	0.00241	0.10017	25F+1	0.00123	0.00237	-0.07201
26F-2	-0.17886	0.00641	-0.07978	25F-1	-0.00376	0.00184	-0.08484
26F+3	-0.08684	0.00028	0.26656	25F-3	-0.03337	-0.00017	-0.05989
26F-3	0.05093	-0.00175	0.03716	26F+1	0.00085	0.00148	-0.05585
27F 0	-0.01810	-0.02854	-0.16495	27F-1	-0.00377	0.00147	-0.05119
27F+1	0.05531	0.00180	0.08266	Ir			
27F-1	-0.07112	0.00146	0.07017	4S	-0.05001	-0.00013	0.00929
27F-2	-0.11788	0.00503	-0.05593	5S	0.03317	0.01416	-0.17048
27F+3	-0.05828	-0.00204	0.18924	6S	0.04566	0.01044	-0.32958
28F 0	-0.00937	-0.01485	-0.08874	10PX	-0.00702	-0.02695	0.05457
Ir				10PY	-0.00334	0.00179	0.05774
4S	-0.05951	-0.00582	-0.00360	10PZ	0.01004	-0.00283	0.04731
12D+2	-0.01205	0.05872	-0.05382	11PX	-0.01496	-0.00764	0.06425
12D-2	0.00277	-0.00723	0.05686	11PY	-0.03708	-0.00659	0.06113
Ir				11PZ	-0.03097	-0.00747	0.15469

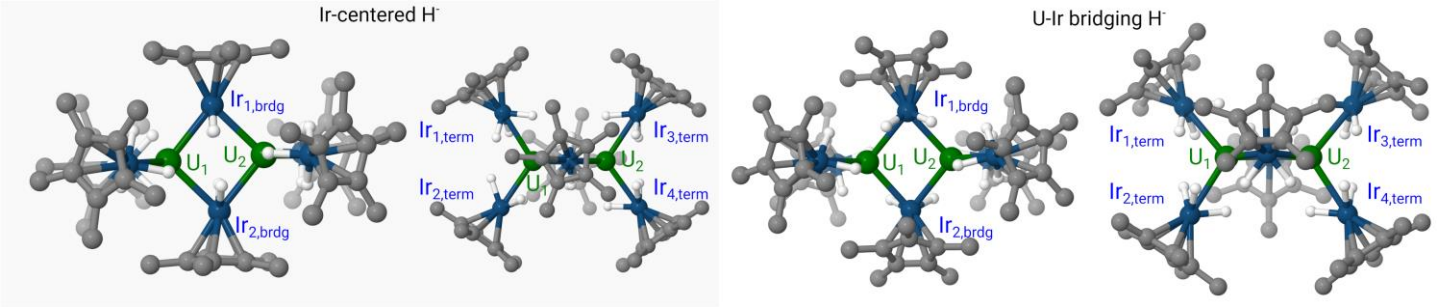
2S	0.05099	0.00206	-0.00112	12D 0	-0.03008	-0.03785	0.08329
4S	-0.06711	0.00249	-0.00094	12D+1	0.01429	0.01250	-0.06067
12D+1	0.05890	-0.00057	0.05956	12D+2	-0.01890	0.06871	0.03858
12D-1	-0.06723	-0.00454	0.00448	12D-2	-0.04015	-0.00755	-0.11091
Ir				Ir			
5S	-0.01259	0.07349	0.03526	5S	0.02093	-0.02211	-0.15621
8PY	-0.10017	-0.13640	0.00223	6S	0.04351	-0.01287	-0.08325
10PY	0.09661	0.15327	-0.01820	10PX	0.00748	-0.04210	-0.05871
12D 0	-0.11971	-0.16604	0.01670	10PY	-0.00653	-0.00571	0.09313
12D+1	-0.14139	-0.06772	0.07594	10PZ	-0.03107	-0.00370	0.05147
12D+2	-0.05741	-0.16188	-0.03442	11PY	-0.03464	0.00906	-0.08269
12D-2	0.17823	0.20961	0.01430	11PZ	0.02568	-0.00966	-0.14340
13D 0	-0.04521	-0.06488	0.00870	12D 0	-0.04055	0.02411	0.34516
13D+1	-0.05219	-0.01599	0.03269	12D-1	0.00407	0.00776	-0.05582
13D+2	-0.02231	-0.06678	-0.01755	12D+2	0.00095	-0.06507	0.14813
13D-2	0.07236	0.09085	0.00179	12D-2	0.02639	0.02265	0.21044
Ir				13D 0	-0.02326	0.00502	0.17714
5S	-0.01873	-0.07483	-0.01094	13D-2	0.00534	0.00667	0.12326
8PY	-0.09795	0.12931	-0.00483	14D 0	-0.00709	0.01017	0.10295
10PX	-0.04067	0.06445	-0.02115	14D-2	-0.00875	0.01919	0.06964
10PY	0.08740	-0.14631	0.02690	Ir			
12D 0	-0.14299	0.14791	-0.05076	5S	-0.00149	0.07369	-0.09849

12D+1	-0.16416	0.10847	-0.04850	8PY	-0.14117	-0.13202	0.00792
12D-1	0.08492	-0.08079	-0.01855	10PY	0.12286	0.15101	-0.01257
12D+2	-0.03785	0.10192	0.04034	10PZ	-0.02212	-0.01091	0.07029
12D-2	-0.10548	0.21735	0.01509	12D 0	-0.14936	-0.16355	-0.12334
13D 0	-0.05342	0.05444	-0.02469	12D+1	-0.16130	-0.09526	0.03995
13D+1	-0.06242	0.03655	-0.02213	12D-1	-0.04134	-0.06675	-0.03702
13D-2	-0.04534	0.09796	0.00193	12D+2	-0.04683	-0.13625	-0.01306
C (Cp)				12D-2	0.14503	0.19964	0.00557
2S	-0.01573	0.01363	-0.00303	13D 0	-0.05506	-0.06027	-0.06488
2PX	-0.10441	0.15155	0.00660	13D+1	-0.05968	-0.03002	0.02533
2PZ	0.06743	-0.10337	-0.00478	13D+2	-0.01694	-0.05485	-0.00076
3S	0.06537	-0.07991	-0.00940	13D-2	0.06293	0.08649	0.01132
3PX	-0.09104	0.13271	0.00295	Ir			
3PY	-0.07665	0.10211	-0.00226	4S	0.02747	-0.02282	-0.05385
3PZ	0.05881	-0.08706	-0.00452	5S	-0.00862	-0.06296	-0.10531
C (Cp)				6S	-0.02011	-0.01423	0.05690
2PX	0.09218	0.14721	0.00943	8PX	0.06024	-0.05065	-0.00758
2PZ	-0.07709	-0.11187	-0.00728	8PY	-0.13151	0.12553	0.00202
3S	0.05660	0.07716	0.01217	10PX	-0.06675	0.05063	0.08342
3PX	0.08705	0.13896	0.00622	10PY	0.10944	-0.14522	0.03730
3PY	-0.04596	-0.06782	0.00097	11PX	0.02485	0.00348	-0.11660
3PZ	-0.07849	-0.10868	-0.00672	11PZ	-0.01391	-0.00691	-0.08252

				12D 0	-0.13236	0.14068	0.16520
				12D+1	-0.19409	0.13444	-0.16703
				12D-1	0.06351	-0.10701	0.00500
				12D+2	-0.00896	0.07993	-0.17182
				12D-2	-0.11988	0.20770	-0.03939
				13D 0	-0.04778	0.05021	0.09248
				13D+1	-0.07428	0.04742	-0.08405
				13D-1	0.02914	-0.05054	-0.00005
				13D+2	0.00130	0.02938	-0.09269
				13D-2	-0.05415	0.09168	-0.02538
				C (Cp)			
				2PX	-0.14333	0.15415	-0.01730
				2PZ	0.08987	-0.09714	0.03344
				3S	0.06825	-0.08173	0.02480
				3PX	-0.11966	0.12969	-0.01549
				3PY	-0.09561	0.10938	-0.02864
				3PZ	0.07632	-0.08322	0.04630
				C (Cp)			
				2PX	0.14516	0.15478	0.03554
				2PZ	-0.09103	-0.09707	-0.01069
				3S	0.06612	0.07776	0.03933
				3PX	0.13152	0.14065	0.05352

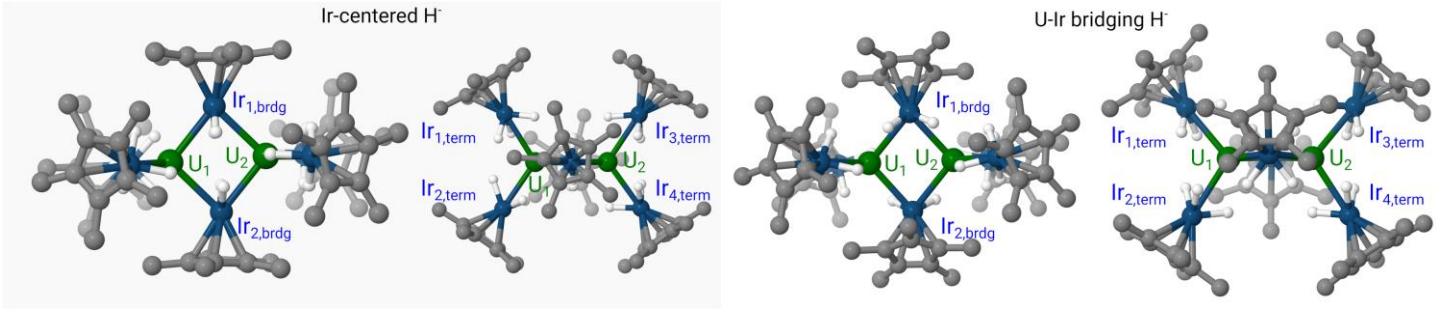
				3PY	-0.06889	-0.08091	-0.02102
				3PZ	-0.08535	-0.09200	-0.00281

Table S10. Tabulated calculated bond distances/angles for **3**



	Ir-centered H^-			Experimental	U-Ir bridging H^-		
Multiplicity	singlet	triplet	quintet	–	singlet	triplet	quintet
$\Delta_r G$ (kcal/mol)	55.6	7.3	0.0	–	78.0	20.7	13.6
Ir_{brdg}–H_{brdg} dist. (Å)	[1.628–1.631]	[1.627–1.630]	[1.627–1.631]	–	[1.602–1.608]	[1.609–1.610]	[1.608–1.612]
Ir_{term}–H_{term} dist. (Å)	[1.624–1.630]	[1.622–1.628]	[1.622–1.628]	–	[1.614–1.633]	[1.609–1.630]	[1.620–1.630]
U–H_{brdg} dist. (Å)	[2.440–2.584]	[2.445–2.613]	[2.445–2.613]	–	[2.413–2.485] [3.254–3.396]	[2.379–2.394] [3.575–3.579]	[2.361–2.394] [3.484–3.666]
U–H_{term} dist. (Å)	[2.365–2.415]	[2.373–2.397]	[2.373–2.394]	–	[2.315–2.439]	[2.368–2.423]	[2.373–2.424]
U–Ir_{brdg} dist. (Å)	2.810/2.829 2.818/2.831	2.827/2.830 2.837/2.840	2.827/2.830 2.837/2.840	2.814/2.840 2.814/2.840	2.785/2.813 2.797/2.800	2.851/2.856 2.850/2.856	2.851/2.866 2.835/2.873
U–Ir_{term} dist. (Å)	2.997/3.002 2.973/2.976	2.978/2.997 2.981/2.983	2.978/2.997 2.981/2.983	2.965/2.972 2.965/2.972	2.964/2.962 2.971/2.975	3.000 /3.003 2.996/2.998	3.004 /3.008 2.998/3.001
U–U dist. (Å)	3.779	3.815	3.815	3.795	2.465	3.703	3.703
Ir_{brdg}–Ir_{brdg} dist. (Å)	4.192	4.191	4.191	4.192	5.024	4.342	4.343
Ir_{brdg}–U–Ir_{brdg} angle (°)	96.0	95.4	95.4	95.6	127.7	99.1	99.0
Ir_{term}–U–Ir_{term} angle (°)	111.5	111.9	111.9	113.5	101.5	107.4	108.5
U–Ir_{brdg}–U angle (°)	84.0	84.6	84.7	84.3	52.2	80.9	80.8

Table S11. Calculated NBO Wiberg Bond Indexes for **3**



	Ir-centered H^-	U-Ir bridging H^-
Multiplicity	quintet	quintet
Ir_{brdg}–H_{brdg}	0.47	0.54
Ir_{brdg}–C(Cp)	[0.18-0.30]	[0.18-0.30]
Ir_{term}–H_{term}	0.58	[0.57-0.59]
Ir_{term}–C(Cp)	[0.32-0.35]	[0.32-0.35]
U_1–H_{brdg}	0.17 (H-$Ir_{1,brdg}$) / 0.20 (H-$Ir_{2,brdg}$)	0.24 / 0.04 (H-$Ir_{1,brdg}$) / 0.24 / 0.05 (H-$Ir_{2,brdg}$)
U_2–H_{brdg}	0.19 (H-$Ir_{1,brdg}$) / 0.22 (H-$Ir_{2,brdg}$)	0.22 / 0.04 (H-$Ir_{1,brdg}$) / 0.23 / 0.03 (H-$Ir_{2,brdg}$)
U_1–H_{term}	[0.23-0.25]	[0.23-0.25]
U_2–H_{term}	[0.24-0.26]	[0.24-0.25]
U–$Ir_{1,brdg}$	0.85 (U_1) / 0.83 (U_2)	0.88 (U_1) / 0.84 (U_2)
U–$Ir_{2,brdg}$	0.83 (U_1) / 0.85 (U_2)	0.84 (U_1) / 0.89 (U_2)
U_1–Ir_{term}	0.64 ($Ir_{1,term}$) / 0.66 ($Ir_{2,term}$)	0.X ($Ir_{1,term}$) / 0.X ($Ir_{2,term}$)
U_2–Ir_{term}	0.65 ($Ir_{3,term}$) / 0.65 ($Ir_{4,term}$)	0.X ($Ir_{3,term}$) / 0.X ($Ir_{4,term}$)
U_1–U_2	0.26	0.36
$Ir_{1,brdg}$–$Ir_{2,brdg}$	0.03	0.03

Table S12. Atomic coordinates for the computed structures of **1** at different spin states (singlet (sing), triplet (t) and quintet (q)), with or without dispersion corrections (disp)

1-linear-sing

U	6.12294	5.09344	4.16193
Ir	3.83891	3.37355	4.84564
Ir	6.76321	6.90294	6.39049
C	5.99518	7.97527	8.20707
C	7.08518	7.12941	8.59599
C	6.51276	8.95164	7.26402
C	8.27728	7.56075	7.90602
C	5.73906	10.09346	6.68170
H	6.15349	10.40480	5.71998
H	5.75605	10.96214	7.35337
H	4.69412	9.82033	6.51539
C	9.66498	7.04306	8.12500
H	9.65465	5.98565	8.40096
H	10.17368	7.59298	8.92887
H	10.27145	7.13794	7.22083
C	7.91031	8.69605	7.08792
C	4.60752	7.95241	8.76892
H	3.87523	8.29293	8.03255
H	4.52640	8.60628	9.64795
H	4.31829	6.94412	9.07462
C	8.85735	9.51244	6.26392
H	9.65173	8.89221	5.84195
H	9.32756	10.29373	6.87514
H	8.34262	9.99995	5.43297
C	2.11405	3.42787	7.72124
H	3.00654	3.28569	8.33476

H	1.26598	2.97158	8.24794
H	1.92657	4.50179	7.65150
C	0.60322	4.34791	5.05889
H	0.81088	5.15008	5.77157
H	-0.41017	3.97454	5.26116
H	0.60034	4.79274	4.06062
C	3.42367	0.15323	3.94221
H	3.53004	0.34200	2.87135
H	2.76092	-0.71354	4.06683
H	4.40896	-0.12223	4.32590
C	1.45738	2.35552	2.71000
H	1.27088	3.37823	2.37423
H	0.51103	1.80265	2.64689
H	2.15953	1.90057	2.00745
C	3.81135	0.80218	7.04645
H	4.67982	0.32877	6.58166
H	3.17213	0.00466	7.44920
H	4.17543	1.39496	7.88922
C	1.99052	2.33149	4.10934
C	2.87669	1.35049	4.65633
C	3.06201	1.64912	6.06460
C	2.28171	2.81464	6.36524
C	1.61763	3.25131	5.16316
C	7.02123	6.03399	9.61512
H	6.02559	5.58670	9.65743
H	7.25858	6.42360	10.61348
H	7.73301	5.23686	9.38815
H	5.37372	2.89386	4.60259

H	6.70304	5.27861	6.43091
H	3.98804	4.32568	3.53916
H	7.59430	6.72699	5.00176
H	5.42953	6.91546	5.45487
H	4.43101	4.60048	5.72950
Ir	8.52049	3.50387	3.54520
Ir	5.48888	6.74009	1.80855
C	6.21604	7.65662	-0.10416
C	5.11088	6.78621	-0.39899
C	5.71974	8.71027	0.76067
C	3.93970	7.27796	0.27653
C	6.51295	9.89103	1.22804
H	6.10100	10.31016	2.14893
H	6.51321	10.68432	0.46880
H	7.55218	9.61740	1.42632
C	2.54658	6.74703	0.14018
H	2.55003	5.67114	-0.05086
H	2.01379	7.23288	-0.68891
H	1.96717	6.91449	1.05166
C	4.32797	8.47659	0.99435
C	7.58844	7.58620	-0.69889
H	8.34181	7.96539	-0.00376
H	7.65294	8.18067	-1.62054
H	7.86211	6.55764	-0.94632
C	3.39819	9.36650	1.75993
H	2.60636	8.79005	2.24414
H	2.92223	10.09632	1.09189
H	3.92665	9.91999	2.53951

C	10.42575	3.35629	2.37399
C	9.59743	2.23890	2.04091
C	11.68363	4.18125	4.52626
H	11.65503	5.20027	4.13226
H	12.71798	3.81995	4.44475
H	11.43221	4.23591	5.58822
C	8.69518	0.12935	3.31726
H	8.30016	-0.05924	4.31852
H	9.38416	-0.69020	3.07052
H	7.85521	0.07828	2.61990
C	10.21249	1.60193	5.71480
H	10.35020	2.42205	6.42309
H	11.07175	0.92571	5.81012
H	9.31700	1.05296	6.01498
C	9.11799	1.86698	0.67190
H	8.14694	1.36753	0.71370
H	9.82602	1.18393	0.18426
H	9.00825	2.74704	0.03402
C	10.96279	4.37521	1.41715
H	10.29135	4.51570	0.56709
H	11.94136	4.06521	1.02755
H	11.08753	5.34673	1.90131
C	10.09542	2.10794	4.30989
C	9.38632	1.45553	3.24425
C	10.73748	3.28578	3.78827
C	5.15166	5.60828	-1.32313
H	6.13797	5.13882	-1.32652
H	4.92164	5.91823	-2.35063

H	4.42437	4.84735	-1.03072
H	7.04507	3.35843	2.87551
H	5.77631	5.13934	1.84885
H	7.81535	3.70356	4.99811
H	4.62854	6.60503	3.18132
H	6.80093	6.87084	2.76439
H	8.33456	5.11229	3.36939

1-linear-t

U	6.15106	5.17560	4.13648
Ir	3.87838	3.41650	4.81095
Ir	6.81033	6.89986	6.44483
C	6.06813	7.90496	8.30592
C	7.15462	7.02591	8.65462
C	6.60117	8.91342	7.41207
C	8.34244	7.46884	7.98127
C	5.83683	10.08491	6.87777
H	6.26824	10.45103	5.94335
H	5.84331	10.91271	7.59889
H	4.79506	9.82153	6.67950
C	9.72280	6.91593	8.15565
H	9.69510	5.85284	8.40642
H	10.25964	7.43635	8.96057
H	10.31091	7.02077	7.24063
C	7.99210	8.64864	7.21025
C	4.68745	7.88169	8.88511
H	3.95573	8.28895	8.18268
H	4.63160	8.47535	9.80801
H	4.37506	6.86223	9.12440

C	8.95359	9.49426	6.43396
H	9.73463	8.88486	5.97287
H	9.44246	10.22937	7.08702
H	8.44794	10.04051	5.63436
C	1.87024	3.75506	7.49199
H	2.67290	3.70621	8.23151
H	0.95968	3.35482	7.95761
H	1.69461	4.80999	7.26751
C	0.60449	4.22500	4.59760
H	0.74496	5.14430	5.17152
H	-0.40322	3.84575	4.81525
H	0.63936	4.49188	3.53868
C	3.68105	0.06865	4.34042
H	3.89306	0.11331	3.26920
H	3.02650	-0.79648	4.51513
H	4.62801	-0.12173	4.85169
C	1.76990	1.98158	2.63703
H	1.48546	2.92304	2.16178
H	0.91621	1.29542	2.56475
H	2.59327	1.55477	2.05967
C	3.79578	1.20101	7.32469
H	4.72084	0.72455	6.99173
H	3.17146	0.43110	7.79643
H	4.05898	1.93528	8.08927
C	2.15734	2.18678	4.06901
C	3.04622	1.33565	4.82307
C	3.07045	1.83815	6.17983
C	2.21919	2.98615	6.25549

C	1.64687	3.20550	4.93784
C	7.07257	5.88845	9.62534
H	6.08308	5.42580	9.61225
H	7.26681	6.24061	10.64663
H	7.80457	5.11158	9.39291
H	5.42049	3.25860	5.30276
H	6.40990	5.32458	6.47857
H	4.47206	3.71565	3.32744
H	7.77065	6.54341	5.18102
H	5.60437	7.11416	5.37507
H	4.01832	5.00967	5.11670
Ir	8.49244	3.49428	3.50343
Ir	5.44064	6.82293	1.78957
C	6.16379	7.79171	-0.09872
C	5.09125	6.88235	-0.42321
C	5.61226	8.81191	0.76612
C	3.89852	7.32297	0.23849
C	6.35595	10.00805	1.27456
H	5.92340	10.38039	2.20597
H	6.32601	10.82270	0.53934
H	7.40448	9.77001	1.46884
C	2.52881	6.73727	0.08751
H	2.57580	5.66824	-0.13304
H	1.97853	7.22463	-0.72878
H	1.94350	6.85782	1.00244
C	4.22543	8.52958	0.97862
C	7.54223	7.78003	-0.68342
H	8.26936	8.21807	0.00497

H	7.58326	8.35104	-1.62134
H	7.87242	6.76085	-0.89929
C	3.24785	9.38379	1.72492
H	2.47386	8.77725	2.20146
H	2.75030	10.09213	1.04898
H	3.74151	9.96138	2.50998
C	10.36457	3.27015	2.29353
C	9.49290	2.17665	1.98912
C	11.70672	4.07478	4.40188
H	11.70944	5.08929	3.99545
H	12.72431	3.67231	4.30236
H	11.48271	4.15227	5.46866
C	8.54266	0.12277	3.31740
H	8.17474	-0.04186	4.33293
H	9.18869	-0.72561	3.05352
H	7.67791	0.10374	2.64953
C	10.18102	1.56267	5.65701
H	10.32520	2.38984	6.35582
H	11.04588	0.89248	5.74473
H	9.29433	1.01056	5.97653
C	8.98022	1.79746	0.63433
H	7.99672	1.32561	0.70003
H	9.66015	1.08852	0.14315
H	8.88205	2.67071	-0.01481
C	10.90457	4.26352	1.31156
H	10.20829	4.42502	0.48562
H	11.85504	3.91233	0.88924
H	11.08519	5.23159	1.78470

C	10.03996	2.05575	4.24983
C	9.28647	1.41756	3.21019
C	10.70884	3.20858	3.69800
C	5.19442	5.72363	-1.36634
H	6.18710	5.26910	-1.32959
H	5.01128	6.05070	-2.39805
H	4.46545	4.94628	-1.12624
H	6.95476	3.26534	3.02041
H	5.96651	5.28532	1.78875
H	7.89632	3.82225	4.98009
H	4.45795	6.39475	3.01359
H	6.56586	7.15177	2.91519
H	8.29567	5.07142	3.15723

1-linear-t-disp

U	6.14093	5.23245	4.14867
Ir	3.93040	3.45777	4.79185
Ir	6.81276	6.91297	6.43165
C	6.08912	7.90140	8.28984
C	7.15905	6.99811	8.62494
C	6.63905	8.90814	7.40677
C	8.35211	7.42564	7.95437
C	5.88867	10.07724	6.85669
H	6.32161	10.41387	5.91239
H	5.90776	10.91864	7.56051
H	4.84478	9.81746	6.66735
C	9.71247	6.82145	8.08383
H	9.64793	5.75328	8.30280
H	10.28618	7.29881	8.88901

H	10.27840	6.93089	7.15583
C	8.02318	8.62030	7.19866
C	4.70254	7.87811	8.84577
H	3.98812	8.29790	8.13353
H	4.63319	8.45776	9.77584
H	4.38408	6.85543	9.06068
C	8.99020	9.43604	6.40397
H	9.74046	8.80010	5.92849
H	9.51322	10.15847	7.04346
H	8.48029	9.99065	5.61337
C	1.91960	3.71487	7.44079
H	2.72563	3.67911	8.17682
H	1.01695	3.29795	7.90564
H	1.72797	4.76627	7.21449
C	0.67571	4.19092	4.54069
H	0.79822	5.09903	5.13545
H	-0.33250	3.79854	4.72703
H	0.73785	4.47744	3.48849
C	3.90627	0.15734	4.24987
H	4.12223	0.24991	3.18299
H	3.31339	-0.75532	4.39624
H	4.86139	0.02586	4.76367
C	1.94599	2.03170	2.55810
H	1.65450	2.98420	2.11066
H	1.11703	1.32503	2.42931
H	2.80537	1.65360	2.00031
C	3.93698	1.23825	7.25401
H	4.87048	0.79291	6.90337

H	3.34760	0.45248	7.74255
H	4.19075	1.99045	8.00376
C	2.27770	2.19728	4.00582
C	3.18606	1.36420	4.75597
C	3.17509	1.84340	6.11990
C	2.28402	2.95887	6.20467
C	1.72028	3.18007	4.88500
C	7.04830	5.83300	9.55412
H	6.04946	5.39354	9.51269
H	7.24210	6.14396	10.58802
H	7.76556	5.05189	9.29366
H	5.46299	3.33414	5.31916
H	6.36784	5.35034	6.46914
H	4.52149	3.77727	3.31205
H	7.78338	6.54480	5.18027
H	5.62236	7.17920	5.35632
H	4.01293	5.05236	5.11416
Ir	8.42183	3.54343	3.53031
Ir	5.43543	6.83285	1.82039
C	6.16028	7.77128	-0.06296
C	5.09603	6.84999	-0.37626
C	5.59953	8.79826	0.78587
C	3.89963	7.29077	0.27577
C	6.34111	9.98570	1.30819
H	5.90116	10.34566	2.24059
H	6.32076	10.80708	0.58127
H	7.38536	9.73666	1.50958
C	2.54350	6.67379	0.16193

H	2.61398	5.60071	-0.02941
H	1.96810	7.12725	-0.65563
H	1.97631	6.80527	1.08636
C	4.21544	8.50965	0.99835
C	7.54756	7.74347	-0.61687
H	8.25968	8.18146	0.08660
H	7.61473	8.30353	-1.55909
H	7.87115	6.71820	-0.81108
C	3.23739	9.34757	1.75560
H	2.48831	8.72470	2.24987
H	2.71312	10.04215	1.08674
H	3.73758	9.93544	2.52828
C	10.26247	3.26173	2.31355
C	9.36466	2.18259	2.04229
C	11.61323	4.10452	4.39815
H	11.61281	5.10682	3.96344
H	12.63106	3.70074	4.31524
H	11.37881	4.21051	5.45989
C	8.34292	0.20998	3.43337
H	7.99913	0.08814	4.46297
H	8.92957	-0.67835	3.16521
H	7.45704	0.23590	2.79460
C	10.04210	1.66050	5.72182
H	10.22459	2.51115	6.38182
H	10.87090	0.95207	5.84174
H	9.12497	1.17225	6.05793
C	8.80359	1.80498	0.71014
H	7.81107	1.36108	0.81593

H	9.44892	1.07519	0.20454
H	8.70575	2.67724	0.06024
C	10.78793	4.23800	1.31167
H	10.06569	4.40469	0.50984
H	11.71953	3.87153	0.86297
H	10.99299	5.20467	1.77671
C	9.92780	2.10150	4.29843
C	9.15060	1.45756	3.28144
C	10.61897	3.22371	3.71477
C	5.21866	5.66074	-1.27271
H	6.21700	5.22304	-1.20723
H	5.03798	5.94379	-2.31701
H	4.49877	4.88601	-1.00083
H	6.88388	3.32217	3.04968
H	5.97302	5.29999	1.82425
H	7.85402	3.89961	5.01107
H	4.44081	6.41392	3.03749
H	6.55503	7.19362	2.94154
H	8.25881	5.11772	3.15287

1-linear-q

U	6.28174	4.97359	3.74388
Ir	3.95764	3.57522	5.15231
Ir	6.53746	6.85307	6.29026
C	5.56611	7.63096	8.27438
C	6.84951	7.03252	8.53734
C	5.76170	8.72535	7.36239
C	7.84964	7.79022	7.83381
C	4.69399	9.66042	6.88463

H	4.96364	10.12009	5.93169
H	4.53287	10.46517	7.61309
H	3.74327	9.14148	6.74265
C	9.33191	7.61975	7.94988
H	9.59898	6.57715	8.13487
H	9.72667	8.22191	8.77836
H	9.84210	7.93219	7.03590
C	7.16906	8.84251	7.09844
C	4.26722	7.23355	8.89366
H	3.43156	7.37785	8.20446
H	4.06794	7.83963	9.78808
H	4.27573	6.18589	9.20007
C	7.83183	9.93307	6.31677
H	8.76632	9.58903	5.86781
H	8.06418	10.78708	6.96586
H	7.19020	10.28977	5.50816
C	3.00286	3.37712	8.41160
H	3.99933	3.08928	8.75612
H	2.26814	2.89465	9.07029
H	2.89990	4.45650	8.54172
C	1.05200	4.86132	6.35310
H	1.55228	5.53371	7.05495
H	0.08799	4.57564	6.79659
H	0.84555	5.43435	5.44574
C	2.86394	0.58412	4.06901
H	2.76100	0.91678	3.03326
H	2.10348	-0.18834	4.25037
H	3.84562	0.11365	4.16511

C	1.01058	3.15313	3.65122
H	0.83214	4.22344	3.52633
H	0.03645	2.65634	3.74757
H	1.48472	2.78933	2.73686
C	4.13961	0.75458	6.99461
H	4.81113	0.29518	6.26535
H	3.52625	-0.04239	7.43576
H	4.75871	1.17840	7.78893
C	1.86204	2.87852	4.85233
C	2.71270	1.72502	5.02519
C	3.27680	1.79995	6.35737
C	2.77745	2.98152	6.98649
C	1.89406	3.65979	6.05530
C	7.10791	5.91326	9.49879
H	6.29823	5.18027	9.48413
H	7.19901	6.29673	10.52287
H	8.03228	5.38593	9.25463
H	5.45155	3.01211	4.86613
H	7.05884	5.33888	6.19223
H	3.97661	4.35295	3.73287
H	7.64439	6.87089	5.16551
H	5.70506	7.13075	4.94008
H	4.71822	4.92540	5.73257
Ir	8.83036	3.36674	3.39933
Ir	5.50686	6.63404	1.32853
C	6.09130	7.35187	-0.71819
C	4.85525	6.61188	-0.81379
C	5.83816	8.49502	0.12899

C	3.85334	7.28393	-0.03984
C	6.82289	9.58348	0.42762
H	6.60389	10.06909	1.38156
H	6.80020	10.35311	-0.35516
H	7.84147	9.19185	0.48269
C	2.40150	6.92491	0.03711
H	2.25282	5.84819	-0.07480
H	1.82539	7.42761	-0.75200
H	1.97143	7.21495	0.99916
C	4.46886	8.46058	0.54943
C	7.34885	7.07976	-1.48454
H	8.22974	7.42791	-0.93894
H	7.34059	7.58296	-2.46173
H	7.48140	6.00966	-1.66286
C	3.75387	9.51617	1.33526
H	2.96148	9.08362	1.95135
H	3.29261	10.25988	0.67095
H	4.43771	10.04524	2.00368
C	11.00758	3.38324	2.88431
C	10.32009	2.55949	1.92794
C	11.52407	3.26097	5.45145
H	11.69110	4.34122	5.44618
H	12.50080	2.77344	5.57968
H	10.91926	3.02783	6.33183
C	9.00115	0.30003	2.03952
H	8.30484	-0.15697	2.74664
H	9.70512	-0.47571	1.70983
H	8.42264	0.61808	1.16877

C	9.73900	0.63081	5.13711
H	9.57630	1.14270	6.08892
H	10.56211	-0.08299	5.27650
H	8.83519	0.05924	4.91319
C	10.34010	2.71869	0.43917
H	9.42554	2.32769	-0.01390
H	11.18953	2.18403	-0.00858
H	10.41926	3.77028	0.15258
C	11.82854	4.59274	2.55616
H	11.42948	5.11811	1.68538
H	12.86494	4.30751	2.33297
H	11.84681	5.29962	3.38909
C	10.05560	1.60302	4.04263
C	9.72999	1.45327	2.65793
C	10.84961	2.80789	4.19362
C	4.63891	5.39702	-1.66285
H	5.54606	4.79151	-1.72704
H	4.35299	5.68451	-2.68314
H	3.84678	4.76248	-1.25855
H	7.43012	3.22333	2.58029
H	5.83197	5.04072	1.38491
H	7.93235	3.49165	4.74818
H	4.65685	6.43452	2.69809
H	6.82051	6.81809	2.26890
H	8.64723	4.97520	3.24649

1-1 lig bend-t

U	9.16623	9.90284	4.34232
Ir	10.19459	11.57660	6.55813

Ir	7.86605	11.59039	2.28216
Ir	7.20512	7.95910	5.33451
Ir	11.36599	8.42778	3.11116
C	7.24287	11.84975	0.13784
C	11.69979	13.08361	7.28904
C	9.61605	12.83814	8.31688
C	10.38890	13.64657	7.39915
C	11.75579	11.91311	8.14684
C	8.03666	12.97856	0.51446
C	10.47525	11.77426	8.77560
C	7.35708	13.66725	1.59536
C	6.14216	12.95158	1.86510
C	9.91854	14.91474	6.75688
H	10.43090	15.09830	5.80972
H	10.10809	15.77295	7.41466
H	8.84609	14.88163	6.55155
C	6.21666	7.02736	7.11909
C	13.54250	7.98099	2.68105
C	12.97834	11.10062	8.44199
H	12.71968	10.07754	8.72522
H	13.55245	11.54237	9.26763
H	13.63954	11.04220	7.57426
C	12.58496	11.64065	2.57672
H	11.73035	12.01855	2.01050
H	13.48426	12.15586	2.20915
H	12.43548	11.92843	3.62116
C	9.27395	13.46687	-0.17275
H	9.97087	13.92343	0.53456

H	9.02210	14.22447	-0.92661
H	9.79914	12.65609	-0.68217
C	10.11260	10.74943	9.80548
H	9.04967	10.50160	9.76290
H	10.33111	11.12468	10.81355
H	10.67427	9.82363	9.66231
C	7.77308	14.97614	2.19124
H	7.37098	15.10293	3.19916
H	7.41628	15.81759	1.58167
H	8.86102	15.05379	2.26027
C	12.72105	10.15700	2.42279
C	8.24266	13.14941	8.82621
H	7.63625	13.64169	8.06184
H	8.28409	13.81429	9.69984
H	7.71437	12.24057	9.12437
C	6.41737	7.33188	8.57105
H	7.45645	7.17518	8.87121
H	5.78715	6.69048	9.20249
H	6.16499	8.37098	8.79714
C	4.89992	10.88963	0.82368
H	5.22551	9.89830	0.49910
H	4.18329	11.26683	0.08128
H	4.36562	10.76332	1.76825
C	12.82000	8.03990	1.42894
C	6.30168	5.93068	5.05628
C	11.56001	9.90898	0.10294
H	11.08949	9.10161	-0.46303
H	12.23554	10.44648	-0.57556

H	10.76996	10.59419	0.42192
C	12.30923	9.37645	1.28490
C	6.88958	5.99670	6.36061
C	5.19834	7.59023	6.26352
C	12.85594	13.67367	6.54225
H	13.54304	12.89960	6.19146
H	13.42741	14.35686	7.18459
H	12.52132	14.23918	5.66919
C	4.20230	8.63082	6.67286
H	4.63472	9.33910	7.38347
H	3.33291	8.16199	7.15157
H	3.84410	9.20113	5.81289
C	5.09049	13.35746	2.85110
H	4.55586	12.48894	3.24221
H	4.35596	14.02083	2.37675
H	5.52506	13.88899	3.70070
C	14.13719	9.69569	4.56160
H	13.52204	10.41263	5.11145
H	15.10626	10.16617	4.34870
H	14.31632	8.84131	5.21841
C	6.06200	11.82110	0.97551
C	7.51823	10.91316	-0.99758
H	8.58806	10.83603	-1.20306
H	7.02343	11.26148	-1.91356
H	7.15109	9.90722	-0.78102
C	13.46295	9.27718	3.29211
C	4.29451	7.11942	3.85470
H	3.90171	8.13871	3.83247

H	3.44133	6.43219	3.93282
H	4.78381	6.93596	2.89511
C	5.24479	6.92577	4.99527
C	12.74963	6.94840	0.40502
H	12.76189	5.96175	0.87481
H	13.60108	6.99907	-0.28699
H	11.83391	7.01481	-0.18761
C	6.62276	4.93330	3.98689
H	6.47263	5.35623	2.99066
H	5.98137	4.04624	4.07548
H	7.66223	4.60335	4.04769
C	7.96470	5.09536	6.88473
H	8.63345	4.76602	6.08652
H	7.52511	4.20338	7.34939
H	8.57384	5.60027	7.63804
C	14.34018	6.81466	3.17919
H	14.40689	6.81301	4.26990
H	15.36357	6.83809	2.78129
H	13.88837	5.86591	2.87908
H	8.79494	8.01301	5.67555
H	10.89370	6.93801	3.36047
H	10.98541	8.37852	4.68301
H	9.83235	8.40652	2.59651
H	7.15891	9.57684	5.52311
H	7.60362	8.24175	3.78112
H	11.08292	10.84399	5.40482
H	9.16280	12.02004	5.38548
H	9.37170	10.18297	6.68061

H	7.35481	11.26630	3.78852
H	9.36480	11.78926	2.88791
H	8.22963	10.00846	2.16380

1-1 lig bend-t-disp

U	9.16876	9.87182	4.38071
Ir	10.31005	11.52012	6.50601
Ir	7.89765	11.45533	2.28194
Ir	7.16556	8.04391	5.38165
Ir	11.27614	8.37908	3.17819
C	7.51585	11.75795	0.09627
C	11.90277	12.95663	7.13671
C	9.83050	12.86728	8.21148
C	10.61110	13.59113	7.25490
C	11.90924	11.83237	8.04179
C	8.06597	12.96108	0.63657
C	10.64002	11.76601	8.69805
C	7.16450	13.46175	1.65098
C	6.05097	12.55043	1.71945
C	10.18542	14.82732	6.53102
H	10.64306	14.87854	5.54069
H	10.47947	15.72467	7.08912
H	9.10228	14.84995	6.39526
C	6.19906	7.10330	7.15589
C	13.47108	8.15102	2.71793
C	13.07269	10.93296	8.30568
H	12.74437	9.91616	8.53131
H	13.65469	11.30132	9.15937
H	13.73966	10.88282	7.44344

C	12.22009	11.70851	2.87600
H	11.34620	12.06473	2.32580
H	13.08683	12.30636	2.56191
H	12.03700	11.90266	3.93607
C	9.32451	13.63687	0.19825
H	9.82633	14.11408	1.04344
H	9.11074	14.41075	-0.54905
H	10.02437	12.92514	-0.24353
C	10.24458	10.80303	9.76968
H	9.17642	10.57965	9.72152
H	10.46095	11.21107	10.76536
H	10.78267	9.85812	9.66790
C	7.30236	14.75315	2.38918
H	6.80486	14.70620	3.36064
H	6.86169	15.58529	1.82435
H	8.35311	14.99054	2.57168
C	12.46375	10.25703	2.61853
C	8.46422	13.22266	8.70108
H	7.90615	13.77961	7.94526
H	8.51876	13.84100	9.60624
H	7.88870	12.32522	8.93953
C	6.51434	7.33438	8.59747
H	7.55990	7.10150	8.81194
H	5.88897	6.70832	9.24751
H	6.34839	8.37790	8.87507
C	5.31970	10.37893	0.45637
H	5.86526	9.48651	0.14131
H	4.63297	10.65890	-0.35314

H	4.72147	10.10551	1.32817
C	12.73166	8.23473	1.47753
C	6.11841	6.11595	5.04299
C	11.27176	10.07148	0.32020
H	10.86344	9.26702	-0.29484
H	11.86671	10.72762	-0.32817
H	10.42764	10.64056	0.72086
C	12.10597	9.52678	1.43255
C	6.76596	6.06801	6.31603
C	5.19478	7.77927	6.37980
C	13.06188	13.46427	6.34253
H	13.70508	12.64716	6.00796
H	13.67743	14.15571	6.93259
H	12.72296	13.99740	5.45107
C	4.32252	8.88949	6.86930
H	4.83961	9.49572	7.61606
H	3.41085	8.48814	7.32840
H	4.02832	9.54965	6.05071
C	4.85322	12.70622	2.59949
H	4.42109	11.73501	2.84916
H	4.08264	13.30420	2.09790
H	5.11441	13.20447	3.53548
C	13.89308	9.77158	4.72655
H	13.19542	10.39667	5.28917
H	14.82327	10.33419	4.57483
H	14.12045	8.89369	5.33501
C	6.26182	11.49352	0.77550
C	8.05326	10.95817	-1.04511

H	9.10895	11.17089	-1.22064
H	7.50661	11.19081	-1.96755
H	7.95752	9.88632	-0.85688
C	13.28586	9.38578	3.41894
C	4.17490	7.52150	3.98369
H	3.86894	8.56875	4.03852
H	3.27093	6.90174	4.04666
H	4.62413	7.36274	3.00067
C	5.13870	7.18525	5.07442
C	12.72753	7.21218	0.38754
H	12.83008	6.20335	0.79411
H	13.55425	7.37801	-0.31541
H	11.79321	7.24335	-0.17765
C	6.35908	5.19143	3.89442
H	6.19330	5.69918	2.94181
H	5.68508	4.32680	3.94118
H	7.38695	4.82318	3.89494
C	7.80719	5.08309	6.73735
H	8.39507	4.74145	5.88323
H	7.34401	4.20656	7.20729
H	8.49908	5.52710	7.45627
C	14.35505	7.02106	3.13756
H	14.42629	6.95921	4.22594
H	15.37044	7.14602	2.73970
H	13.96979	6.06374	2.77902
H	8.73810	8.07882	5.80059
H	10.91060	6.84676	3.34667
H	10.86955	8.21391	4.73856

H	9.74287	8.27030	2.67976
H	7.13719	9.66809	5.49800
H	7.62569	8.22858	3.83274
H	11.04392	10.26539	5.78020
H	9.79476	12.02664	5.05311
H	8.99322	10.57634	6.61238
H	7.34932	11.17948	3.78205
H	9.35389	11.73528	2.93862
H	8.30626	9.88297	2.20428

1-2 lig bend-t

U	9.15979	10.07401	4.36246
Ir	10.15811	11.75107	6.60495
Ir	7.94524	11.77588	2.24848
Ir	7.16847	8.17936	5.29680
Ir	11.33288	8.53319	3.21333
C	7.40565	12.04704	0.08047
C	11.66306	13.29214	7.23552
C	9.66221	13.00425	8.40751
C	10.34927	13.82460	7.43525
C	11.80466	12.12718	8.09112
C	8.23677	13.14151	0.48186
C	10.57676	11.96240	8.80865
C	7.54297	13.86470	1.53228
C	6.29158	13.20553	1.75997
C	9.80935	15.07849	6.82000
H	10.24906	15.26097	5.83695
H	10.03163	15.94536	7.45563
H	8.72549	15.02576	6.69357

C	5.99665	7.12965	6.91760
C	13.47254	7.94914	2.71497
C	13.06069	11.34041	8.30309
H	12.84214	10.31192	8.59998
H	13.67777	11.79347	9.09063
H	13.66470	11.29621	7.39392
C	12.64013	11.62520	2.36599
H	11.70585	11.98614	1.92876
H	13.47284	12.08471	1.81414
H	12.68031	11.99315	3.39404
C	9.51236	13.58117	-0.16693
H	10.20993	13.99948	0.56313
H	9.31584	14.35573	-0.92012
H	10.01519	12.75288	-0.67054
C	10.32664	10.94610	9.87918
H	9.26462	10.70809	9.96754
H	10.66463	11.32662	10.85167
H	10.86015	10.01418	9.67933
C	7.99575	15.15348	2.14511
H	7.56616	15.29663	3.13937
H	7.69595	16.00908	1.52496
H	9.08318	15.18389	2.24945
C	12.72486	10.13086	2.31900
C	8.32982	13.29823	9.02456
H	7.65837	13.78350	8.31194
H	8.43309	13.96494	9.89151
H	7.83786	12.38478	9.36816
C	6.35968	5.86373	7.63192

H	6.46252	5.02919	6.93374
H	5.59301	5.59024	8.36941
H	7.31067	5.96277	8.16087
C	4.99807	11.19932	0.66359
H	5.28733	10.19191	0.35455
H	4.33917	11.61160	-0.11288
H	4.41004	11.10253	1.57898
C	12.68204	7.93565	1.50551
C	4.94447	8.62462	5.47878
C	11.44290	9.74781	0.08391
H	10.87351	8.93017	-0.36397
H	12.11672	10.14925	-0.68460
H	10.73322	10.52979	0.36565
C	12.22020	9.28048	1.27486
C	5.14903	7.23260	5.75276
C	6.28960	8.47112	7.35866
C	12.75070	13.90562	6.40928
H	13.44568	13.14788	6.03928
H	13.33116	14.62561	7.00138
H	12.34595	14.43460	5.54306
C	7.04828	8.83717	8.59595
H	7.77686	8.06713	8.85979
H	6.36432	8.95908	9.44631
H	7.59342	9.77344	8.45533
C	5.21746	13.66980	2.69453
H	4.61842	12.83333	3.06189
H	4.54041	14.36655	2.18394
H	5.63805	14.18440	3.56154

C	14.24031	9.77625	4.41343
H	13.71112	10.59433	4.90798
H	15.23353	10.14098	4.12003
H	14.37940	8.98004	5.14832
C	6.19700	12.07128	0.87112
C	7.67873	11.09404	-1.04158
H	8.74927	10.99136	-1.22995
H	7.20733	11.44846	-1.96732
H	7.28361	10.09900	-0.82436
C	13.47911	9.29174	3.21902
C	5.52582	10.88287	6.67596
H	6.43115	11.29135	7.13133
H	4.67500	11.13985	7.32332
H	5.38281	11.39641	5.72194
C	5.62963	9.40138	6.48526
C	12.51451	6.76973	0.57961
H	12.50371	5.82484	1.12862
H	13.33408	6.72335	-0.15011
H	11.57617	6.83232	0.02315
C	4.07195	9.19401	4.40342
H	4.50322	10.11195	3.99644
H	3.07454	9.43062	4.79661
H	3.94768	8.49214	3.57568
C	4.51393	6.08523	5.02843
H	4.33536	6.32398	3.97722
H	3.54863	5.82246	5.48106
H	5.14846	5.19615	5.05782
C	14.24541	6.79183	3.26985

H	14.36781	6.87359	4.35255
H	15.24728	6.73934	2.82323
H	13.74132	5.84336	3.06906
H	7.78085	6.93236	4.54053
H	10.84156	7.09990	3.66583
H	11.04722	8.69266	4.79831
H	9.79599	8.46613	2.72304
H	8.72713	8.17576	5.72033
H	7.32311	8.70400	3.77547
H	11.03973	11.04212	5.43695
H	9.08124	12.17350	5.46469
H	9.36251	10.33683	6.72893
H	7.32254	11.38313	3.69658
H	9.37949	12.00348	2.98284
H	8.38550	10.21525	2.11094

1-2 lig bend-t-disp

U	9.18330	9.77537	4.34826
Ir	10.22080	11.46101	6.50824
Ir	7.91147	11.46281	2.31548
Ir	7.19752	8.04354	5.38486
Ir	11.35508	8.41526	3.15170
C	7.45338	11.89935	0.16484
C	11.72861	13.01170	7.06366
C	9.70756	12.80612	8.21829
C	10.41291	13.55849	7.20969
C	11.84548	11.90044	7.98846
C	8.21891	12.98323	0.70004
C	10.60843	11.78382	8.69456

C	7.45186	13.57324	1.78088
C	6.22066	12.85420	1.88585
C	9.87241	14.74562	6.47973
H	10.32211	14.83736	5.48891
H	10.07804	15.66855	7.03547
H	8.79168	14.66432	6.34545
C	5.78758	7.54709	7.07221
C	13.55254	8.29436	2.63019
C	13.08082	11.10181	8.24808
H	12.83553	10.08077	8.54829
H	13.67762	11.55761	9.04832
H	13.70973	11.04078	7.35800
C	12.10538	11.77678	2.80032
H	11.19965	12.07309	2.26803
H	12.92734	12.42655	2.46990
H	11.92850	11.96350	3.86353
C	9.51569	13.50685	0.17519
H	10.13087	13.91641	0.98043
H	9.34574	14.30759	-0.55554
H	10.09541	12.72271	-0.31559
C	10.33065	10.82301	9.80388
H	9.26313	10.61624	9.89473
H	10.67480	11.23562	10.76018
H	10.84151	9.87176	9.64141
C	7.84967	14.77425	2.57571
H	7.38206	14.76406	3.56271
H	7.55382	15.70146	2.06855
H	8.93126	14.80228	2.72637

C	12.43169	10.34174	2.54053
C	8.35797	13.12565	8.77290
H	7.71006	13.56456	8.01038
H	8.42937	13.83903	9.60406
H	7.86058	12.22813	9.14633
C	5.87369	6.37149	7.99107
H	5.84842	5.43209	7.43414
H	5.03814	6.36424	8.70290
H	6.80328	6.38694	8.56455
C	5.07131	10.90073	0.56355
H	5.42460	9.91782	0.24328
H	4.45812	11.31996	-0.24486
H	4.42182	10.74948	1.42804
C	12.77502	8.32407	1.41227
C	5.13250	8.94890	5.33684
C	11.20005	10.06983	0.27005
H	10.79414	9.23631	-0.30692
H	11.75891	10.71889	-0.41639
H	10.35494	10.62987	0.68051
C	12.08197	9.58223	1.37133
C	5.03382	7.61018	5.84049
C	6.33632	8.85049	7.31119
C	12.82588	13.55750	6.21004
H	13.48265	12.76218	5.85111
H	13.44108	14.27143	6.77218
H	12.42671	14.07522	5.33502
C	7.13268	9.27243	8.50035
H	7.67042	8.42998	8.94022

H	6.48052	9.70244	9.27148
H	7.87099	10.02219	8.20792
C	5.09780	13.18257	2.81452
H	4.52677	12.29117	3.08062
H	4.40834	13.89489	2.34526
H	5.46705	13.63124	3.73935
C	13.94709	9.94994	4.61215
H	13.23862	10.54591	5.19198
H	14.84531	10.55399	4.43054
H	14.23235	9.08909	5.22031
C	6.21380	11.80432	0.89476
C	7.82064	11.04971	-1.00772
H	8.89969	11.03391	-1.16863
H	7.34829	11.43431	-1.91985
H	7.48955	10.01891	-0.86418
C	13.32187	9.52374	3.32562
C	6.11203	11.21571	6.22429
H	7.11898	11.49685	6.54716
H	5.38805	11.71413	6.88336
H	5.97731	11.60910	5.21471
C	5.91983	9.73304	6.25415
C	12.79277	7.29005	0.33338
H	12.96028	6.29280	0.74666
H	13.58839	7.49118	-0.39559
H	11.84179	7.26508	-0.20339
C	4.48155	9.48033	4.10259
H	5.16663	10.14682	3.57294
H	3.56715	10.03444	4.34983

H	4.21398	8.67257	3.41842
C	4.21390	6.50337	5.26015
H	4.13450	6.59685	4.17485
H	3.19812	6.50587	5.67577
H	4.66108	5.52964	5.47230
C	14.49929	7.21262	3.03974
H	14.59720	7.16372	4.12662
H	15.49798	7.38400	2.61809
H	14.15327	6.23471	2.69766
H	7.64164	6.57755	4.98667
H	11.10064	6.86861	3.36926
H	11.00688	8.25271	4.72322
H	9.83405	8.16735	2.66977
H	8.75065	7.93048	5.82276
H	7.51332	8.13408	3.80133
H	11.09801	10.58042	5.46661
H	9.23820	11.89753	5.29675
H	9.34406	10.10418	6.68919
H	7.24155	10.85035	3.65326
H	9.25197	11.77737	3.16393
H	8.47923	9.95761	2.07583

Table S8. Atomic coordinates for the computed structures of **2** at different spin states (singlet (sing), triplet (t) and quintet (q)), with or without dispersion corrections (disp)

2-linear-s

Th	6.15591	5.14189	4.12698
Ir	3.81221	3.37323	4.84146
Ir	6.80912	6.91070	6.48837
C	6.06475	7.90866	8.35422
C	7.16173	7.04379	8.69763
C	6.58086	8.92218	7.45347
C	8.34299	7.49806	8.01639
C	5.80182	10.08719	6.92625
H	6.22190	10.45775	5.98839
H	5.80667	10.91495	7.64757
H	4.76076	9.81490	6.73648
C	9.73096	6.96443	8.19089
H	9.71783	5.90016	8.43809
H	10.26029	7.48939	8.99792
H	10.31858	7.07959	7.27677
C	7.97340	8.67163	7.24588
C	4.68805	7.87418	8.94238
H	3.94579	8.25833	8.23804
H	4.62945	8.48292	9.85518
H	4.39237	6.85472	9.20189
C	8.91950	9.52529	6.45938
H	9.70867	8.92404	6.00162
H	9.39808	10.27300	7.10552
H	8.40309	10.05673	5.65674
C	1.75923	3.83545	7.46176
H	2.55045	3.81893	8.21485

H	0.84003	3.45986	7.93045
H	1.59111	4.87879	7.18420
C	0.53781	4.16864	4.52719
H	0.65056	5.10741	5.07527
H	-0.47328	3.78655	4.72406
H	0.60403	4.40304	3.46198
C	3.61392	0.00342	4.51950
H	3.82977	-0.01231	3.44838
H	2.96043	-0.85184	4.74033
H	4.55920	-0.15623	5.04430
C	1.74432	1.84487	2.69216
H	1.50371	2.77002	2.16368
H	0.86896	1.18527	2.63368
H	2.56521	1.36155	2.15748
C	3.66894	1.26567	7.45181
H	4.60647	0.78453	7.16315
H	3.03681	0.50814	7.93347
H	3.90573	2.02848	8.19708
C	2.10524	2.10986	4.12136
C	2.97347	1.29360	4.92829
C	2.97411	1.85722	6.26449
C	2.12357	3.00673	6.26898
C	1.57981	3.17251	4.93256
C	7.09936	5.90678	9.67035
H	6.11217	5.43918	9.67265
H	7.30721	6.26125	10.68813
H	7.83185	5.13349	9.42780
H	5.36376	3.14458	5.26642

H	6.49229	5.31870	6.52647
H	4.34009	3.71249	3.34395
H	7.74692	6.63833	5.18944
H	5.54408	7.07557	5.48209
H	3.99198	4.94618	5.20613
Ir	8.56750	3.44893	3.45531
Ir	5.44087	6.85017	1.73852
C	6.15244	7.82712	-0.15042
C	5.06919	6.93574	-0.46993
C	5.62364	8.84709	0.73535
C	3.88499	7.38042	0.21201
C	6.38479	10.03507	1.23693
H	5.96596	10.41231	2.17269
H	6.35767	10.85091	0.50268
H	7.43251	9.78578	1.42149
C	2.50611	6.81707	0.05945
H	2.53730	5.74791	-0.16377
H	1.96131	7.31389	-0.75505
H	1.92309	6.94233	0.97525
C	4.23750	8.57490	0.95821
C	7.52560	7.80668	-0.74732
H	8.26607	8.21273	-0.05351
H	7.56856	8.40259	-1.66941
H	7.83559	6.78821	-0.99385
C	3.28021	9.42608	1.73384
H	2.50830	8.81901	2.21290
H	2.77971	10.14788	1.07495
H	3.79174	9.98769	2.51892

C	10.45796	3.25873	2.26592
C	9.59388	2.16886	1.92458
C	11.76910	4.02355	4.40680
H	11.77881	5.04510	4.01847
H	12.78803	3.62217	4.31689
H	11.52803	4.08262	5.47104
C	8.63321	0.08522	3.19748
H	8.24962	-0.09976	4.20359
H	9.28468	-0.75652	2.92636
H	7.77921	0.07919	2.51575
C	10.24116	1.47635	5.58777
H	10.35555	2.28976	6.30801
H	11.11918	0.82331	5.67483
H	9.36195	0.89734	5.87927
C	9.10969	1.81194	0.55335
H	8.12663	1.33603	0.59047
H	9.80120	1.11433	0.06183
H	9.02091	2.69665	-0.08163
C	11.00660	4.27522	1.31276
H	10.32558	4.44373	0.47567
H	11.96869	3.94036	0.90387
H	11.16796	5.23623	1.80669
C	10.11205	1.99982	4.19043
C	9.37738	1.38256	3.12762
C	10.78213	3.17070	3.67154
C	5.14613	5.78245	-1.42225
H	6.13980	5.32878	-1.41790
H	4.93154	6.11576	-2.44577

H	4.42513	5.00331	-1.16461
H	7.02854	3.16456	3.01460
H	5.79970	5.26677	1.72499
H	8.01861	3.80553	4.94146
H	4.51465	6.57451	3.04523
H	6.70405	7.06535	2.73720
H	8.33844	5.00653	3.05881

2-linear-s-disp

Th	6.14742	5.14451	4.12253
Ir	3.83869	3.40404	4.84131
Ir	6.80110	6.88042	6.45179
C	6.05982	7.87447	8.30073
C	7.14190	6.99277	8.64593
C	6.59499	8.88134	7.40588
C	8.33149	7.43074	7.97219
C	5.82876	10.03612	6.84755
H	6.25665	10.37209	5.90071
H	5.83623	10.88299	7.54512
H	4.78844	9.76095	6.66039
C	9.70127	6.85240	8.11761
H	9.65286	5.78543	8.34633
H	10.26109	7.34674	8.92243
H	10.27233	6.96198	7.19281
C	7.98334	8.61141	7.20396
C	4.67274	7.83637	8.85484
H	3.95286	8.23396	8.13546
H	4.59239	8.42849	9.77605
H	4.37041	6.81199	9.08432

C	8.93690	9.43193	6.39790
H	9.70273	8.80273	5.93877
H	9.44067	10.17721	7.02630
H	8.41909	9.95978	5.59430
C	1.85670	3.90068	7.46350
H	2.67147	3.88400	8.19050
H	0.94588	3.54782	7.96341
H	1.70013	4.94073	7.16902
C	0.60597	4.23731	4.54193
H	0.74016	5.16863	5.09694
H	-0.41460	3.87760	4.72815
H	0.69087	4.47538	3.47918
C	3.67266	0.06917	4.50294
H	3.88252	0.07485	3.43089
H	3.04176	-0.80334	4.71849
H	4.62507	-0.06831	5.02028
C	1.79061	1.91822	2.69685
H	1.57516	2.85727	2.18290
H	0.90656	1.27393	2.61623
H	2.61430	1.43256	2.16952
C	3.74971	1.32176	7.43466
H	4.68661	0.85565	7.12173
H	3.14018	0.55754	7.93311
H	3.99332	2.09307	8.16829
C	2.13756	2.15750	4.13063
C	3.00884	1.33820	4.92775
C	3.02298	1.89961	6.26409
C	2.17691	3.05058	6.27714

C	1.62205	3.21989	4.94713
C	7.04861	5.83507	9.58625
H	6.05395	5.38547	9.55597
H	7.24667	6.15771	10.61571
H	7.77182	5.05876	9.32799
H	5.39161	3.14679	5.24164
H	6.43928	5.29964	6.50739
H	4.32971	3.75552	3.33464
H	7.76018	6.58885	5.17406
H	5.55306	7.08751	5.43309
H	4.02403	4.96796	5.23578
Ir	8.52875	3.48231	3.45828
Ir	5.44495	6.82550	1.76632
C	6.17594	7.80865	-0.09162
C	5.11571	6.89712	-0.43130
C	5.61117	8.81568	0.78342
C	3.91267	7.31851	0.22716
C	6.34792	9.99341	1.33369
H	5.90730	10.32842	2.27499
H	6.32458	10.83268	0.62741
H	7.39323	9.74402	1.52896
C	2.55608	6.70988	0.08064
H	2.62620	5.64114	-0.13385
H	1.99229	7.18276	-0.73422
H	1.97672	6.82150	1.00010
C	4.22762	8.51834	0.98041
C	7.56727	7.79394	-0.63596
H	8.27371	8.21480	0.08353

H	7.64170	8.37645	-1.56380
H	7.89230	6.77337	-0.85117
C	3.24762	9.33151	1.76183
H	2.50004	8.69267	2.23749
H	2.72270	10.04295	1.11179
H	3.74648	9.89828	2.55080
C	10.40328	3.30446	2.27278
C	9.54306	2.21256	1.93408
C	11.68301	4.09774	4.41920
H	11.66846	5.11582	4.02312
H	12.71234	3.72181	4.34779
H	11.41950	4.15704	5.47775
C	8.55648	0.15269	3.21852
H	8.17685	-0.01358	4.22897
H	9.18245	-0.70646	2.94481
H	7.69642	0.17228	2.54532
C	10.16823	1.54880	5.60214
H	10.26807	2.37706	6.30687
H	11.04395	0.89789	5.71554
H	9.28158	0.97758	5.88489
C	9.03344	1.86888	0.57248
H	8.04830	1.40022	0.62977
H	9.71060	1.17184	0.06199
H	8.93608	2.76117	-0.04987
C	10.92094	4.33838	1.32616
H	10.22682	4.49545	0.49814
H	11.88770	4.03151	0.90841
H	11.05769	5.29743	1.83033

C	10.06201	2.04937	4.19811
C	9.32892	1.42893	3.13816
C	10.72828	3.22033	3.67715
C	5.24216	5.72894	-1.35462
H	6.24428	5.29798	-1.30549
H	5.05180	6.03437	-2.39077
H	4.52990	4.94293	-1.09542
H	6.99427	3.17819	3.01717
H	5.87744	5.26217	1.73156
H	7.99832	3.84027	4.95000
H	4.47669	6.50002	3.02908
H	6.65772	7.10401	2.80928
H	8.30412	5.03555	3.04651

2-1 lig bend-s

Th	9.16591	9.90364	4.34191
Ir	10.21925	11.60494	6.60983
Ir	7.85213	11.60943	2.20169
Ir	7.15536	7.91768	5.36389
Ir	11.42503	8.38059	3.12404
C	7.22844	11.83843	0.05322
C	11.72437	13.11290	7.34309
C	9.64525	12.85334	8.38088
C	10.41029	13.66929	7.46684
C	11.78643	11.93623	8.19301
C	8.03775	12.96661	0.41062
C	10.51208	11.78673	8.82791
C	7.35500	13.67656	1.47786
C	6.13790	12.97936	1.76117

C	9.93236	14.94040	6.83554
H	10.44000	15.13287	5.88759
H	10.12303	15.79374	7.49912
H	8.85900	14.90556	6.63550
C	6.20209	6.94892	7.14985
C	13.61302	8.01396	2.67717
C	13.01157	11.12043	8.46777
H	12.75537	10.09469	8.74332
H	13.59336	11.55477	9.29178
H	13.66386	11.07088	7.59282
C	12.51595	11.63583	2.61463
H	11.62862	11.98157	2.07777
H	13.37984	12.19563	2.22830
H	12.38441	11.90618	3.66645
C	9.26555	13.44586	-0.29960
H	9.96835	13.92055	0.38987
H	9.00625	14.18523	-1.06934
H	9.79006	12.62574	-0.79460
C	10.15866	10.75631	9.85539
H	9.09891	10.49571	9.80874
H	10.36901	11.13232	10.86499
H	10.73171	9.83741	9.71292
C	7.79031	14.98224	2.06748
H	7.39150	15.11844	3.07533
H	7.44318	15.82354	1.45279
H	8.87924	15.04531	2.13351
C	12.71290	10.16055	2.44245
C	8.27746	13.16018	8.90788

H	7.66467	13.66479	8.15687
H	8.32899	13.81253	9.79044
H	7.74977	12.24869	9.19905
C	6.44886	7.19729	8.60535
H	7.49003	6.99976	8.87233
H	5.81605	6.55299	9.23121
H	6.23427	8.23469	8.87424
C	4.87814	10.90926	0.74812
H	5.18911	9.91814	0.40902
H	4.15031	11.29842	0.02291
H	4.36084	10.77868	1.70163
C	12.87970	8.05681	1.42987
C	6.20088	5.91619	5.05163
C	11.55214	9.89308	0.12412
H	11.10365	9.07536	-0.44492
H	12.20852	10.45456	-0.55375
H	10.74318	10.55256	0.44998
C	12.32307	9.37617	1.29911
C	6.82870	5.92981	6.33930
C	5.16958	7.55956	6.34343
C	12.87781	13.71909	6.60477
H	13.56713	12.95335	6.24005
H	13.44868	14.39425	7.25638
H	12.54053	14.29774	5.74128
C	4.21035	8.60825	6.81595
H	4.67860	9.27661	7.54232
H	3.33998	8.14430	7.29762
H	3.84854	9.22097	5.98717

C	5.08159	13.41109	2.73111
H	4.55266	12.55228	3.15070
H	4.34185	14.05207	2.23426
H	5.50992	13.97447	3.56319
C	14.16635	9.73274	4.56516
H	13.53890	10.43387	5.12156
H	15.12278	10.22633	4.34734
H	14.36999	8.88095	5.21822
C	6.05106	11.82941	0.88610
C	7.50178	10.88027	-1.06474
H	8.57185	10.78956	-1.26270
H	7.01664	11.22190	-1.98813
H	7.12155	9.88205	-0.83612
C	13.49419	9.30118	3.29892
C	4.18098	7.18083	3.95247
H	3.79401	8.20213	3.98489
H	3.32607	6.49566	4.02910
H	4.63915	7.03429	2.97143
C	5.16347	6.93444	5.05510
C	12.84342	6.97269	0.39641
H	12.89693	5.98314	0.85714
H	13.68691	7.06195	-0.30144
H	11.92114	7.00932	-0.18861
C	6.46597	4.94237	3.94553
H	6.29098	5.39484	2.96648
H	5.81117	4.06482	4.03166
H	7.50042	4.59161	3.96270
C	7.89953	4.99042	6.80190

H	8.53385	4.66883	5.97301
H	7.45463	4.09566	7.25600
H	8.54467	5.46009	7.54794
C	14.45535	6.87260	3.15949
H	14.53208	6.86567	4.24950
H	15.47352	6.93499	2.75256
H	14.03452	5.91074	2.85625
H	8.75395	7.90374	5.64234
H	11.00639	6.87600	3.38380
H	11.05433	8.32689	4.69538
H	9.89614	8.28392	2.61431
H	7.16374	9.51714	5.65975
H	7.47424	8.25469	3.80666
H	11.12108	10.79615	5.52292
H	9.26661	12.08800	5.39029
H	9.31560	10.26647	6.73726
H	7.21732	11.12376	3.61113
H	9.23142	11.96731	2.98432
H	8.42448	10.10148	2.01512

2-1 lig bend-s-disp

Th	9.14708	9.84227	4.30613
Ir	10.28281	11.45554	6.54956
Ir	7.86706	11.52712	2.20051
Ir	7.14931	7.94568	5.40050
Ir	11.30130	8.33894	3.04122
C	7.35243	11.82089	0.04452
C	11.87087	12.87540	7.23173
C	9.79133	12.75181	8.28994

C	10.57660	13.50452	7.36039
C	11.87170	11.72452	8.10149
C	8.13227	12.95251	0.49320
C	10.59811	11.63665	8.74956
C	7.38179	13.59613	1.54197
C	6.15819	12.87854	1.74249
C	10.15684	14.76323	6.67263
H	10.61359	14.84029	5.68351
H	10.45700	15.64266	7.25549
H	9.07355	14.79683	6.53974
C	6.14859	7.14196	7.21965
C	13.51633	8.25986	2.66457
C	13.03317	10.81570	8.34058
H	12.70150	9.79669	8.55058
H	13.62329	11.16608	9.19622
H	13.69272	10.77769	7.47198
C	11.99403	11.71675	2.78816
H	11.03165	11.96380	2.32950
H	12.74777	12.40069	2.37461
H	11.90768	11.92099	3.85914
C	9.39763	13.45638	-0.12076
H	10.01645	13.97258	0.61725
H	9.19012	14.16212	-0.93574
H	9.99408	12.63936	-0.53331
C	10.19757	10.64555	9.79321
H	9.13022	10.42150	9.73142
H	10.40611	11.02714	10.80104
H	10.73797	9.70451	9.67019

C	7.79393	14.84035	2.25985
H	7.37528	14.87059	3.26782
H	7.44952	15.73071	1.71978
H	8.88066	14.89826	2.35077
C	12.37454	10.29372	2.53306
C	8.42181	13.09210	8.78141
H	7.86733	13.66985	8.03864
H	8.47089	13.68470	9.70388
H	7.84603	12.18775	8.99138
C	6.37703	7.54837	8.63912
H	7.42381	7.41469	8.92183
H	5.76179	6.95649	9.32959
H	6.13097	8.60227	8.78876
C	5.01881	10.80330	0.62515
H	5.37748	9.84968	0.23196
H	4.27036	11.19929	-0.07301
H	4.52010	10.60041	1.57558
C	12.83032	8.30754	1.39120
C	6.22438	5.93080	5.22458
C	11.32751	10.05670	0.16586
H	10.93124	9.23262	-0.43139
H	11.94778	10.68468	-0.48648
H	10.48053	10.65024	0.51934
C	12.12363	9.55124	1.32310
C	6.80798	6.05814	6.52352
C	5.14577	7.67050	6.32974
C	13.03479	13.41156	6.46363
H	13.70315	12.60944	6.14293

H	13.62230	14.11451	7.06859
H	12.70465	13.93992	5.56575
C	4.18871	8.76983	6.65826
H	4.63578	9.48817	7.34858
H	3.28407	8.36447	7.12768
H	3.89023	9.31390	5.75981
C	5.04311	13.25991	2.66077
H	4.53040	12.37520	3.04523
H	4.30148	13.88263	2.14389
H	5.41496	13.82294	3.51971
C	13.77739	9.89343	4.68338
H	13.04493	10.49524	5.22595
H	14.69214	10.48568	4.55233
H	14.01856	9.02609	5.30158
C	6.14427	11.76900	0.80779
C	7.71840	10.90401	-1.07707
H	8.80161	10.80814	-1.17235
H	7.32792	11.28434	-2.02900
H	7.31101	9.90350	-0.91767
C	13.22459	9.47807	3.36085
C	4.26172	7.09923	3.93659
H	3.90501	8.12861	3.85753
H	3.38646	6.44343	4.03108
H	4.76592	6.85476	2.99894
C	5.18576	6.93755	5.09924
C	12.94368	7.29376	0.29875
H	13.06097	6.28687	0.70594
H	13.81007	7.50114	-0.34261

H	12.05190	7.29097	-0.33211
C	6.55894	4.89611	4.20048
H	6.41495	5.28423	3.18985
H	5.92215	4.01016	4.31805
H	7.60065	4.58024	4.28399
C	7.88047	5.18736	7.09279
H	8.54512	4.81792	6.30944
H	7.44323	4.32315	7.60795
H	8.49110	5.73667	7.81249
C	14.46156	7.19197	3.11191
H	14.48975	7.12232	4.20173
H	15.48166	7.39351	2.75993
H	14.16134	6.21390	2.72892
H	8.70586	8.04676	5.84453
H	10.99038	6.78724	3.11978
H	10.89274	8.05516	4.57602
H	9.77611	8.18536	2.53836
H	7.05703	9.56656	5.45835
H	7.61999	8.04209	3.84941
H	11.00975	10.19787	5.82881
H	9.81122	12.01115	5.10355
H	8.94311	10.54816	6.61263
H	7.10371	10.53294	3.22616
H	8.79695	12.04847	3.42028
H	8.91611	10.32186	1.93728

2-2 lig bend-s

Th	9.18582	10.00961	4.36764
Ir	10.23559	11.70123	6.65949

Ir	7.86759	11.74594	2.23899
Ir	7.16784	8.09066	5.38399
Ir	11.40477	8.46454	3.13841
C	7.33011	12.03176	0.07267
C	11.74497	13.23680	7.30224
C	9.74623	12.93421	8.47592
C	10.43123	13.76601	7.51292
C	11.88821	12.06110	8.14376
C	8.14970	13.13332	0.48890
C	10.66252	11.88611	8.86188
C	7.43587	13.83520	1.54078
C	6.19335	13.16142	1.75791
C	9.88942	15.02770	6.91507
H	10.32807	15.22442	5.93425
H	10.11175	15.88579	7.56242
H	8.80548	14.97588	6.78908
C	5.83406	7.25544	7.00662
C	13.57317	8.01134	2.66829
C	13.14560	11.27243	8.34058
H	12.92932	10.24075	8.62778
H	13.76639	11.71780	9.12951
H	13.74470	11.23844	7.42771
C	12.55593	11.64319	2.35089
H	11.60479	11.96090	1.91613
H	13.36277	12.14693	1.79931
H	12.58271	12.00773	3.38066
C	9.41463	13.60056	-0.16137
H	10.09510	14.05308	0.56421

H	9.20191	14.35424	-0.93148
H	9.94591	12.77759	-0.64448
C	10.41149	10.85419	9.91739
H	9.35256	10.59517	9.98174
H	10.72436	11.22940	10.90029
H	10.96539	9.93434	9.71708
C	7.87505	15.11684	2.17836
H	7.44350	15.23764	3.17463
H	7.56600	15.97860	1.57199
H	8.96191	15.15656	2.28351
C	12.71560	10.15532	2.29263
C	8.41798	13.22458	9.10367
H	7.74223	13.71514	8.39871
H	8.52736	13.88540	9.97441
H	7.92771	12.30940	9.44479
C	6.07962	6.04009	7.84775
H	6.19333	5.14553	7.23040
H	5.24635	5.86390	8.54117
H	6.99122	6.14276	8.44153
C	4.92951	11.15333	0.62487
H	5.22888	10.14881	0.31599
H	4.27931	11.56546	-0.15891
H	4.32787	11.05035	1.53072
C	12.81145	7.97844	1.43887
C	4.96977	8.66656	5.37031
C	11.49742	9.74362	0.02644
H	10.99287	8.90347	-0.45614
H	12.15760	10.21125	-0.71599

H	10.73242	10.46943	0.31346
C	12.27970	9.29611	1.22188
C	5.08168	7.29377	5.77234
C	6.16830	8.61142	7.35254
C	12.83275	13.86454	6.48677
H	13.52753	13.11355	6.10273
H	13.41396	14.57380	7.09108
H	12.42836	14.40952	5.63025
C	6.86332	9.04966	8.60385
H	7.50151	8.25782	9.00262
H	6.13291	9.31596	9.37921
H	7.49590	9.91997	8.41247
C	5.10302	13.60677	2.68279
H	4.52796	12.75863	3.06194
H	4.40551	14.27569	2.16229
H	5.50525	14.14614	3.54347
C	14.21986	9.85271	4.40239
H	13.64303	10.63376	4.90360
H	15.19537	10.27329	4.12449
H	14.39410	9.05366	5.12660
C	6.11981	12.03223	0.85288
C	7.62473	11.09361	-1.05661
H	8.69875	10.99079	-1.22427
H	7.17396	11.46396	-1.98628
H	7.22188	10.09693	-0.86277
C	13.49897	9.34606	3.19222
C	5.57163	10.98978	6.42768
H	6.42530	11.39186	6.97969

H	4.65624	11.32762	6.93448
H	5.58697	11.44266	5.43212
C	5.62247	9.49423	6.35549
C	12.72146	6.81980	0.49334
H	12.75220	5.86705	1.02762
H	13.55455	6.82908	-0.22223
H	11.79062	6.84175	-0.07852
C	4.20174	9.17723	4.19155
H	4.68717	10.05639	3.76106
H	3.18105	9.45665	4.48446
H	4.12991	8.42246	3.40516
C	4.43132	6.12017	5.10554
H	4.33257	6.27671	4.02865
H	3.42660	5.94375	5.51214
H	5.01393	5.20708	5.25008
C	14.40306	6.89108	3.21665
H	14.49935	6.96016	4.30287
H	15.41457	6.90490	2.78916
H	13.95918	5.91862	2.99015
H	7.79928	6.73684	4.86673
H	10.95011	6.99047	3.48670
H	11.10551	8.48227	4.72377
H	9.86962	8.37693	2.65261
H	8.69920	8.12156	5.88888
H	7.45586	8.34862	3.81710
H	11.11781	10.96844	5.50944
H	9.18001	12.15559	5.51530
H	9.41039	10.30875	6.79230

H	7.18316	11.17158	3.59277
H	9.18766	12.11248	3.11049
H	8.48572	10.25917	2.02876

2-2 lig bend-s-disp

Th	9.17719	9.74899	4.35817
Ir	10.28835	11.42056	6.58079
Ir	7.85159	11.44158	2.26655
Ir	7.16864	7.98176	5.48175
Ir	11.40226	8.38397	3.09648
C	7.40198	11.86604	0.10921
C	11.82226	12.93862	7.16144
C	9.79601	12.74696	8.31194
C	10.51450	13.50333	7.31813
C	11.91877	11.80856	8.06555
C	8.16710	12.96551	0.65898
C	10.67882	11.69789	8.76855
C	7.38515	13.53976	1.71878
C	6.14716	12.81826	1.82865
C	9.99571	14.71375	6.61118
H	10.44218	14.81274	5.61954
H	10.22563	15.62201	7.18135
H	8.91248	14.65929	6.48352
C	5.67562	7.66924	7.14205
C	13.60471	8.38785	2.60782
C	13.13924	10.98091	8.30359
H	12.87519	9.96488	8.60472
H	13.75852	11.42047	9.09564
H	13.75158	10.90841	7.40285

C	11.91683	11.76780	2.78623
H	10.92124	11.95096	2.36973
H	12.60742	12.50181	2.34943
H	11.85470	11.96029	3.86165
C	9.45558	13.49980	0.12436
H	10.03727	13.98779	0.90993
H	9.27748	14.23741	-0.66863
H	10.07538	12.70428	-0.29521
C	10.37852	10.71795	9.85512
H	9.30948	10.50756	9.91569
H	10.69954	11.11276	10.82685
H	10.89374	9.77025	9.68632
C	7.77237	14.72844	2.53851
H	7.32028	14.68451	3.53163
H	7.44241	15.65564	2.05455
H	8.85527	14.77987	2.66955
C	12.37295	10.37050	2.50881
C	8.45461	13.08592	8.87489
H	7.80291	13.52134	8.11341
H	8.54071	13.80861	9.69659
H	7.95303	12.19851	9.26534
C	5.67917	6.56138	8.14509
H	5.62026	5.58673	7.65549
H	4.82564	6.64654	8.82997
H	6.59333	6.57312	8.74281
C	5.04401	10.84288	0.51329
H	5.41442	9.88198	0.15011
H	4.39134	11.26981	-0.25837

H	4.43294	10.65007	1.39670
C	12.85355	8.38602	1.37261
C	5.13854	8.95962	5.28445
C	11.24654	10.06000	0.18485
H	10.83895	9.21329	-0.37137
H	11.83217	10.67524	-0.51035
H	10.40542	10.65109	0.55343
C	12.09712	9.60287	1.32212
C	4.97285	7.66614	5.87809
C	6.26667	8.96316	7.30809
C	12.92788	13.49004	6.32219
H	13.59582	12.69916	5.97499
H	13.53029	14.21073	6.88967
H	12.53646	14.00144	5.43979
C	7.03324	9.43737	8.49720
H	7.50278	8.60399	9.02401
H	6.37281	9.95916	9.20161
H	7.82480	10.12262	8.18596
C	4.99583	13.17044	2.71258
H	4.40334	12.28817	2.96485
H	4.32804	13.89185	2.22436
H	5.33866	13.61352	3.65067
C	13.89729	10.05003	4.59390
H	13.16513	10.61592	5.17348
H	14.77265	10.68774	4.41615
H	14.21344	9.19862	5.20013
C	6.16761	11.77693	0.82337
C	7.78995	11.03805	-1.07181

H	8.87413	10.93977	-1.14961
H	7.42722	11.49720	-1.99992
H	7.36975	10.03228	-1.00491
C	13.29846	9.60150	3.30276
C	6.20649	11.23911	6.01647
H	7.15801	11.51391	6.48220
H	5.41482	11.84105	6.48258
H	6.27123	11.52307	4.96229
C	5.92919	9.77770	6.16831
C	12.95589	7.36452	0.28638
H	13.13418	6.36825	0.69738
H	13.78028	7.59918	-0.39936
H	12.03500	7.31713	-0.29910
C	4.51894	9.42550	4.00955
H	5.16412	10.15819	3.52027
H	3.54180	9.88784	4.19958
H	4.37462	8.59641	3.31375
C	4.12104	6.55652	5.35165
H	4.06571	6.58542	4.26113
H	3.09797	6.62465	5.74348
H	4.52428	5.58123	5.63335
C	14.60869	7.36156	3.02325
H	14.68838	7.30368	4.11109
H	15.60289	7.59928	2.62356
H	14.33010	6.36903	2.66221
H	7.59943	6.47501	5.25729
H	11.20494	6.82254	3.26518
H	11.08281	8.16095	4.66205

H	9.88806	8.08571	2.63193
H	8.70360	7.89307	5.96855
H	7.56316	7.87063	3.92243
H	11.14729	10.50364	5.56125
H	9.36469	11.91190	5.34632
H	9.35124	10.10928	6.75708
H	7.15736	10.22887	3.08243
H	8.58324	11.93534	3.62229
H	9.03833	10.36982	2.01363

Table S9. Atomic coordinates for the computed structures of **3** (Ir-centered H^-) at different spin states (singlet (sing), triplet (t) and quintet (q))

3-Ir-centered-H-sing

C	7.77553	-1.50989	14.79934
C	7.81070	-0.11101	14.44151
C	9.11304	0.39247	14.81757
C	9.86968	-0.67974	15.38973
C	9.03666	-1.86928	15.37614
Ir	9.37058	-1.20263	13.25879
U	10.35233	-1.97267	10.52888
U	11.03756	0.54779	7.79814
Ir	12.00832	-0.10419	5.06126
C	13.60223	0.23407	3.52657
C	13.56074	-1.17242	3.84453
C	12.25434	-1.65908	3.45838
C	11.50364	-0.56838	2.91689
C	12.34098	0.61674	2.96249
C	14.71048	-2.01488	4.30232
C	11.81554	-3.08946	3.52070
C	10.15381	-0.64853	2.27471
C	11.99430	1.95237	2.38113
C	14.79651	1.12499	3.67816
C	6.65572	0.70954	13.95746
C	9.54573	1.82275	14.71881
C	11.21670	-0.57637	16.03503
C	9.39017	-3.18762	15.99197
C	6.58352	-2.40815	14.67547
Ir	12.68114	-0.57420	9.81173
C	14.96328	-0.32204	9.39216

C	14.71007	-1.61440	9.99714
C	14.25189	-1.40677	11.34161
C	14.09569	0.00585	11.52242
C	14.57453	0.67731	10.32843
C	14.03710	-2.46558	12.37882
C	15.05693	-2.94015	9.39137
C	15.62241	-0.08990	8.06814
C	14.74087	2.15658	10.16919
C	13.69211	0.68498	12.79550
Ir	10.66093	-4.93419	10.18635
C	9.62276	-6.92220	10.18631
C	10.64312	-6.94003	11.18983
C	11.92284	-6.76088	10.52687
C	11.66907	-6.63338	9.12158
C	10.24748	-6.72735	8.89598
C	10.44898	-7.22595	12.64682
C	13.26409	-6.85993	11.18546
C	12.70652	-6.52227	8.04741
C	9.56957	-6.80253	7.56350
C	8.16369	-7.16886	10.41729
Ir	8.70782	-0.86883	8.50839
C	6.48184	-1.47176	8.90421
C	6.56925	-0.06382	8.60062
C	6.98754	0.08724	7.22835
C	7.28014	-1.21615	6.72758
C	6.96530	-2.18250	7.76510
C	7.03073	1.36668	6.45209
C	6.09595	1.04613	9.48907

C	5.89672	-2.07338	10.14412
C	6.98116	-3.67039	7.59760
C	7.68819	-1.54660	5.32536
Ir	10.75792	3.49207	8.10488
C	11.78409	5.48399	8.05842
C	10.74799	5.48055	7.06604
C	9.48328	5.31047	7.75771
C	9.75422	5.20617	9.15818
C	11.18455	5.30879	9.35665
C	10.91570	5.75937	5.60458
C	8.13296	5.37554	7.11433
C	8.73802	5.11942	10.25468
C	11.88473	5.39624	10.67710
C	13.23919	5.72342	7.79689
H	6.32398	-3.05850	10.35029
H	4.80847	-2.19697	10.04537
H	6.08315	-1.44847	11.02109
H	12.91564	5.04149	10.60357
H	11.38333	4.78837	11.43450
H	11.91362	6.43133	11.04479
H	13.46175	6.79786	7.82605
H	13.53465	5.34588	6.81524
H	13.86555	5.23210	8.54479
H	7.37477	4.87470	7.72084
H	8.13673	4.90027	6.13034
H	7.81686	6.41867	6.98088
H	6.25419	0.80419	10.54266
H	5.02401	1.23727	9.34358

H	6.63355	1.97444	9.28036
H	9.10438	4.51544	11.08817
H	7.80621	4.66924	9.90530
H	8.50261	6.11950	10.64192
H	10.16415	5.23363	5.01028
H	11.89711	5.43673	5.24865
H	10.81904	6.83305	5.39279
H	9.57797	0.26565	2.43967
H	9.56978	-1.48351	2.66818
H	10.24907	-0.79014	1.18980
H	7.75557	-3.98168	6.89276
H	6.01625	-4.03404	7.21786
H	7.18728	-4.17304	8.54585
H	7.78455	1.32714	5.66087
H	7.28273	2.21530	7.09202
H	6.05950	1.57595	5.98080
H	12.23917	1.99275	1.31099
H	12.53968	2.75760	2.87898
H	10.92781	2.16618	2.48676
H	6.81042	-1.64440	4.67160
H	8.23904	-2.48961	5.28599
H	8.34127	-0.77467	4.91093
H	15.41851	0.81817	4.52213
H	14.50009	2.16310	3.84510
H	15.41721	1.09241	2.77344
H	14.37298	-2.84047	4.93391
H	15.42727	-1.42870	4.88261
H	15.25068	-2.44656	3.44833

H	12.13716	-3.63016	2.62093
H	10.72881	-3.17299	3.59123
H	12.24361	-3.59791	4.38783
H	15.34614	0.88283	7.65386
H	16.71728	-0.11785	8.16319
H	15.33058	-0.84717	7.33676
H	8.53897	-6.44500	7.62065
H	10.08607	-6.19097	6.81941
H	9.54412	-7.83514	7.18862
H	7.94060	-8.24205	10.35749
H	7.85007	-6.81546	11.40231
H	7.54952	-6.65991	9.67079
H	14.03083	-6.32700	10.61794
H	13.24558	-6.43638	12.19276
H	13.58230	-7.90774	11.27082
H	15.00267	-2.90123	8.30064
H	16.07538	-3.24685	9.66605
H	14.36359	-3.71554	9.72759
H	12.34011	-5.93613	7.20151
H	13.61514	-6.04051	8.41484
H	12.98035	-7.51775	7.67447
H	11.19522	-6.71069	13.25661
H	9.46422	-6.89855	12.98851
H	10.53487	-8.30181	12.85033
H	11.80254	-1.48673	15.88456
H	11.79321	0.25940	15.63197
H	11.11764	-0.42015	17.11758
H	13.95873	2.70357	10.70066

H	15.71140	2.48927	10.56349
H	14.68264	2.45243	9.11873
H	13.27611	-2.16522	13.10465
H	13.70603	-3.40619	11.93002
H	14.96442	-2.66790	12.93400
H	9.14104	-3.20229	17.06171
H	8.85224	-4.00863	15.51218
H	10.45854	-3.39665	15.89641
H	14.55572	0.81946	13.46111
H	13.26710	1.67217	12.59779
H	12.93542	0.10458	13.32953
H	5.96270	-2.13307	13.81976
H	6.88144	-3.45122	14.54666
H	5.96001	-2.34417	15.57657
H	6.99148	1.53918	13.33049
H	5.96229	0.10920	13.36300
H	6.08935	1.13373	14.79811
H	9.22515	2.38259	15.60710
H	10.63172	1.90976	14.64143
H	9.11183	2.30901	13.84199
H	10.32874	2.34767	9.18008
H	12.13060	2.64771	7.89053
H	10.09587	2.55404	6.95120
H	11.58200	-1.14825	6.23570
H	10.66449	0.73337	5.44949
H	12.76807	0.77063	6.20093
H	9.83840	-0.19166	12.07746
H	8.58233	-2.03951	12.11233

H	10.70903	-2.05719	12.90069
H	11.32039	-3.77473	9.25999
H	11.12461	-4.04716	11.46553
H	9.29015	-4.05772	10.14303
H	10.01402	-1.74491	8.07330
H	9.35602	0.12202	9.62623
H	11.39987	0.35657	10.20337
H	12.05279	-1.51252	8.63893

3-Ir-centered-H-t

C	10.99011	5.25709	9.56623
C	11.59813	5.54165	8.28468
C	10.57240	5.56067	7.28730
C	9.30575	5.29301	7.94539
C	9.57219	5.11266	9.34260
Ir	10.64665	3.50800	8.20220
U	11.04691	0.57229	7.75170
Ir	8.75346	-0.91998	8.46430
C	6.88748	-2.19421	7.93680
C	6.48456	-1.20670	8.88149
C	6.71081	0.09292	8.28291
C	7.16937	-0.09814	6.93629
C	7.34654	-1.50702	6.74505
C	5.82936	-1.45779	10.20384
C	6.34340	1.40827	8.89860
C	7.37157	0.97364	5.90964
C	7.74524	-2.17154	5.46364
C	6.74576	-3.67713	8.08574
C	13.04328	5.86494	8.06186

C	10.74399	5.92461	5.84485
C	7.95873	5.36321	7.29539
C	8.54643	4.91340	10.41518
C	11.67210	5.29044	10.89866
Ir	11.99402	-0.08181	5.00513
C	12.61456	0.71653	3.00495
C	13.71614	-0.01988	3.56449
C	13.28427	-1.39567	3.71189
C	11.93472	-1.49476	3.25137
C	11.50823	-0.18009	2.81079
C	15.10589	0.49362	3.78242
C	14.15038	-2.53346	4.15595
C	11.14118	-2.75731	3.11885
C	10.21938	0.14261	2.11990
C	12.64896	2.15895	2.60280
Ir	12.72038	-0.52035	9.75574
C	14.61478	0.77545	10.09061
C	14.97758	-0.34397	9.28443
C	14.75505	-1.54524	10.06766
C	14.31167	-1.16107	11.37321
C	14.14650	0.26512	11.36163
C	15.61473	-0.29106	7.93040
C	15.10424	-2.93752	9.63761
C	14.11861	-2.06040	12.55491
C	13.74308	1.10114	12.53797
C	14.79967	2.22045	9.74682
U	10.41198	-1.99884	10.49739
Ir	10.73903	-4.94982	10.22799

C	10.33838	-6.78597	9.00203
C	9.75166	-6.95883	10.30734
C	10.79470	-6.92621	11.29064
C	12.05138	-6.73840	10.58826
C	11.76798	-6.65484	9.18855
C	8.30287	-7.22176	10.58095
C	10.64432	-7.19154	12.75651
C	13.40726	-6.77445	11.22279
C	12.77449	-6.56084	8.08367
C	9.62905	-6.90418	7.68895
Ir	9.37140	-1.30403	13.20532
C	9.02458	-1.99434	15.31170
C	7.76569	-1.62873	14.73303
C	7.80147	-0.22611	14.39340
C	9.10207	0.27348	14.77980
C	9.85696	-0.80476	15.34236
C	6.57599	-2.52699	14.58879
C	6.64805	0.60167	13.91828
C	9.53169	1.70588	14.70082
C	11.20581	-0.70795	15.98465
C	9.37548	-3.31994	15.91315
H	6.10778	-2.43587	10.60357
H	4.73427	-1.43042	10.11124
H	6.12306	-0.71060	10.94466
H	12.72254	5.00085	10.81501
H	11.19915	4.60303	11.60458
H	11.64041	6.29713	11.33799
H	13.22047	6.94061	8.19093

H	13.36346	5.59135	7.05377
H	13.68576	5.33460	8.76844
H	7.22020	4.76663	7.83611
H	7.99342	4.99257	6.26782
H	7.59154	6.39796	7.26382
H	6.39830	1.36154	9.98892
H	5.32013	1.70030	8.62586
H	7.02420	2.19718	8.56808
H	8.93684	4.29680	11.22801
H	7.65044	4.42317	10.02847
H	8.24430	5.87958	10.83992
H	10.02429	5.39822	5.21296
H	11.74381	5.66978	5.48547
H	10.59710	7.00232	5.69267
H	9.92594	1.18166	2.28984
H	9.40381	-0.49073	2.47823
H	10.30297	-0.00790	1.03487
H	7.52816	-4.20715	7.53765
H	5.77479	-4.02156	7.70275
H	6.82409	-3.98057	9.13271
H	8.14649	0.69731	5.18920
H	7.67842	1.91639	6.37136
H	6.44606	1.16260	5.34691
H	13.00544	2.26118	1.56967
H	13.31686	2.73578	3.24674
H	11.65749	2.61391	2.66169
H	6.86991	-2.34990	4.82425
H	8.22560	-3.13536	5.64904

H	8.45436	-1.55447	4.90635
H	15.59968	-0.02898	4.60531
H	15.10384	1.55898	4.02655
H	15.72361	0.35868	2.88388
H	13.56174	-3.32818	4.61982
H	14.89482	-2.20500	4.88504
H	14.68821	-2.96688	3.30234
H	11.29845	-3.21095	2.13124
H	10.07081	-2.57168	3.23185
H	11.42923	-3.49155	3.87468
H	15.26015	0.56711	7.35383
H	16.70839	-0.21851	8.01183
H	15.38361	-1.18646	7.34836
H	8.59719	-6.55209	7.76236
H	10.12256	-6.31058	6.91534
H	9.60235	-7.94690	7.34340
H	8.09865	-8.30005	10.56293
H	8.00689	-6.83969	11.56065
H	7.66354	-6.74820	9.83257
H	14.15216	-6.26197	10.60971
H	13.40028	-6.29600	12.20538
H	13.74440	-7.81063	11.35926
H	15.02304	-3.04950	8.55350
H	16.13380	-3.19224	9.92374
H	14.43164	-3.67006	10.09109
H	12.38592	-5.98288	7.24173
H	13.69567	-6.07844	8.41745
H	13.03411	-7.56138	7.71356

H	11.37918	-6.63142	13.34017
H	9.65355	-6.90088	13.11390
H	10.78121	-8.25817	12.98099
H	11.78399	-1.62359	15.83733
H	11.78709	0.12046	15.57303
H	11.11192	-0.54378	17.06652
H	13.97955	2.82989	10.13415
H	15.73915	2.60778	10.16621
H	14.83123	2.37089	8.66470
H	13.29864	-1.71626	13.19152
H	13.88591	-3.08366	12.24839
H	15.02694	-2.09951	13.17355
H	9.12027	-3.34806	16.98117
H	8.84071	-4.13515	15.42013
H	10.44445	-3.52730	15.82077
H	14.60404	1.30997	13.18750
H	13.32615	2.05930	12.21811
H	12.98120	0.59342	13.13519
H	5.96269	-2.24192	13.73088
H	6.87705	-3.56784	14.44943
H	5.94459	-2.47551	15.48522
H	6.98360	1.42898	13.28791
H	5.94514	0.00521	13.33140
H	6.09224	1.03026	14.76378
H	9.19875	2.25593	15.59073
H	10.61818	1.79751	14.63769
H	9.10649	2.19948	13.82383
H	10.05108	2.28804	9.09204

H	12.04996	2.68935	8.18426
H	10.23990	2.65428	6.88136
H	10.60514	-0.56644	5.70102
H	11.70362	1.39196	5.61759
H	12.71613	-0.45410	6.41298
H	9.83338	-0.27979	12.02979
H	8.61826	-2.16829	12.05401
H	10.69231	-2.18832	12.85539
H	11.15403	-3.81159	9.14307
H	11.35498	-3.98778	11.38776
H	9.34981	-4.12864	10.42023
H	10.05262	-1.82346	8.07016
H	9.35594	0.03231	9.63815
H	11.41081	0.33940	10.20008
H	12.09045	-1.52282	8.63815

3-Ir-centered-H-q

C	10.99011	5.25709	9.56623
C	11.59813	5.54165	8.28468
C	10.57240	5.56067	7.28730
C	9.30575	5.29301	7.94539
C	9.57219	5.11266	9.34260
Ir	10.64665	3.50800	8.20220
U	11.04691	0.57229	7.75170
Ir	8.75346	-0.91998	8.46430
C	6.88748	-2.19421	7.93680
C	6.48456	-1.20670	8.88149
C	6.71081	0.09292	8.28291
C	7.16937	-0.09814	6.93629

C	7.34654	-1.50702	6.74505
C	5.82936	-1.45779	10.20384
C	6.34340	1.40827	8.89860
C	7.37157	0.97364	5.90964
C	7.74524	-2.17154	5.46364
C	6.74576	-3.67713	8.08574
C	13.04328	5.86494	8.06186
C	10.74399	5.92461	5.84485
C	7.95873	5.36321	7.29539
C	8.54643	4.91340	10.41518
C	11.67210	5.29044	10.89866
Ir	11.99402	-0.08181	5.00513
C	12.61456	0.71653	3.00495
C	13.71614	-0.01988	3.56449
C	13.28427	-1.39567	3.71189
C	11.93472	-1.49476	3.25137
C	11.50823	-0.18009	2.81079
C	15.10589	0.49362	3.78242
C	14.15038	-2.53346	4.15595
C	11.14118	-2.75731	3.11885
C	10.21938	0.14261	2.11990
C	12.64896	2.15895	2.60280
Ir	12.72038	-0.52035	9.75574
C	14.61478	0.77545	10.09061
C	14.97758	-0.34397	9.28443
C	14.75505	-1.54524	10.06766
C	14.31167	-1.16107	11.37321
C	14.14650	0.26512	11.36163

C	15.61473	-0.29106	7.93040
C	15.10424	-2.93752	9.63761
C	14.11861	-2.06040	12.55491
C	13.74308	1.10114	12.53797
C	14.79967	2.22045	9.74682
U	10.41198	-1.99884	10.49739
Ir	10.73903	-4.94982	10.22799
C	10.33838	-6.78597	9.00203
C	9.75166	-6.95883	10.30734
C	10.79470	-6.92621	11.29064
C	12.05138	-6.73840	10.58826
C	11.76798	-6.65484	9.18855
C	8.30287	-7.22176	10.58095
C	10.64432	-7.19154	12.75651
C	13.40726	-6.77445	11.22279
C	12.77449	-6.56084	8.08367
C	9.62905	-6.90418	7.68895
Ir	9.37140	-1.30403	13.20532
C	9.02458	-1.99434	15.31170
C	7.76569	-1.62873	14.73303
C	7.80147	-0.22611	14.39340
C	9.10207	0.27348	14.77980
C	9.85696	-0.80476	15.34236
C	6.57599	-2.52699	14.58879
C	6.64805	0.60167	13.91828
C	9.53169	1.70588	14.70082
C	11.20581	-0.70795	15.98465
C	9.37548	-3.31994	15.91315

H	6.10778	-2.43587	10.60357
H	4.73427	-1.43042	10.11124
H	6.12306	-0.71060	10.94466
H	12.72254	5.00085	10.81501
H	11.19915	4.60303	11.60458
H	11.64041	6.29713	11.33799
H	13.22047	6.94061	8.19093
H	13.36346	5.59135	7.05377
H	13.68576	5.33460	8.76844
H	7.22020	4.76663	7.83611
H	7.99342	4.99257	6.26782
H	7.59154	6.39796	7.26382
H	6.39830	1.36154	9.98892
H	5.32013	1.70030	8.62586
H	7.02420	2.19718	8.56808
H	8.93684	4.29680	11.22801
H	7.65044	4.42317	10.02847
H	8.24430	5.87958	10.83992
H	10.02429	5.39822	5.21296
H	11.74381	5.66978	5.48547
H	10.59710	7.00232	5.69267
H	9.92594	1.18166	2.28984
H	9.40381	-0.49073	2.47823
H	10.30297	-0.00790	1.03487
H	7.52816	-4.20715	7.53765
H	5.77479	-4.02156	7.70275
H	6.82409	-3.98057	9.13271
H	8.14649	0.69731	5.18920

H	7.67842	1.91639	6.37136
H	6.44606	1.16260	5.34691
H	13.00544	2.26118	1.56967
H	13.31686	2.73578	3.24674
H	11.65749	2.61391	2.66169
H	6.86991	-2.34990	4.82425
H	8.22560	-3.13536	5.64904
H	8.45436	-1.55447	4.90635
H	15.59968	-0.02898	4.60531
H	15.10384	1.55898	4.02655
H	15.72361	0.35868	2.88388
H	13.56174	-3.32818	4.61982
H	14.89482	-2.20500	4.88504
H	14.68821	-2.96688	3.30234
H	11.29845	-3.21095	2.13124
H	10.07081	-2.57168	3.23185
H	11.42923	-3.49155	3.87468
H	15.26015	0.56711	7.35383
H	16.70839	-0.21851	8.01183
H	15.38361	-1.18646	7.34836
H	8.59719	-6.55209	7.76236
H	10.12256	-6.31058	6.91534
H	9.60235	-7.94690	7.34340
H	8.09865	-8.30005	10.56293
H	8.00689	-6.83969	11.56065
H	7.66354	-6.74820	9.83257
H	14.15216	-6.26197	10.60971
H	13.40028	-6.29600	12.20538

H	13.74440	-7.81063	11.35926
H	15.02304	-3.04950	8.55350
H	16.13380	-3.19224	9.92374
H	14.43164	-3.67006	10.09109
H	12.38592	-5.98288	7.24173
H	13.69567	-6.07844	8.41745
H	13.03411	-7.56138	7.71356
H	11.37918	-6.63142	13.34017
H	9.65355	-6.90088	13.11390
H	10.78121	-8.25817	12.98099
H	11.78399	-1.62359	15.83733
H	11.78709	0.12046	15.57303
H	11.11192	-0.54378	17.06652
H	13.97955	2.82989	10.13415
H	15.73915	2.60778	10.16621
H	14.83123	2.37089	8.66470
H	13.29864	-1.71626	13.19152
H	13.88591	-3.08366	12.24839
H	15.02694	-2.09951	13.17355
H	9.12027	-3.34806	16.98117
H	8.84071	-4.13515	15.42013
H	10.44445	-3.52730	15.82077
H	14.60404	1.30997	13.18750
H	13.32615	2.05930	12.21811
H	12.98120	0.59342	13.13519
H	5.96269	-2.24192	13.73088
H	6.87705	-3.56784	14.44943
H	5.94459	-2.47551	15.48522

H	6.98360	1.42898	13.28791
H	5.94514	0.00521	13.33140
H	6.09224	1.03026	14.76378
H	9.19875	2.25593	15.59073
H	10.61818	1.79751	14.63769
H	9.10649	2.19948	13.82383
H	10.05108	2.28804	9.09204
H	12.04996	2.68935	8.18426
H	10.23990	2.65428	6.88136
H	10.60514	-0.56644	5.70102
H	11.70362	1.39196	5.61759
H	12.71613	-0.45410	6.41298
H	9.83338	-0.27979	12.02979
H	8.61826	-2.16829	12.05401
H	10.69231	-2.18832	12.85539
H	11.15403	-3.81159	9.14307
H	11.35498	-3.98778	11.38776
H	9.34981	-4.12864	10.42023
H	10.05262	-1.82346	8.07016
H	9.35594	0.03231	9.63815
H	11.41081	0.33940	10.20008
H	12.09045	-1.52282	8.63815

Table S10. Atomic coordinates for the computed structures of **3** (U–Ir bridging H^-) at different spin states (singlet (sing), triplet (t) and quintet (q))

3-U-Ir brid. H-sing

C	14.32570	-1.51889	11.39171
C	14.59633	-1.46638	9.97872
C	14.99485	-0.12305	9.64815
C	14.99644	0.64296	10.87054
C	14.58862	-0.20521	11.93197
Ir	12.80479	-0.12854	10.36832
U	10.37309	-1.46559	10.02249
Ir	10.84588	-4.40194	9.97151
C	11.02510	-6.36112	11.08149
C	12.19650	-6.20590	10.23982
C	11.75173	-6.15445	8.87892
C	10.31538	-6.28060	8.85582
C	9.87838	-6.41282	10.22695
C	14.63460	-2.63544	9.04546
C	15.57635	0.32821	8.34554
C	9.46119	-6.42541	7.63490
C	13.61660	-6.29712	10.70441
C	8.46791	-6.66277	10.66506
C	15.41396	2.07557	10.99207
C	12.63454	-6.09661	7.67100
C	11.04225	-6.57669	12.56290
C	14.50556	0.16735	13.37940
C	14.09846	-2.75316	12.20715
Ir	8.48694	-1.09047	7.98675
C	6.82550	0.30937	7.23557
C	6.68330	0.13336	8.65447

C	6.37239	-1.25120	8.90752
C	6.30310	-1.91925	7.63107
C	6.58176	-0.97117	6.61051
C	6.69010	1.23050	9.67239
C	5.90493	-1.82993	10.20504
C	5.93788	-3.35712	7.43061
C	6.55433	-1.22169	5.13445
C	6.94113	1.61504	6.51410
U	10.96051	0.15884	8.26443
Ir	10.52184	3.08604	8.10800
C	9.85079	4.95495	7.01784
C	9.21286	4.92380	8.31196
C	10.26059	4.96640	9.30818
C	11.52271	5.02065	8.63814
C	11.26731	5.01138	7.20748
C	12.86179	5.19226	9.28523
C	7.74536	5.06418	8.57352
C	12.30043	5.17980	6.13710
C	10.05090	5.04608	10.78875
C	9.14020	5.02571	5.70170
Ir	12.36399	-0.38220	5.71225
C	13.99260	-1.41238	4.52852
C	12.70314	-1.90850	4.09920
C	11.95664	-0.81947	3.55034
C	12.78232	0.37272	3.63391
C	14.02910	-0.00169	4.22928
C	12.43768	1.71296	3.06203
C	10.61787	-0.90620	2.88566

C	12.27378	-3.34245	4.12829
C	15.21109	0.89886	4.41299
C	15.14530	-2.25078	4.98682
Ir	9.05715	-1.13282	12.66515
C	7.40605	-0.27908	13.96625
C	8.67789	0.28983	14.36292
C	9.51752	-0.76832	14.82861
C	8.77653	-2.01242	14.71985
C	7.48058	-1.69827	14.19617
C	9.23485	-3.34702	15.22060
C	10.87250	-0.61756	15.44657
C	9.00719	1.75066	14.38142
C	6.35382	-2.66852	14.01901
C	6.17632	0.49752	13.61084
H	6.17422	-2.88589	10.29582
H	4.81102	-1.75347	10.28926
H	6.35880	-1.31154	11.05131
H	13.65518	4.74877	8.67863
H	12.89265	4.71363	10.26652
H	13.09943	6.25630	9.41940
H	12.51377	6.24294	5.96164
H	11.96764	4.74598	5.19134
H	13.24006	4.69252	6.40913
H	7.46290	4.62055	9.53151
H	7.14736	4.58005	7.79741
H	7.45221	6.12280	8.60176
H	7.01236	0.85833	10.64753
H	5.68427	1.66055	9.78021

H	7.37718	2.02852	9.38070
H	10.87937	4.58771	11.33336
H	9.13544	4.53087	11.08866
H	9.96923	6.09236	11.11147
H	8.18721	4.49259	5.73160
H	9.73959	4.58798	4.90013
H	8.93051	6.06939	5.43332
H	10.05120	0.01945	3.01322
H	10.01821	-1.71912	3.30155
H	10.72733	-1.08523	1.80747
H	6.35553	-3.75306	6.50146
H	4.84753	-3.48058	7.38407
H	6.30600	-3.97697	8.25210
H	7.44888	1.49779	5.55283
H	7.51799	2.33576	7.09686
H	5.94581	2.03871	6.31681
H	12.70517	1.76771	1.99797
H	12.96757	2.51553	3.58062
H	11.36748	1.91783	3.14684
H	5.56290	-0.99741	4.71842
H	6.78326	-2.26429	4.89872
H	7.28158	-0.59638	4.61068
H	15.82875	0.58481	5.25738
H	14.90097	1.93054	4.59492
H	15.84344	0.89046	3.51563
H	14.80625	-3.11745	5.55958
H	15.82842	-1.68315	5.62356
H	15.72551	-2.62472	4.13185

H	12.60226	-3.86261	3.21882
H	11.18728	-3.43258	4.19484
H	12.70217	-3.86514	4.98639
H	15.41098	1.39630	8.18042
H	16.66145	0.15097	8.32159
H	15.11903	-0.20024	7.50719
H	8.44649	-6.06175	7.81302
H	9.86661	-5.85413	6.79625
H	9.38975	-7.47643	7.32186
H	8.25203	-7.73910	10.66856
H	8.28802	-6.28092	11.67258
H	7.75166	-6.18129	9.99523
H	14.29618	-5.74608	10.04980
H	13.73609	-5.89860	11.71492
H	13.95059	-7.34352	10.72268
H	14.37323	-2.33048	8.02969
H	15.64060	-3.07867	9.02571
H	13.92010	-3.40463	9.34864
H	12.14448	-5.57010	6.84903
H	13.57296	-5.57997	7.88501
H	12.87936	-7.10928	7.32460
H	11.82941	-5.98853	13.04145
H	10.09296	-6.28563	13.01847
H	11.22026	-7.63323	12.80498
H	11.49488	-1.49547	15.25667
H	11.39759	0.25375	15.04909
H	10.79163	-0.49517	16.53501
H	14.92854	2.56600	11.83995

H	16.49937	2.15649	11.13959
H	15.15995	2.64151	10.09249
H	13.50853	-2.53828	13.10247
H	13.55654	-3.50824	11.63575
H	15.05552	-3.18422	12.53456
H	9.03748	-3.45449	16.29601
H	8.72188	-4.16340	14.70644
H	10.30753	-3.48554	15.06332
H	15.45151	-0.04814	13.89440
H	14.29477	1.23226	13.50940
H	13.71756	-0.39144	13.88974
H	5.67812	-2.35828	13.21900
H	6.72134	-3.66785	13.77444
H	5.76505	-2.74361	14.94246
H	6.42299	1.42144	13.08143
H	5.50272	-0.07842	12.97157
H	5.61501	0.77556	14.51360
H	8.67679	2.21194	15.32152
H	10.08214	1.91703	14.28300
H	8.51819	2.27811	13.55902
H	10.08275	2.08655	9.31476
H	11.87976	2.24393	7.85752
H	9.81566	1.99496	7.13856
H	11.90747	-1.45847	6.85175
H	11.03334	0.50098	5.96774
H	12.99069	0.44667	6.95364
H	9.31995	0.01870	11.54405
H	8.49889	-2.03531	11.44093

H	10.48470	-1.80972	12.32568
H	11.30034	-3.29718	8.85972
H	11.40448	-3.36708	11.08817
H	9.44661	-3.62011	10.16060
H	11.65315	0.04133	11.47382
H	9.14884	-2.54112	8.14600
H	9.52024	-1.07572	6.75828
H	12.24992	1.31895	9.94222

3-U-Ir brid. H-t

C	11.78785	-0.86073	3.06646
C	12.25505	0.50965	2.94488
C	13.60362	0.55114	3.43296
C	13.97963	-0.76989	3.86793
C	12.84394	-1.63831	3.63498
Ir	12.24067	-0.05545	5.11109
U	11.11928	0.52969	7.82682
Ir	12.57830	-0.29866	10.13839
C	14.70028	-0.24606	9.25439
C	14.89179	0.38580	10.54360
C	14.56061	-0.54446	11.54979
C	14.15368	-1.78155	10.91442
C	14.29232	-1.60852	9.48969
C	15.38524	1.78583	10.74077
C	14.63258	-0.33120	13.03003
C	13.97466	-3.08328	11.63623
C	14.27179	-2.70450	8.46853
C	15.19867	0.31334	7.95567
C	11.51583	1.62861	2.27861

C	14.50527	1.74686	3.40939
C	15.34937	-1.20802	4.28401
C	12.82493	-3.11904	3.85736
C	10.47861	-1.38295	2.56135
Ir	10.78083	3.49913	8.06459
C	10.17361	5.19773	9.40367
C	11.55044	5.35848	9.05465
C	11.63018	5.52141	7.61270
C	10.29303	5.46608	7.09612
C	9.38128	5.26121	8.19307
C	12.69762	5.46975	10.01041
C	12.86954	5.84918	6.83884
C	9.89715	5.67945	5.66767
C	7.88656	5.31352	8.12083
C	9.62646	5.08733	10.79317
Ir	8.83296	-1.14750	8.11308
U	10.26349	-1.93236	10.45723
Ir	9.12998	-1.26102	13.15260
C	9.56164	-0.36517	15.16398
C	9.12699	-1.74087	15.33880
C	7.78150	-1.83572	14.85202
C	7.37306	-0.54124	14.36627
C	8.48577	0.36299	14.56712
C	9.89424	-2.81369	16.04809
C	6.91079	-3.05248	14.91977
C	5.99383	-0.15549	13.93009
C	8.46653	1.83416	14.28902
C	10.85632	0.20733	15.65189

C	6.54646	-1.88504	7.66668
C	6.87460	-0.95050	6.66329
C	7.24145	0.29781	7.30133
C	7.07830	0.12688	8.72378
C	6.69821	-1.24385	8.95685
C	6.09333	-3.29827	7.46705
C	6.83841	-1.17040	5.18277
C	7.40705	1.60191	6.58021
C	7.05155	1.22775	9.73984
C	6.19263	-1.81189	10.24926
Ir	10.56255	-4.91900	10.35381
C	11.88732	-6.68115	9.88755
C	10.69192	-6.76314	9.06719
C	9.57043	-6.88927	9.94972
C	10.04630	-6.87391	11.31226
C	11.48708	-6.75313	11.25983
C	10.66412	-6.85178	7.57263
C	8.14778	-7.10054	9.53208
C	9.22722	-7.11991	12.54114
C	12.40298	-6.80064	12.44403
C	13.29203	-6.68029	9.36951
H	6.37726	-2.88836	10.31405
H	5.10722	-1.65827	10.33798
H	6.67605	-1.35015	11.11351
H	13.62696	5.11180	9.56112
H	12.52202	4.88134	10.91392
H	12.85417	6.51409	10.31229
H	13.06312	6.93041	6.84536

H	12.78459	5.53236	5.79660
H	13.74610	5.35181	7.26148
H	7.42524	4.73435	8.92491
H	7.51530	4.91279	7.17417
H	7.52335	6.34676	8.20865
H	7.32952	0.86138	10.73119
H	6.04173	1.65856	9.80549
H	7.74616	2.02836	9.47427
H	10.34676	4.62211	11.46981
H	8.71550	4.48464	10.81651
H	9.38119	6.08079	11.19107
H	8.99236	5.12094	5.41677
H	10.68543	5.35796	4.98334
H	9.69904	6.74246	5.47873
H	9.68885	-0.63298	2.64860
H	10.15825	-2.26541	3.11972
H	10.55499	-1.66395	1.50235
H	6.39034	-3.68221	6.48751
H	4.99988	-3.37611	7.53484
H	6.51808	-3.96129	8.22575
H	7.91666	1.46562	5.62163
H	8.00026	2.31388	7.15923
H	6.42693	2.05506	6.37158
H	11.67712	1.61576	1.19212
H	11.84400	2.60135	2.65271
H	10.43985	1.55610	2.45621
H	5.90596	-0.78495	4.74881
H	6.90444	-2.23195	4.93000

H	7.66822	-0.66040	4.68632
H	15.23627	1.71080	4.22044
H	13.93983	2.67559	3.51396
H	15.05691	1.79262	2.46152
H	15.30841	-2.05741	4.97069
H	15.89168	-0.40482	4.78871
H	15.94615	-1.51493	3.41409
H	13.19646	-3.64810	2.96995
H	11.81478	-3.47860	4.06604
H	13.45615	-3.40231	4.70291
H	15.04848	1.39561	7.90092
H	16.27663	0.12480	7.84541
H	14.68311	-0.12558	7.09825
H	9.71572	-6.48998	7.16846
H	11.45900	-6.25106	7.12365
H	10.79838	-7.88908	7.23656
H	7.92723	-8.17332	9.45816
H	7.45091	-6.66565	10.25251
H	7.94566	-6.65006	8.55774
H	13.34611	-6.28713	12.24293
H	11.94833	-6.32721	13.31753
H	12.63701	-7.84004	12.70877
H	13.97069	-2.32954	7.48717
H	15.27170	-3.15194	8.37121
H	13.57337	-3.49520	8.75162
H	13.37073	-6.12435	8.43200
H	13.98540	-6.22679	10.08180
H	13.63550	-7.70555	9.17765

H	9.65232	-6.60850	13.40849
H	8.20474	-6.75444	12.41640
H	9.17324	-8.19168	12.77711
H	11.66528	-0.52439	15.58887
H	11.15487	1.07866	15.06460
H	10.77247	0.52147	16.70104
H	15.11829	2.17223	11.72789
H	16.47875	1.83530	10.65104
H	14.96290	2.46418	9.99447
H	13.46985	-2.94053	12.59632
H	13.36826	-3.78730	11.06103
H	14.95006	-3.54844	11.84126
H	9.73852	-2.75588	17.13388
H	9.58492	-3.80902	15.72014
H	10.96741	-2.72554	15.86081
H	15.56982	-0.72974	13.44130
H	14.58503	0.73005	13.28816
H	13.80844	-0.83305	13.54394
H	6.18871	-3.07164	14.10020
H	7.50191	-3.96918	14.86171
H	6.34946	-3.07141	15.86288
H	6.01529	0.67304	13.21750
H	5.47809	-0.98930	13.44737
H	5.38262	0.16102	14.78652
H	8.05667	2.38337	15.14678
H	9.47075	2.21671	14.09334
H	7.84945	2.06652	13.41794
H	10.08797	2.33256	8.96345

H	12.16581	2.65595	8.12637
H	10.44768	2.59804	6.75756
H	12.20892	-1.03610	6.41177
H	10.72191	0.37810	5.48229
H	12.70062	1.13701	6.11123
H	9.17413	-0.31754	11.82518
H	8.67433	-2.48218	12.18794
H	10.64740	-1.71920	12.80410
H	11.25003	-3.81239	9.37375
H	10.90871	-3.93770	11.59786
H	9.18921	-4.06973	10.21266
H	11.51333	-0.08500	11.32597
H	9.47591	-2.61023	8.31388
H	9.92359	-1.33677	6.94417
H	11.96136	1.17726	9.95584

3-U-Ir brid. H-q

C	7.63249	-2.05615	14.83986
C	7.38727	-0.67759	14.51254
C	8.59576	0.06209	14.82250
C	9.56398	-0.85547	15.33482
C	8.97282	-2.18182	15.34262
Ir	9.07521	-1.44937	13.23003
U	10.20375	-1.91375	10.48836
U	11.03915	0.54698	7.85013
Ir	12.23505	-0.28261	5.22176
C	13.58057	0.22111	3.50029
C	14.02693	-1.02267	4.07342
C	12.94649	-1.97598	3.92434

C	11.85423	-1.32548	3.27129
C	12.24336	0.04934	3.00830
C	15.41276	-1.33248	4.54772
C	13.01349	-3.42492	4.29569
C	10.57967	-1.96990	2.82166
C	11.44938	1.04823	2.22436
C	14.40872	1.46131	3.36250
C	6.07108	-0.08096	14.12102
C	8.75243	1.54807	14.72317
C	10.91298	-0.50365	15.88088
C	9.59172	-3.41552	15.92338
C	6.62691	-3.16307	14.75976
Ir	12.43184	-0.17778	10.24752
C	14.39989	-0.21733	11.68531
C	14.11693	-1.49709	11.06709
C	14.26708	-1.34031	9.64331
C	14.56199	0.04879	9.38772
C	14.66911	0.71912	10.66636
C	14.03236	-2.79929	11.80446
C	14.35004	-2.45657	8.64792
C	15.03745	0.63033	8.09031
C	15.02713	2.16211	10.84256
C	14.42751	0.02830	13.16209
Ir	10.69021	-4.85318	10.15660
C	9.73591	-6.87632	10.10690
C	10.75767	-6.88261	11.11070
C	12.02838	-6.64167	10.45198
C	11.76802	-6.48793	9.05012

C	10.35026	-6.62634	8.82206
C	10.57629	-7.21680	12.55897
C	13.37205	-6.71052	11.10859
C	12.79955	-6.32195	7.97758
C	9.66880	-6.66950	7.48962
C	8.28616	-7.17745	10.33210
Ir	8.68805	-1.02459	8.21494
C	6.68981	-0.73399	6.85063
C	7.13763	0.49682	7.47045
C	7.02619	0.33275	8.89910
C	6.58349	-1.01595	9.14982
C	6.35319	-1.65005	7.86857
C	7.32112	1.79145	6.73800
C	7.11088	1.42823	9.91719
C	6.08752	-1.54906	10.45994
C	5.81990	-3.03735	7.68336
C	6.58118	-0.95525	5.37371
Ir	10.82504	3.54725	7.89995
C	11.95986	5.46995	7.75004
C	10.95015	5.45875	6.73538
C	9.65725	5.40579	7.39330
C	9.89239	5.38012	8.80778
C	11.31401	5.41543	9.04396
C	11.16726	5.61582	5.26213
C	8.33093	5.53085	6.71050
C	8.84087	5.41162	9.87370
C	11.98403	5.55132	10.37610
C	13.43243	5.61975	7.52152

H	6.17466	-2.63818	10.51009
H	5.02532	-1.29809	10.59612
H	6.64939	-1.14375	11.30411
H	12.99756	5.14407	10.35474
H	11.43597	5.01461	11.15453
H	12.05436	6.60493	10.68020
H	13.71501	6.68050	7.51807
H	13.73475	5.18821	6.56460
H	14.00954	5.12446	8.30590
H	7.52341	5.12595	7.32484
H	8.31932	4.99541	5.75775
H	8.09456	6.58356	6.50462
H	7.43664	1.04594	10.88786
H	6.12836	1.90431	10.04962
H	7.82191	2.19736	9.60811
H	9.16129	4.86568	10.76408
H	7.90543	4.96529	9.52855
H	8.62825	6.44644	10.17159
H	10.41023	5.07405	4.68967
H	12.14492	5.23343	4.95958
H	11.11525	6.67322	4.96979
H	9.75349	-1.25506	2.81481
H	10.29427	-2.79442	3.47907
H	10.68326	-2.36989	1.80410
H	6.09069	-3.44494	6.70576
H	4.72407	-3.05215	7.75570
H	6.20822	-3.71876	8.44520
H	7.80728	1.63817	5.76996

H	7.94499	2.49110	7.29795
H	6.34791	2.26671	6.54739
H	11.62996	0.93701	1.14660
H	11.71063	2.07204	2.50282
H	10.37688	0.92689	2.39625
H	5.63074	-0.56515	4.98520
H	6.62937	-2.01755	5.11986
H	7.38757	-0.45021	4.83540
H	15.11540	1.56218	4.18954
H	13.78333	2.35684	3.34960
H	14.98453	1.43783	2.42830
H	15.40817	-2.09342	5.33241
H	15.90484	-0.44550	4.95460
H	16.03664	-1.70895	3.72538
H	13.47101	-4.00991	3.48698
H	12.01797	-3.83342	4.48361
H	13.61107	-3.57799	5.19745
H	14.75817	1.68411	7.99547
H	16.13365	0.57251	8.02369
H	14.61287	0.10723	7.23063
H	8.63147	-6.33425	7.56311
H	10.16759	-6.01797	6.76787
H	9.66364	-7.68769	7.07632
H	8.09941	-8.25517	10.23903
H	7.96323	-6.86547	11.32802
H	7.65459	-6.66531	9.60259
H	14.12041	-6.13720	10.55631
H	13.33800	-6.31193	12.12563

H	13.72638	-7.74844	11.16883
H	14.07314	-2.11450	7.64790
H	15.37515	-2.85278	8.60463
H	13.67651	-3.27521	8.91453
H	12.42043	-5.71580	7.15177
H	13.70253	-5.83896	8.35759
H	13.08913	-7.30004	7.57196
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H	10.70695	-8.29347	12.73224
H	11.62216	-1.32406	15.74695
H	11.32754	0.37705	15.38523
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H	14.69190	2.54524	11.80997
H	16.11388	2.31113	10.78594
H	14.56857	2.77907	10.06480
H	13.49545	-2.69251	12.75165
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H	13.64767	-0.54176	13.67368
H	5.91158	-2.99631	13.95118
H	7.11015	-4.12646	14.58207
H	6.06240	-3.23733	15.69818

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H	5.45839	-0.79202	13.56179
H	5.49886	0.22284	15.00828
H	8.38394	2.03961	15.63328
H	9.79927	1.82993	14.58918
H	8.19229	1.95088	13.87579
H	10.09909	2.49052	8.89988
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H	10.38484	2.55552	6.68958
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H	9.26474	-2.51868	8.39353
H	9.71974	-1.27731	7.00758
H	11.65767	1.22394	10.06113

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