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Synthesis, structure and bonding of hexaphenyl thorium(IV): Observation of a non-octahedral structure

Elizabeth A. Pedrick,[a] Peter Hrobárik,*[,b] Lani A. Seaman,[a] Guang Wu,[a] Trevor W. Hayton*[,a]

[a] Department of Chemistry and Biochemistry, University of California, Santa Barbara
Santa Barbara, CA 93106, USA

[b] Institut für Chemie, Technische Universität Berlin
Strasse des 17. Juni 135, 10623 Berlin, Germany

E-mail: peter.hrobarik@tu-berlin.de, hayton@chem.ucsb.edu

Supporting Information

1 Experimental Section

All reactions and subsequent manipulations were performed under anaerobic and anhydrous conditions under an atmosphere of nitrogen or argon. Hexanes was dried by passage over activated molecular sieves using a Vacuum Atmospheres DRI-SOLV solvent purification system. Dimethoxyethane (DME) and THF were distilled from sodium benzophenone ketyl. THF-d_8 was dried over activated 3Å molecular sieves for 24 h before use. $ThCl_4(DME)_2$ was prepared according to literature procedure.[S1] All other reagents were purchased from commercial suppliers and used as received.

NMR spectra were recorded on a Varian UNITY INOVA 400 MHz spectrometer, an Agilent Technologies 400-MR DD2 spectrometer, or a Varian UNITY INOVA 500 MHz spectrometer. ^1H and $^{13}C\{^1H\}$ NMR spectra were referenced to external $SiMe_4$ using the residual protio solvent peaks as internal standards. The chemical shifts of $^7Li\{^1H\}$ were referenced indirectly with the ^1H resonance of $SiMe_4$ at 0 ppm, according to IUPAC standard.[S2],[S3] IR spectra were recorded on a Mattson Genesis FTIR/Raman spectrometer. Elemental analyses were performed by the Microanalytical Laboratory at UC Berkeley.

Synthesis of $[Li(DME)_3]_2[Th(C_6H_5)_6]$ (1). To a cold (-25 °C), stirring solution of $ThCl_4(DME)_2$ (181.0 mg, 0.327 mmol) in THF (2 mL) was added a cold (-25 °C) 1.9 M dibutyl ether solution of PhLi (1.40 mL, 2.660 mmol). The solution immediately (< 1 min) turned light amber in color, concomitant with the deposition of a white precipitate. After stirring for few more minutes, the precipitate was removed by filtration through a Celite column (2 cm × 0.5 cm) supported on glass wool. The volatiles were then removed from the filtrate *in vacuo* to give an amber oil that was quickly rinsed with hexanes (3 mL). The oil was then extracted into DME (2 mL) to give an amber solution and small amount of white precipitate. The precipitate was removed by filtration through a Celite column (2 cm × 0.5 cm) supported on glass wool. The solution was reduced in volume *in vacuo* to ca. 1 mL, whereupon crystals began to appear on the walls of the vial. Storage of the solution at -25 °C for 24 h resulted in the deposition of pale yellow crystals (169

mg), which were isolated by decanting away the supernatant. Further concentration of the supernatant *in vacuo*, followed by storage of the solution at -25 °C for 24 h, resulted in the deposition of a second crop of material (60 mg). Total yield: 56%. ^{1}H NMR (400 MHz, 25 °C, THF-d_8): δ 7.61 (d, 12H, *o*-CH), 7.00 (t, 12H, *m*-CH), 6.79 (t, 6H, *p*-CH), 3.44 (s, 24H, CH_2), 3.28 (s, 36H, CH_3). ^{1}H NMR (500 MHz, -55 °C, THF-d_8): δ 7.48 (br s, 12H, *o*-CH), 6.98 (br s, 12H, *m*-CH), 6.80 (br s, 6H, *p*-CH), 3.39 (s, 24H, CH_2-DME), 3.23 (s, 36H, CH_3-DME). ^{1}H NMR (500 MHz, -61 °C, THF-d_8): δ 7.57 (br s, 12H, *o*-CH), 6.97 (br s, 12H, *m*-CH), 6.80 (br s, 6H, *p*-CH), 3.38 (s, 24H, CH_2-DME), 3.23 (s, 36H, CH_3-DME). ^{1}H NMR (500 MHz, -68 °C, THF-d_8): δ 7.76 (br s, 12H, *o*-CH), 6.95 (br s, 18H, *m*-CH and *p*-CH), 3.38 (s, 24H, CH_2-DME), 3.23 (s, 36H, CH_3-DME). ^{1}H NMR (500 MHz, -75 °C, THF-d_8): δ 7.83 (br s), 7.13 (br s), 7.04 (br s), 6.82 (br s), 3.37 (s, 24H, CH_2-DME), 3.21 (s, 36H, CH_3-DME). ^{1}H NMR (500 MHz, -90 °C, THF-d_8): δ 7.84 (br s), 7.16 (br s), 7.01 (br s), 6.78 (br s), 6.60 (br s), 3.37 (s, 24H, CH_2-DME), 3.21 (s, 36H, CH_3-DME). ^{7}Li{^{1}H} NMR (195 MHz, 25 °C, THF-d_8): δ 2.60 (s). ^{13}C{^{1}H} NMR (126 MHz, -4 °C, THF-d_8): δ 220.5 (br s, ipso-C), 136.9 (s, *o*-C), 126.6 (s, *m*-C), 125.2 (s, *p*-CH), 72.9 (s, CH_2 DME), 59.1 (s, CH_3 DME). Anal. Calcd for $C_{60}H_{90}Li_2O_{12}Th$: C, 57.69, H, 7.26. Found: C, 57.09, H, 7.30. The low carbon percentage is likely due to thermal instability of complex **1**. IR (KBr pellet, cm^{-1}): 1591(m), 1483(s), 1450(w), 1410(w), 1367(w), 1288(sh m), 1277(m), 1244(w), 1228(w), 1192(w), 1165(sh w), 1122(s), 1097(sh m), 1082(s), 1039(m), 1028(m), 1009(sh w), 989(sh w), 985(w), 867(m), 847(w), 829(sh w), 764(w), 739(m), 714(sh m), 700(vs), 673(m), 629(w).

Synthesis of [Li(THF)(12-crown-4)]$_2$[Th(C$_6$H$_5$)$_6$] (2). To a cold (-25 °C) amber solution of **1** (45.3 mg, 0.036 mmol) in THF (4 mL) was added 12-crown-4 (5.9 µL, 0.036 mmol), which resulted in a color change to yellow. The solution was layered with hexanes (4 mL) and stored at -25 °C for 24 h, which resulted in the deposition of colorless crystals (18.9 mg, 44% yield). ^{1}H NMR (400 MHz, 25 °C, THF-d_8): δ 7.64 (d, 12H, *o*-CH), 7.03 (t, 12H, *m*-CH), 6.82 (t, 6H, *p*-CH), 3.38 (s, 16H, CH_2-crown). ^{7}Li{^{1}H} NMR (195 MHz, 25 °C, THF-d_8): δ 0.55 (s). Anal. Calcd for

$C_{60}H_{78}Li_2O_{10}Th$: C, 59.80, H, 6.52. Found: C, 58.94, H, 6.63. The low carbon percentage is likely due to thermal instability of complex **2**. IR (KBr pellet, cm^{-1}): 1587(vw), 1560(vw), 1479(w), 1467(sh w), 1448(w), 1410(m), 1363(w), 1300(sh w), 1286(w), 1242(sh w), 1230(w), 1186(vw), 1157(sh w), 1134(s), 1095(vs), 1084(s), 1039(s), 1024(m), 1009(sh w), 985(w), 920(sh m), 914(m), 891(sh w), 860(w), 847(w), 806(vw), 762(vw), 713(sh m), 702(s), 687(sh w), 673(m), 660(sh w), 625(m), 553(w), 474(w), 447(w), 422(w).

X-ray Crystallography. Data for **1** and **2** was collected on a Bruker KAPPA APEX II diffractometer equipped with an APEX II CCD detector using a TRIUMPH monochromator with a Mo Kα X-ray source (α = 0.71073 Å). Crystals of **1**–**2** were mounted on a cryoloop under Paratone-N oil, and all data were collected at 100(2) K using an Oxford nitrogen gas cryostream system. Frame exposures of 40 s, 30s, and 45s were used for **1**, and frames exposures of 10 s and 5 s were used for **2**. SMART was used to determine the cell parameters and data collection.[S4] The raw frame data were processed using SAINT.[S5] Subsequent calculations were carried out using SHELXTL.[S6] Absorption correction of the data was carried out using the multiscan method SADABS.[S7] The structures were solved using Direct methods and difference Fourier techniques. All hydrogen atom positions were idealized, and rode on the atom of attachment. The final refinement included anisotropic temperature factors on all non-hydrogen atoms. Structure solution, refinement, graphics, and creation of publication materials were performed using SHELXTL.[S6] A summary of relevant crystallographic data for complexes **1** and **2** are presented in Table S1. Complexes **1**-**2** have been deposited in the Cambridge Structural Database (**1**: CCDC 1428924; **2**: CCDC 1428925).

Table S1. X-ray crystallographic information for **1** and **2**

	1	**2**
Empirical formula	$C_{60}H_{90}Li_2O_{12}Th$	$C_{60}H_{78}Li_2O_8Th$
Crystal Habit, color	plate, pale-yellow	block, tan
Crystal size (mm)	0.80 × 0.10 × 0.01	0.40 × 0.35 × 0.25
Crystal system	Trigonal	monoclinic
Space group	*R*-3	*P*2(1)/*n*
Volume (Å^3)	4658.9(2)	5605.4(6)
a (Å)	14.8737(4)	16.564(1)
b (Å)	14.8737(4)	16.704(1)
c (Å)	24.3175(8)	21.385(1)
α(°)	90	90
β(°)	90	108.682(1)
γ(°)	120	90
Z	3	4
Formula weight (g/mol)	1249.24	1205.14
Density (calculated) (Mg/m^3)	1.336	1.428
Absorption coefficient (mm^{-1})	2.456	2.717
F_{000}	1926	2456
Total no. reflections	12517	13898
Unique reflections	2963	11374
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0338, wR_2 = 0.0655	R_1 = 0.0297, wR_2 = 0.0701
Largest diff. peak and hole (e$^-$Å^{-3})	1.184 and -0.365	1.892 and -1.412
GOF	1.047	1.007

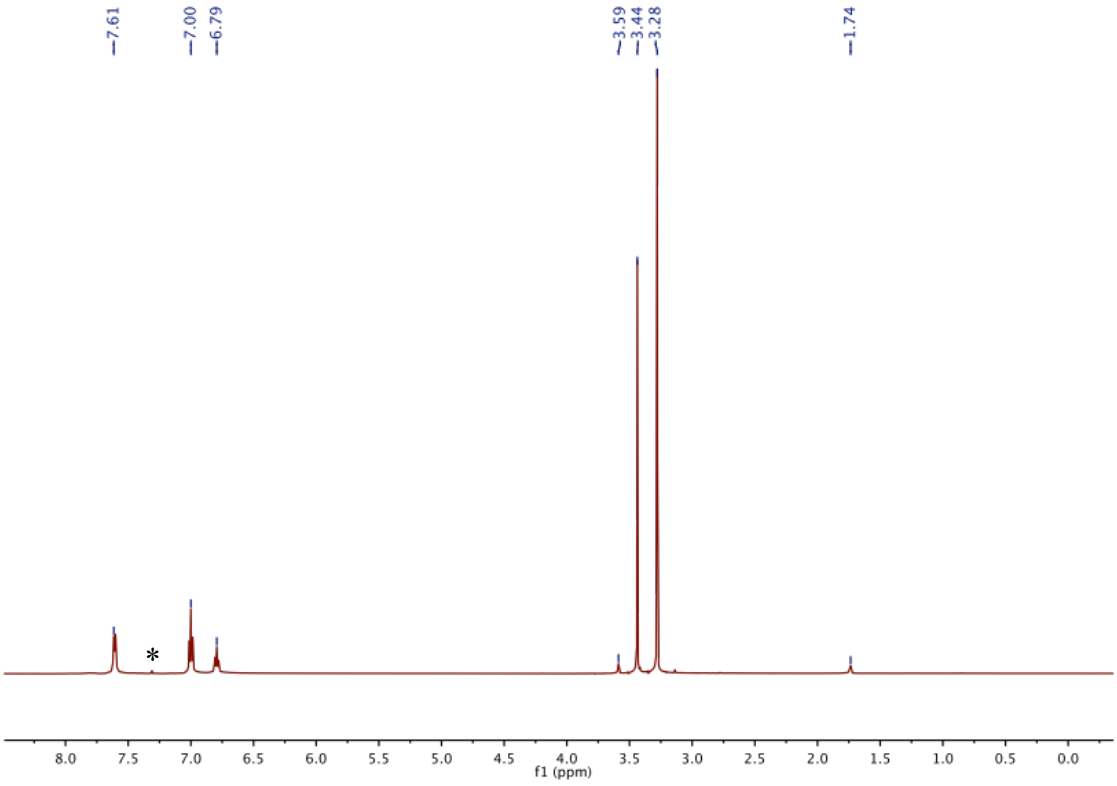


Figure S1. ^{1}H NMR spectrum of **1** in THF-d_8 at room temperature. Asterisk indicates the presence of benzene.

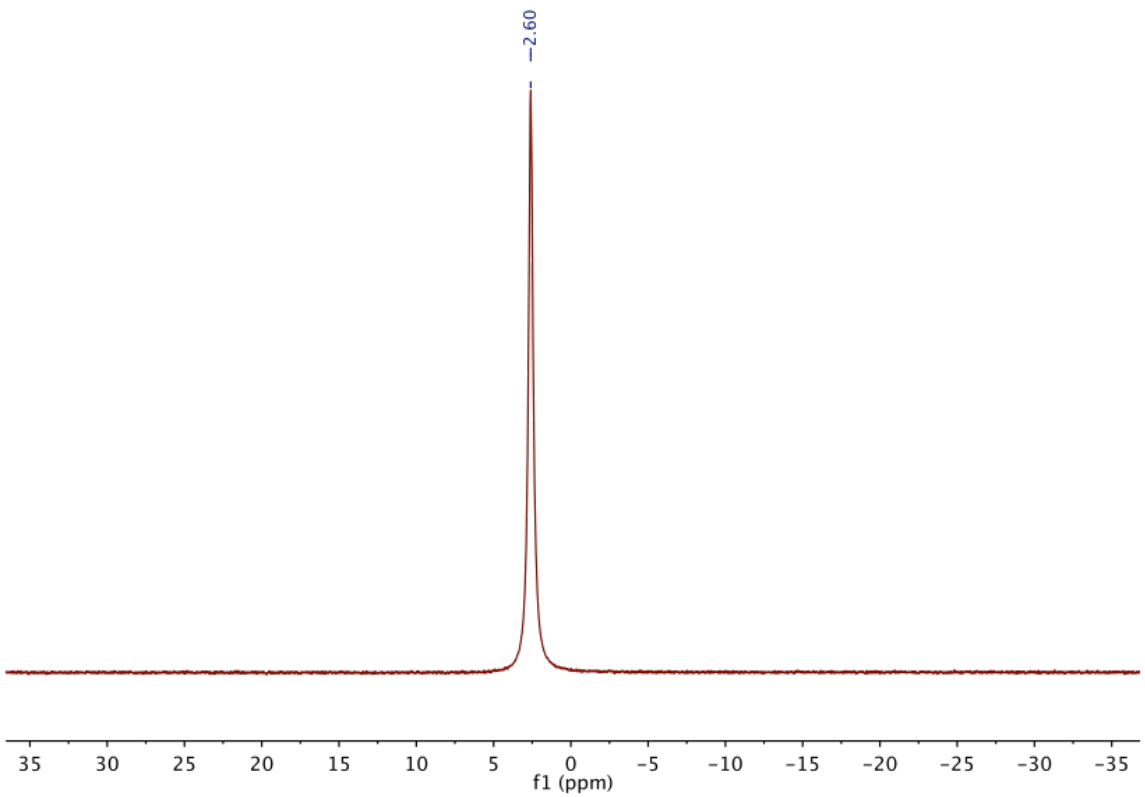


Figure S2. $^{7}Li\{^{1}H\}$ NMR spectrum of **1** in THF-d_8 at room temperature.

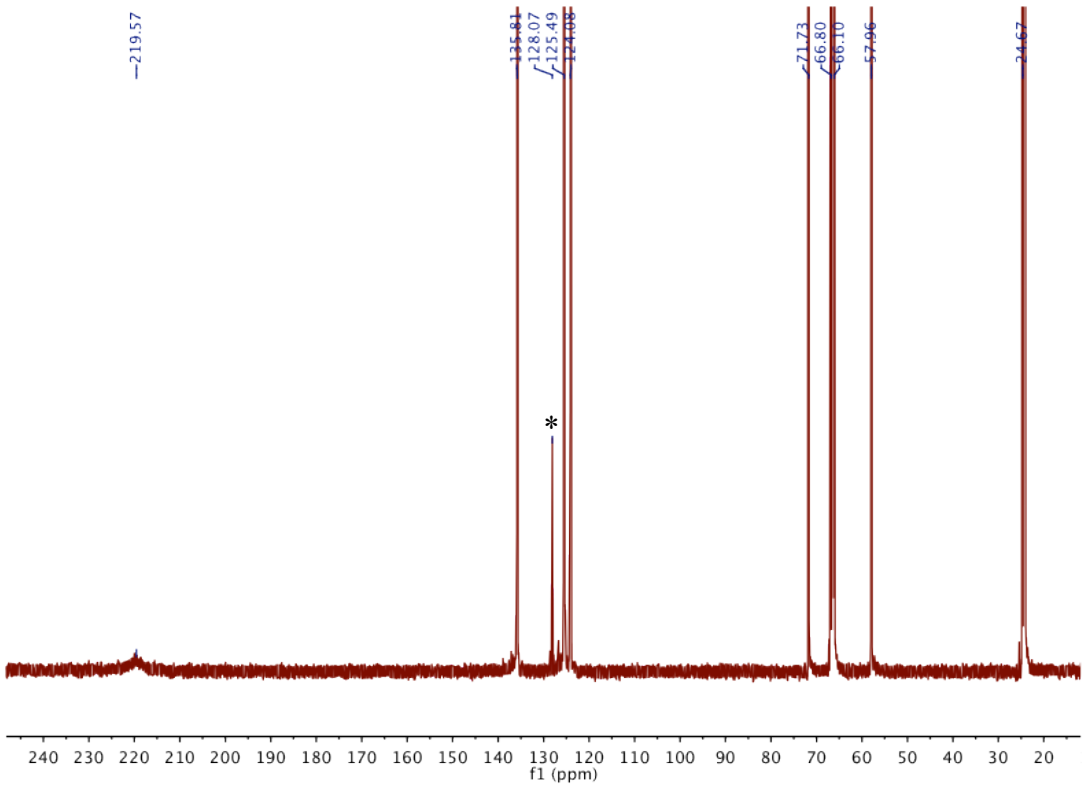


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in THF-d_8 at -4 °C. Asterisk indicates the presence of benzene.

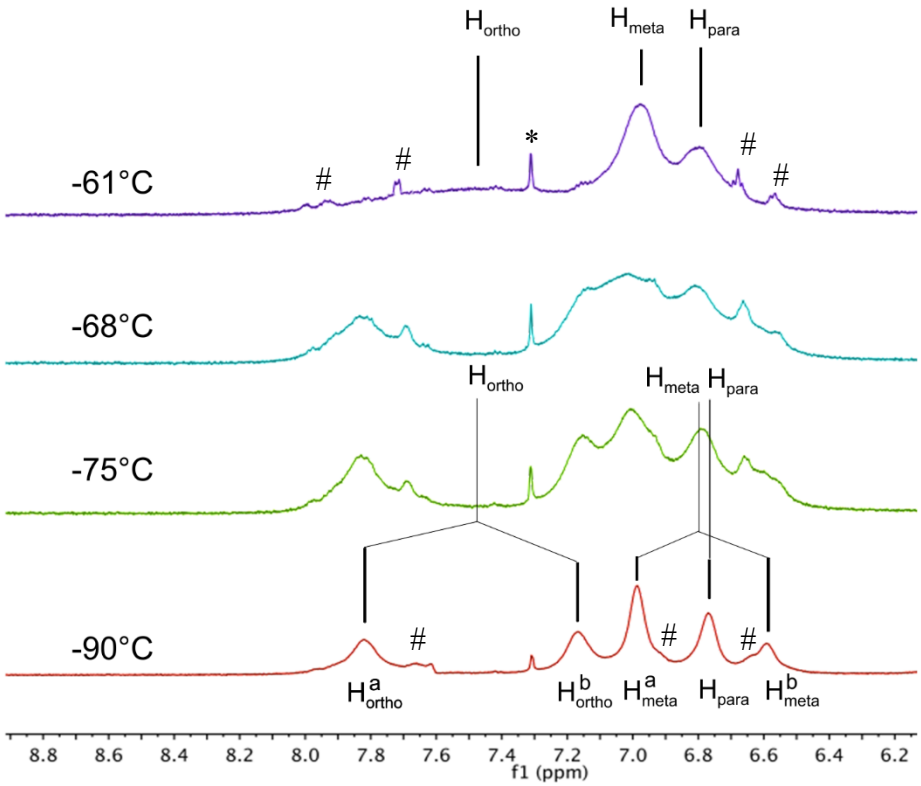


Figure S4. Partial variable temperature ^{1}H NMR spectra of **1** in THF-d_8. Asterisk indicates the presence of benzene, and **#** indicates resonances assignable to an as-yet-unidentified decomposition product.

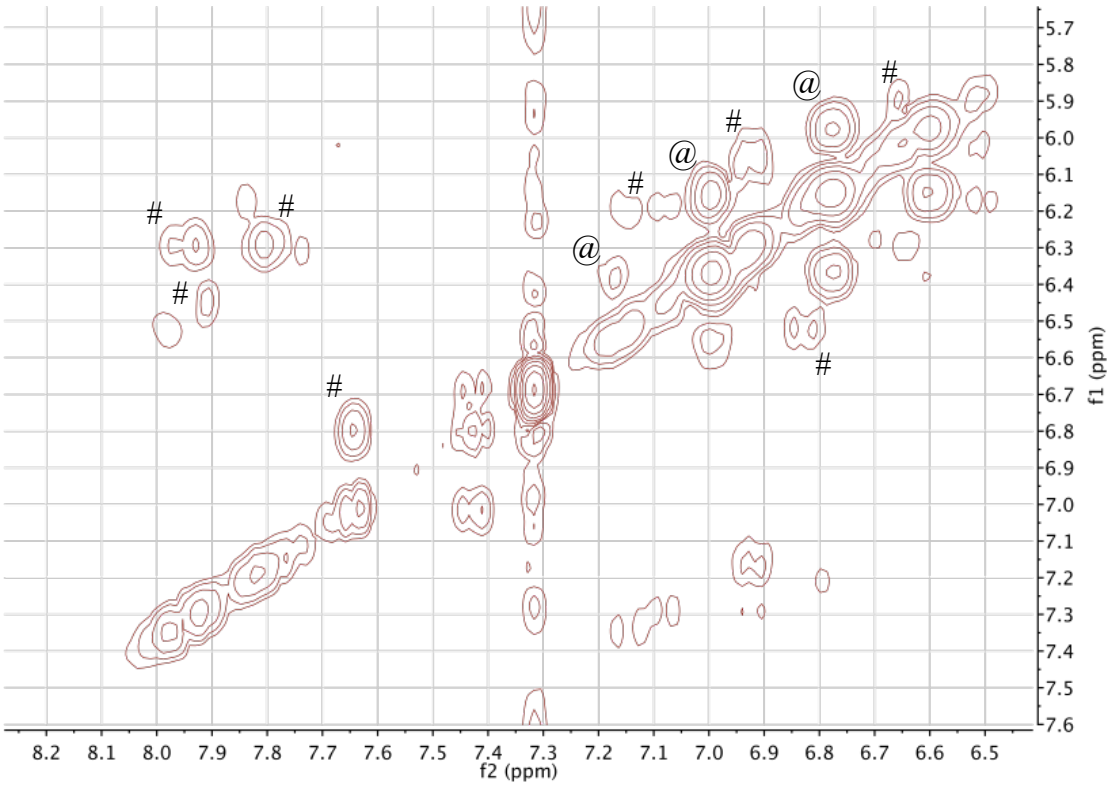


Figure S5. Partial ^{1}H-^{1}H COSY NMR spectrum of **1** in THF-d_8 at -90°C. **Spectrum notes:** The presence of a second species in solution, possibly due to decomposition, is evident in the COSY spectrum. # indicates cross peaks assignable to this second species. @ indicates cross peaks assignable to through-bond coupling in complex **1**.

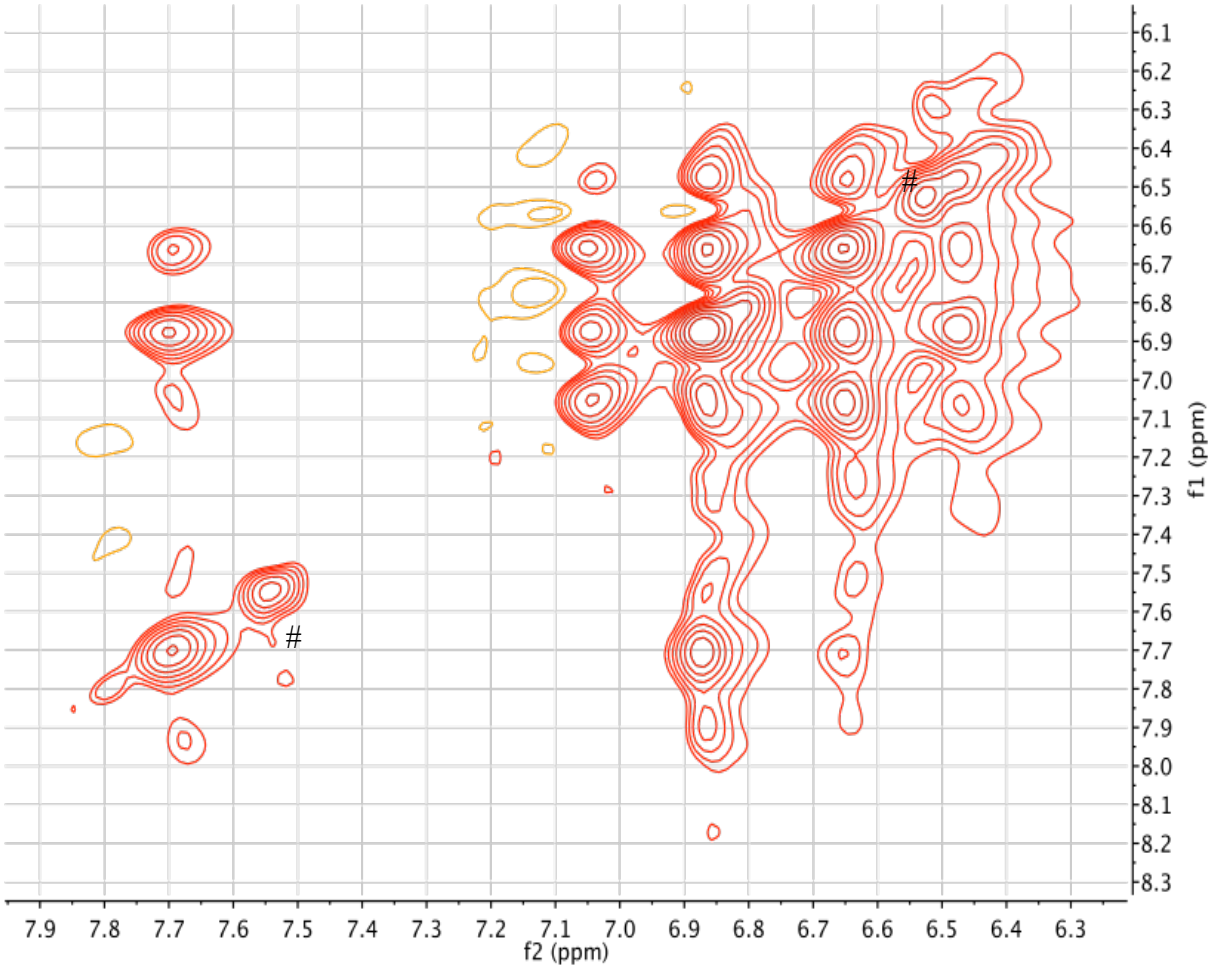


Figure S6. Partial 2D NOESY NMR spectrum of **1** in THF-d_8 at -90°C. **Spectrum notes:** The presence of a second species in solution, possibly due to decomposition, is also evident in the NOESY spectrum. # indicates peaks assignable to this second species.

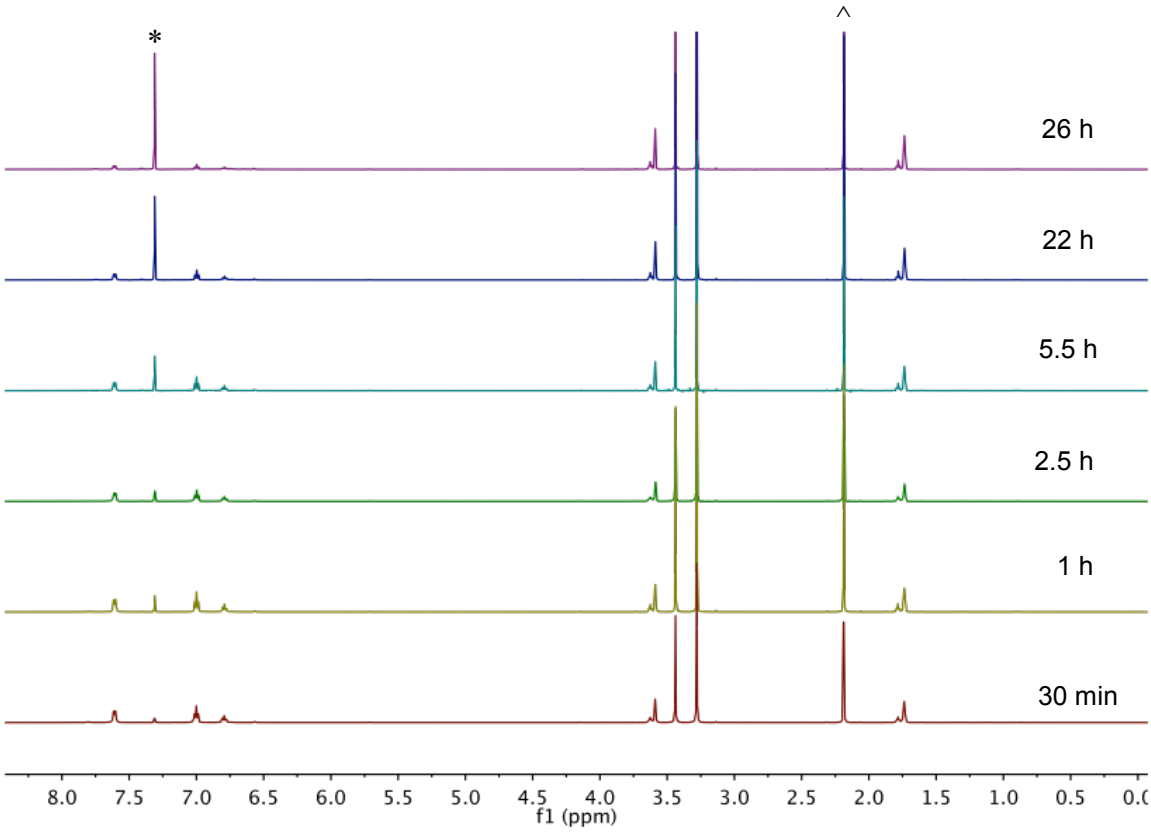


Figure S7: ^{1}H NMR spectra of complex **1** at room temperature in THF-d_8. **Experimental Details:** A light yellow THF-d_8 solution (1 mL) containing **1** (17.2 mg, 0.014 mmol) and hexamethylbenzene (3.1 mg, 0.013 mmol) was sealed in a J. Young NMR tube and the ^{1}H NMR spectrum was obtained (30 min spectrum). The NMR tube was allowed to stand at room temperature, which resulted in a slow color change to dark brown. ^{1}H NMR spectra were collected at 1.5 h, 5.5 h, 22h and 26 h. After 26 h, nearly all of complex **1** had decomposed. Asterisk indicates the presence of benzene, and ^ indicates the presence of hexamethylbenzene.

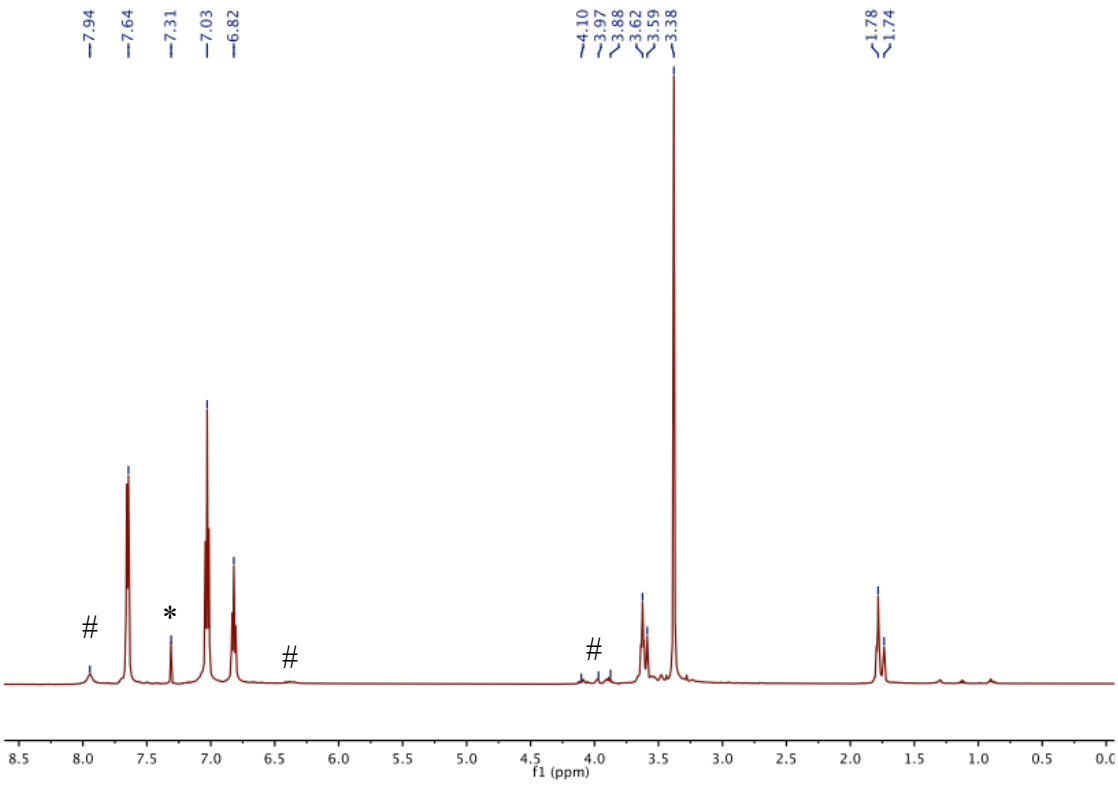


Figure S8. ^{1}H NMR spectrum of **2** in THF-d_8 at room temperature. Asterisk indicates the presence of benzene, and # indicates resonances assignable to an as-yet-unidentified decomposition product.

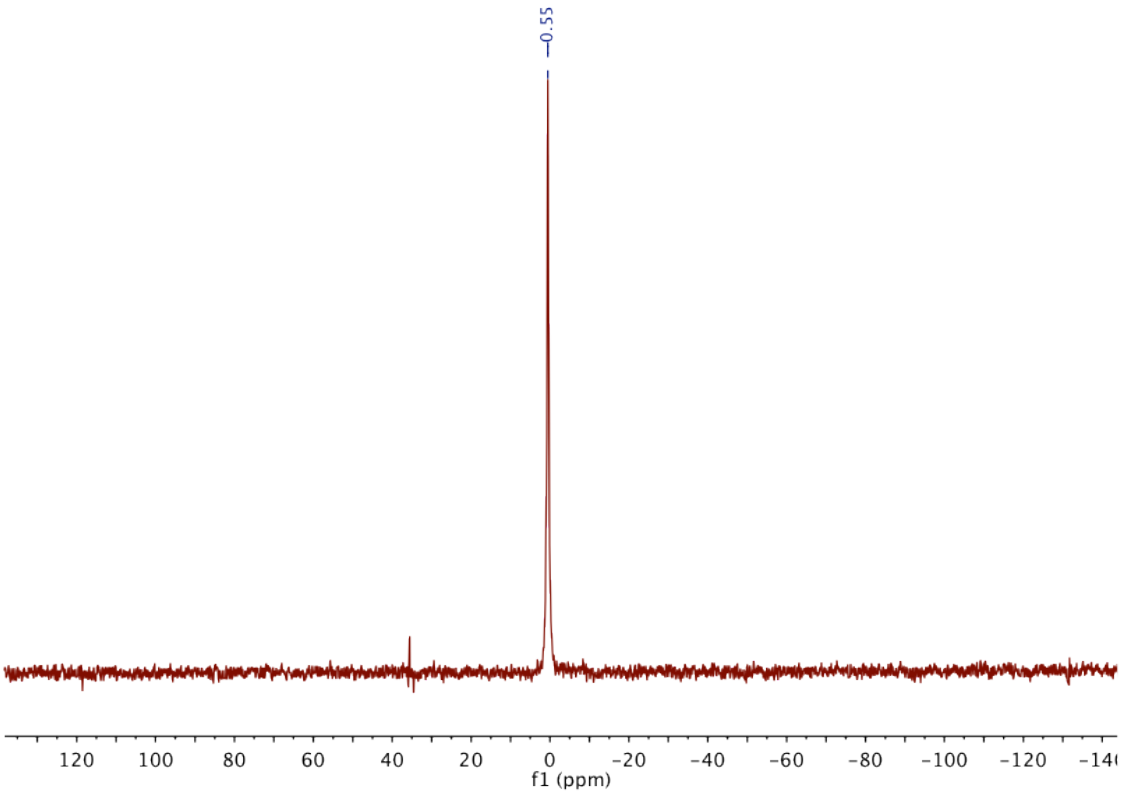


Figure S9. $^{7}Li\{^{1}H\}$ NMR spectrum of **2** in THF-d_8 at room temperature.

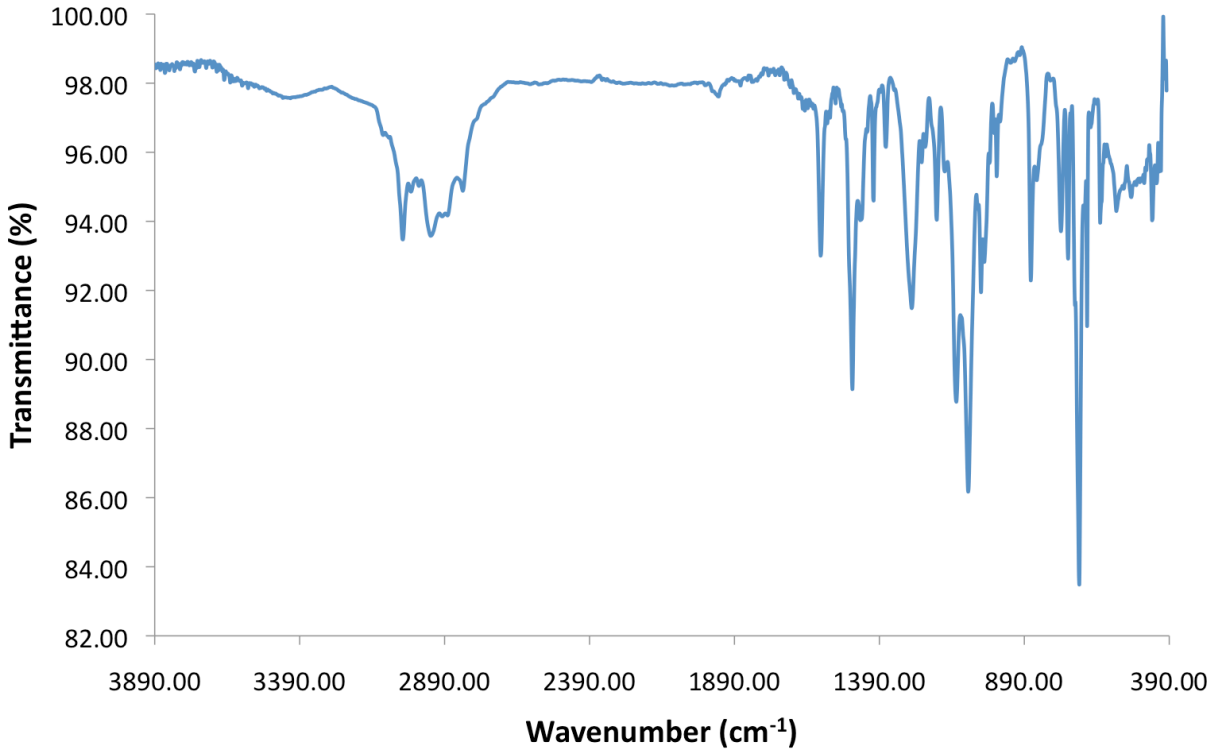


Figure S10. IR spectrum of complex **1** (as KBr pellet).

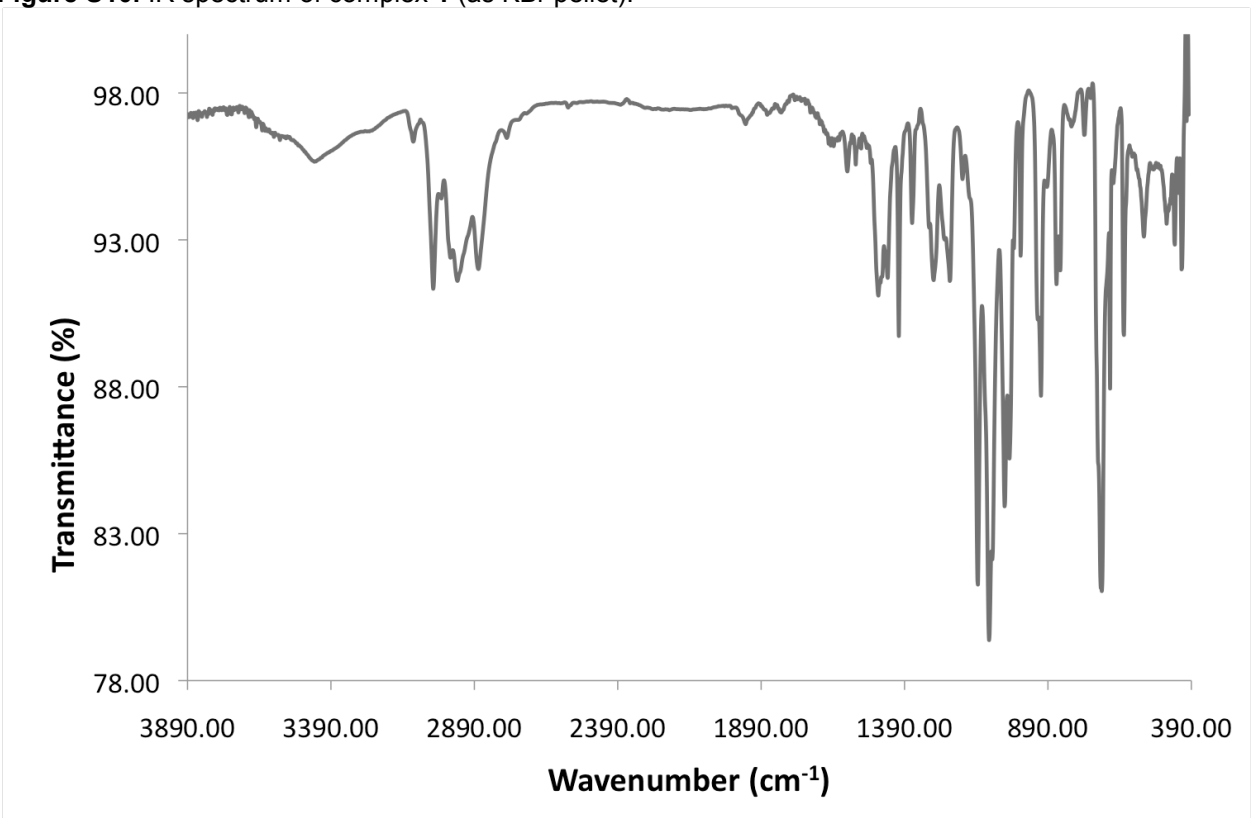


Figure S11. IR spectrum of complex **2** (as KBr pellet).

2 Computational Methods and Results

All investigated structures were fully optimized at the PBE0 level of theory,[S8] including an atom-pairwise correction for dispersion forces via Grimme's D3 model[S9] with Becke-Johnson (BJ)[S10] damping in the Gaussian 09 program.[S11] A quasirelativistic energy-consistent small-core pseudopotential (effective-core potential, ECP)[S12],[S13] in conjunction with the Gaussian-type orbital (GTO) valence basis set of the quality (8s7p6d1f)/[6s4p3d1f] and (14s13p10d8f1g)/[10s9p5d4f1g] was used for transition-metal atoms and actinides, respectively, whereas ligand atoms were treated with an all-electron def2-TZVP basis set.[S14] Relativistic all-electron DFT calculations of the nuclear shieldings were performed using the Amsterdam Density Functional (ADF) program suite,[S15] employing the user-modified PBE0 hybrid exchange-correlation functional with 40% exact-exchange admixture (denoted as PBE0-40HF)[S16] in conjunction with Slater-type orbital (STO) basis sets of triple-zeta doubly polarized (TZ2P) quality and an integration accuracy of 5. Both scalar and spin-orbit relativistic effects were treated by the two-component zeroth-order regular approximation (ZORA).[S17] Bulk solvent effects were simulated by the conductor-like screening model (COSMO) as implemented self-consistently in ADF.[S18] The computed ^{1}H and ^{13}C nuclear shieldings were converted to chemical shifts (δ, in ppm) relative to the shieldings of TMS, computed at the same level, and averaged over the magnetically equivalent nuclei. Natural population analyses (NPA), natural bond orbital (NBO) analyses (including the second-order perturbation theory analysis of Fock matrix in NBO basis) and analyses of natural localized molecular orbitals (NLMOs)[S19] were carried out using the NBO6 code,[S20] interfaced with Gaussian 09.[S11]

To evaluate the degree of distortion away from ideal geometries (octahedron vs. trigonal prism) for the 6-coordinate polyhedra [MC_6] of hexaalkyl and hexaaryl complexes, we performed a systematic analysis of the coordination geometries by the Continuous Symmetry Measure (CSM) method, as implemented in the Shape program.[S21],[S22]

Table S2. Calculated vs. experimental ^{13}C NMR shifts (in ppm with respect to TMS) in $[Th(C_6H_5)_6]^{2-}$ complexes [a]

Structure	$\delta(C_{ipso})$	$\delta^{SO}(C_{ipso})$ [b]	$\delta(C_{ortho})$	$\delta(C_{meta})$	$\delta(C_{para})$
$[Th(C_6H_5)_6]^{2-}$ (***C*₃**)	233.8	35.1	139.5	121.9	117.5
$[Th(C_6H_5)_6]^{2-}$ (***C*₃'**)	233.1	32.3	137.7	121.7	117.7
$[Th(C_6H_5)_6]^{2-}$ (***S*₆**)	242.3	43.6	140.6	122.8	119.0
$[Li(DME)_3]_2[Th(C_6H_5)_6]$ (**1**) [c]	236.3	43.7	138.6	120.7	118.2
$[Li(12\text{-crown-4})(THF)]_2[Th(C_6H_5)_6]$ (**2**) [d]	230.6	34.3	139.6	119.8	114.9
Expt.[e]	220.5		136.9	126.6	125.2

[a] NMR shifts calculated at the 2c-ZORA-SO level using PBE0-40HF hybrid functional and TZ2P all-electron basis set (see Computational Methods). The computed shifts were averaged over magnetically equivalent nuclei, imposing octahedral symmetry. [b] The spin-orbit (SO) contribution to the chemical shift. [c] Calculations done for the crystal structure of **1** with optimized hydrogen positions. [d] Calculations done for the crystal structure of **2** with optimized hydrogen positions. [e] The experimental values as measured for **1** in THF-d_8 at -4 °C.

Table S3. Calculated vs. experimental ^{1}H NMR shifts (in ppm with respect to TMS) in $[Th(C_6H_5)_6]^{2-}$ complexes [a]

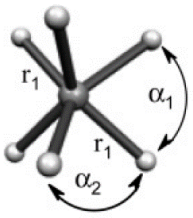
Structure	$\delta(^1H^A_{ortho})$	$\delta(^1H^B_{ortho})$	$\delta(^1H_{ortho})$[b]	$\delta(^1H^A_{meta})$	$\delta(^1H^B_{meta})$	$\delta(^1H_{meta})$[b]	$\delta(^1H_{para})$[b]
$[Th(C_6H_5)_6]^{2-}$ (***C*₃**)	8.19	7.41	7.80	6.81	6.52	6.67	6.32
$[Th(C_6H_5)_6]^{2-}$ (***C*₃'**)	8.22	7.27	7.75	6.94	6.51	6.73	6.38
$[Th(C_6H_5)_6]^{2-}$ (***S*₆**)	8.18	8.18	8.18	6.72	6.72	6.72	6.42
$[Li(DME)_3]_2[Th(C_6H_5)_6]$ (**1**) [c]	8.48	8.48	8.48	6.69	6.69	6.69	6.29
$[Li(12\text{-crown-4})(THF)]_2[Th(C_6H_5)_6]$ (**2**) [d]	8.28	7.54	7.91	6.74	6.23	6.49	6.13
Expt.(**1**, THF, 25 °C)[e]			7.61			7.00	6.79
Expt.(**1**, THF, -61 °C)[f]			7.57			6.97	6.80
Expt.(**1**, THF, -90 °C)[g]	7.84	7.16	(7.50)[b]	7.01	6.60	(6.81)[b]	6.78

[a] NMR shifts calculated at the 2c-ZORA-SO level using PBE0-40HF hybrid functional and TZ2P all-electron basis set (see Computational Methods). [b] NMR shifts averaged over chemically equivalent nuclei (for instance, $\delta(^1H_{ortho}) = (\delta(^1H^A_{ortho}) + \delta(^1H^B_{ortho}))/2$). [c] Calculations done for the solid-state molecular structure of **1** with optimized hydrogen positions. [d] Calculations done for the solid-state molecular structure of **2** with optimized hydrogen positions. [e] The experimental values as measured for **1** in THF-d_8 at 25 °C. [f] Measured for **1** in THF-d_8 at -61 °C. [g] Measured for **1** in THF-d_8 at -90 °C.

Table S4. Relative energies, selected structural parameters and analysis of the M-C bonds in $[M^{IV}(CH_3)_6]^{2-}$ (M = Zr, Hf, Th) and $[M^{V}(CH_3)_6]^{-}$ (M = Nb, Ta, Pa) complexes with different symmetry

Complex		ΔE_{rel}[b]	d(M–C)[c]	α_1(C-M-C)[d]	α_2(C-M-C)[d]	{S(TPM), S(O_h)}[e]	NPA charges		NLMO (M-C)[g]			
		[kJ/mol]	[Å]	[deg]	[deg]		q(M)	q(C)[f]	%M	M(s)	M(d)	M(f)
$[Zr(CH_3)_6]^{2-}$	D_{3h}	0.0	2.385	77.7	84.8	{0.0,16.7}	2.16	−1.23	12.6	23	76	0
	S_6	32.4	2.411	90.0	90.0	{16.7,0.0}	2.35	−1.29	11.9	31	68	0
$[Hf(CH_3)_6]^{2-}$	D_{3h}	0.0	2.387	77.6	84.9	{0.0,16.7}	2.28	−1.25	11.6	28	72	0
	S_6	9.9	2.408	90.0	90.0	{16.7,0.0}	2.45	−1.30	11.1	35	65	0
$[Th(CH_3)_6]^{2-}$	D_{3h}	0.0	2.633	76.5	85.7	{0.0,16.7}	1.98	−1.23	13.2	21	66	13
	S_6	6.4	2.653	90.0	90.0	{16.7,0.0}	2.20	−1.28	11.2	28	52	20
$[Th(CH_3)_6]^{2-}$ "d-only"	D_{3h}	0.0	2.675	76.1	86.0	{0.0,16.7}	2.29	−1.25	13.0	24	76	0
	S_6	48.5	2.711	90.0	90.0	{16.7,0.0}	2.59	−1.32	11.4	34	66	0
$[Nb(CH_3)_6]^{-}$	D_{3h}	0.0	2.238	77.8	84.7	{0.0,16.7}	1.69	−1.06	24.1	13	87	0
	S_6	165.5	2.270	90.0	90.0	{16.7,0.0}	2.12	−1.18	21.0	17	83	0
$[Ta(CH_3)_6]^{-}$	D_{3h}	0.0	2.246	77.6	84.9	{0.0,16.7}	2.11	−1.14	20.3	17	83	0
	S_6	112.8	2.273	90.0	90.0	{16.7,0.0}	2.46	−1.23	19.2	25	75	0
$[Pa(CH_3)_6]^{-}$	D_{3h}	34.8	2.461	75.5	86.5	{0.0,16.7}	1.98	−1.14	19.7	13	54	33
	S_6	0.0	2.468	90.0	90.0	{16.7,0.0}	2.13	−1.19	18.2	17	35	48
$[Pa(CH_3)_6]^{-}$ "d-only"	D_{3h}	0.0	2.515	76.3	86.0	{0.0,16.7}	2.47	−1.20	18.8	17	83	0
	S_6	153.3	2.552	90.0	90.0	{16.7,0.0}	2.97	−1.32	15.9	28	72	0

[a] PBE0-D3(BJ)/ECP/def2-TZVP results (see Computational Methods). [b] Relative zero-point corrected electronic energies. [c] The average M-C bond length. [d] C-M-C angles (see the Figure below for labeling). [e] CSM coordinates evaluated for the $[MC_6]$ core unit (see Computational Methods). [f] The averaged NPA charges on C atoms. [g] The averaged metal and metal AO contributions (%) to the σ(M-C) bonding NLMOs.



D_{3h}

Table S5. Relative energies, selected structural parameters and analysis of the M-C bonds in $[M^{IV}(C_6H_5)_6]^{2-}$ (M = Zr, Hf, Th) and $[M^{V}(C_6H_5)_6]^{-}$ (M = Nb, Ta, Pa) complexes with different symmetry

Complex		ΔE_{rel}[b]	d(M–C)[c]		α(M-C-C)[d]	d(M···H_{ortho})[e]	{S(TPM), $S(O_h)$}[f]	NPA charges		NLMO (M-C)[h]			
		[kJ/mol]	[Å]		[deg]	[Å]		q(M)	q(C)[g]	%M	M(s)	M(d)	M(f)
$[Zr(C_6H_5)_6]^{2-}$	C_3	0.0	2.373	2.371	117.2	3.242	{1.2,9.8}	2.12	–0.44	12.5	20	80	0
	C_3'	18.1	2.346	2.413	109.0	2.986	{5.1,4.5}	2.02	–0.42	13.2	20	80	0
	S_6	34.1	2.406	2.403	122.6	3.404	{16.7,0.0}	2.39	–0.51	11.1	30	70	0
$[Hf(C_6H_5)_6]^{2-}$	C_3	0.0	2.371	2.369	117.5	3.247	{1.8,8.3}	2.22	–0.46	11.8	24	76	0
	C_3'	12.1	2.365	2.408	114.6	3.159	{8.4,1.8}	2.29	–0.48	11.0	28	72	0
	S_6	9.4	2.397	2.397	122.8	3.392	{16.7,0.0}	2.45	–0.52	10.8	34	66	0
$[Th(C_6H_5)_6]^{2-}$	C_3	6.5	2.589	2.614	110.2	3.198	{2.5,8.8}	1.69	–0.39	14.8	15	70	15
	C_3'	0.0	2.567	2.615	106.4	3.064	{5.1,5.4}	1.55	–0.37	15.2	14	71	15
	S_6	18.7	2.640	2.640	122.4	3.590	{16.7,0.0}	2.14	–0.48	11.5	24	52	24
$[Th(C_6H_5)_6]^{2-}$ "d-only"	C_3	0.0	2.648	2.653	115.3	3.397	{0.8,13.4}	2.19	–0.42	13.7	19	81	0
	C_3'	4.6	2.619	2.652	109.2	3.190	{2.9,8.3}	2.03	–0.39	14.7	17	83	0
	S_6	55.4	2.692	2.692	122.7	3.629	{16.7,0.0}	2.61	–0.51	11.0	31	69	0
$[Nb(C_6H_5)_6]^{-}$	C_3	0.0	2.240	2.224	109.7	2.944	{1.7,9.9}	1.45	–0.28	26.0	9	91	0
	C_3'	25.2	2.218	2.258	105.2	2.797	{5.3,5.7}	1.18	–0.22	27.9	10	90	0
	S_6	142.7	2.270	2.270	122.3	3.298	{16.7,0.0}	2.06	–0.43	22.1	17	83	0
$[Ta(C_6H_5)_6]^{-}$	C_3	0.0	2.245	2.244	115.8	3.119	{1.0,10.4}	2.03	–0.40	20.5	15	85	0
	C_3'	30.5	2.227	2.269	106.2	2.831	{5.1,5.2}	1.73	–0.34	22.9	13	87	0
	S_6	95.8	2.275	2.273	122.3	3.301	{16.7,0.0}	2.45	–0.51	18.1	23	77	0
$[Pa(C_6H_5)_6]^{-}$	C_3'	0.0	2.406	2.462	103.5	2.866	{6.2,4,9}	1.47	–0.35	21.8	9	55	36
	S_6	15.7	2.475	2.475	122.0	3.438	{16.7,0.0}	2.14	–0.46	18.5	14	35	51
$[Pa(C_6H_5)_6]^{-}$ "d-only"	C_3'	0.0	2.487	2.477	107.1	3.038	{2.8,10.4}	2.06	–0.36	22.0	11	89	0
	S_6	167.9	2.546	2.546	122.0	3.511	{16.7,0.0}	2.93	–0.56	15.0	25	75	0

[a] PBE0-D3(BJ)/ECP/def2-TZVP results (see Computational Methods). [b] Relative zero-point corrected electronic energies. [c] M-C_{ipso} bond lengths. [d] The most acute α(M-C_{ipso}-C_{ortho}) angle. [e] The shortest d(M···H_{ortho}) contact. [f] CSM coordinates evaluated for the [MC_6] core unit (see Computational Methods). [g] The averaged NPA charges on C_{ipso} atoms. [h] The averaged metal and metal AO contributions (%) to the σ(M-C) bonding NLMOs.

Table S6. NBO second-order perturbation analysis of *ortho* C-H···Th interactions in $[Th(C_6H_5)_6]^{2-}$ in comparison with the agostic C-H···Th interaction in $H_2C{=}ThH_2$

System	Symm.	d(Th···H-C)[a]	occ. σ(C-H)[b]	occ.Th [b]	$E^{(2)}$ (σ(C-H)→Th) [c]	$E^{(2)}$ (Th→σ*(C-H)) [d]
		[Å]			[kcal/mol]	[kcal/mol]
$[Th(C_6H_5)_6]^{2-}$	C_3	3.198	1.961	0.057	4.9	1.1
	C_3'	3.064	1.936	0.077	15.7	10.9
		3.239	1.950	0.051	11.1	2.9
	S_6	3.590	1.969	0.041	2.9	0.0
$H_2C{=}ThH_2$	C_1	2.368	1.913	0.094	32.3	0.0

[a] Interatomic distances between C-H hydrogen atoms and the central atom. [b] Occupancy of the σ(C-H) donor and metal-centered acceptor NBO orbitals. [c] NBO stabilizing energy associated with the $\sigma(C_{ortho}\text{-}H)\rightarrow Th$ interaction. [d] NBO stabilizing energy associated with the back-donation $Th\rightarrow\sigma^*(C_{ortho}\text{-}H)$. Since NBO delocalization energy of the back-donation is smaller than $E^{(2)}$ of $\sigma(C_{ortho}\text{-}H)\rightarrow Th$, this excludes the hydrogen bonding nature of this interaction (see also ref. [S23]).

Table S7. CSM analysis of the X-ray characterized structures of the hexacoordinate $[M(C_6H_5)_6]^q$ anions

Complex	d(M–C) [Å]	{S(TPM),S(O_h)}[a]	Classification	
$[Li(THF)_4]_2[Zr(C_6H_5)_6]$	2.345(6)–2.378(5)	{2.40,7.30}	Distorted Prismatic	Ref. [S24]
$[Li(THF)_4][Li(THF)][Hf(C_6H_5)_6]$	2.330(3)–2.399(3)	{7.05,2.73}	Distorted Octahedral	Ref. [S24]
$[Li(THF)_4]_2[Hf(C_6H_5)_6]$	2.385(3)–2.398(3)	{16.51,0.02}	Octahedral	Ref. [S24]
$[Li(DME)_3]_2[Th(C_6H_5)_6]$ (**1**)	2.589(3)	{16.43, 0.03}	Octahedral	This work
$[Li(12\text{-crown-}4)(THF)]_2[Th(C_6H_5)_6]$ (**2**)	2.553(3)–2.636(3)	{4.83, 6.17}	Intermediate	This work
$[Li(THF)_4][Ta(C_6H_5)_6]$	2.31(1)–2.27(1)	{1.36,9.78}	Prismatic	Ref. [S25]

[a] CSM coordinates evaluated for the $[MC_6]$ core unit (see Computational Methods).

3 Cartesian Coordinates of Selected Optimized Structures

(PBE0-D3(BJ)/ECP/def2-TZVP results)

$[Th(C_6H_5)_6]^{2-}$ (symm. C_3)

Th	0.00000	0.00000	0.16791
C	-0.83329	-1.67656	-1.61016
C	1.86859	0.11663	-1.61016
C	-1.03530	1.55994	-1.61016
C	-1.64885	-1.52905	1.49972
C	2.14862	-0.66342	1.49972
C	-0.49977	2.19247	1.49972
C	-0.91348	2.06265	2.83468
C	-1.10824	3.15207	3.68055
C	-0.87925	4.43835	3.21307
C	-0.46797	4.61378	1.89673
C	-0.29321	3.51146	1.06798
C	-0.24987	-2.92531	-1.35869
C	-0.40312	-4.02216	-2.19925
C	-1.17842	-3.90462	-3.34628
C	-1.77888	-2.68421	-3.63134
C	-1.59985	-1.59814	-2.77919
C	-0.58411	2.18458	-2.77919
C	-1.43515	2.88266	-3.63134
C	-2.79229	2.97285	-3.34628
C	-3.28174	2.36019	-2.19925
C	-2.40846	1.67905	-1.35869
C	3.18762	-1.50180	1.06798
C	4.22964	-1.90162	1.89673
C	4.28335	-1.45772	3.21307
C	3.28389	-0.61627	3.68055
C	2.24305	-0.24023	2.83468
C	-1.32957	-1.82242	2.83468
C	-2.17565	-2.53580	3.68055
C	-3.40410	-2.98063	3.21307
C	-3.76167	-2.71216	1.89673
C	-2.89440	-2.00966	1.06798
C	2.65833	1.24626	-1.35869
C	3.68485	1.66197	-2.19925
C	3.97071	0.93177	-3.34628
C	3.21403	-0.19845	-3.63134

C	2.18396	-0.58644	-2.77919
H	-2.06322	-0.64953	-3.04311
H	-2.38294	-2.57737	-4.53058
H	-1.30958	-4.75364	-4.01205
H	0.07647	-4.96945	-1.96132
H	0.35935	-3.06426	-0.45955
H	0.00000	3.68531	0.03404
H	-0.29033	5.61739	1.51544
H	-1.02451	5.29606	3.86462
H	-1.43958	2.99728	4.70537
H	-1.10680	1.06934	3.24281
H	-2.83340	1.22093	-0.45955
H	-4.34190	2.41850	-1.96132
H	-3.46199	3.51095	-4.01205
H	-1.04060	3.35237	-4.53058
H	0.46910	2.11156	-3.04311
H	1.47948	0.42385	3.24281
H	3.31551	-0.25193	4.70537
H	5.09878	-1.76078	3.86462
H	5.00997	-2.55726	1.51544
H	3.19157	-1.84265	0.03404
H	-3.19157	-1.84265	0.03404
H	-4.71964	-3.06013	1.51544
H	-4.07427	-3.53529	3.86462
H	-1.87593	-2.74535	4.70537
H	-0.37268	-1.49319	3.24281
H	1.59412	-1.46203	-3.04311
H	3.42354	-0.77500	-4.53058
H	4.77157	1.24269	-4.01205
H	4.26543	2.55095	-1.96132
H	2.47406	1.84334	-0.45955

$[Th(C_6H_5)_6]^{2-}$ (symm. C_3')

Th	0.00000	0.00000	0.12156
C	0.35684	1.84351	-1.62901
C	-1.77495	-0.61272	-1.62901
C	2.22595	-0.48145	1.40620
C	-1.52992	-1.68700	1.40620
C	-0.69603	2.16845	1.40620
C	1.41811	-1.23079	-1.62901

C	1.21794	-2.59982	-1.40916
C	1.85066	-3.59199	-2.15221
C	2.72843	-3.23314	-3.16689
C	2.94993	-1.88386	-3.42084
C	2.30266	-0.91193	-2.66538
C	-0.36158	2.45012	-2.66538
C	0.15651	3.49664	-3.42084
C	1.43577	3.97946	-3.16689
C	2.18543	3.39872	-2.15221
C	1.64254	2.35468	-1.40916
C	-0.51758	3.53968	1.17043
C	-0.98138	4.51871	2.04218
C	-1.66011	4.15993	3.20165
C	-1.86626	2.81453	3.47179
C	-1.38825	1.85130	2.58666
C	-2.86048	0.24514	-1.40916
C	-4.03609	0.19328	-2.15221
C	-4.16420	-0.74632	-3.16689
C	-3.10644	-1.61278	-3.42084
C	-1.94108	-1.53820	-2.66538
C	3.32424	-1.32160	1.17043
C	4.40400	-1.40945	2.04218
C	4.43266	-0.64227	3.20165
C	3.37058	0.20897	3.47179
C	2.29739	0.27661	2.58666
C	-2.80666	-2.21808	1.17043
C	-3.42263	-3.10925	2.04218
C	-2.77255	-3.51766	3.20165
C	-1.50432	-3.02349	3.47179
C	-0.90914	-2.12791	2.58666
H	-1.36151	2.08746	-2.89650
H	-2.02661	4.92195	3.88459
H	0.52942	-2.92524	-0.62074
H	3.23096	-3.99554	-3.75624
H	0.00000	3.85286	0.26622
H	2.26862	1.92111	-0.62074
H	-0.43776	3.94058	-4.21766
H	1.66032	-4.64251	-1.94243
H	-0.81677	5.57081	1.81741
H	-4.41608	-3.49275	1.81741

H	2.48855	0.13537	-2.89650
H	-1.57605	0.80416	2.83488
H	3.19037	3.75914	-1.94243
H	1.84476	4.79586	-3.75624
H	-3.33667	-1.92643	0.26622
H	-2.79804	1.00413	-0.62074
H	3.63153	-1.59118	-4.21766
H	-2.40023	2.51517	4.37119
H	-1.12704	-2.22284	-2.89650
H	3.33667	-1.92643	0.26622
H	1.48445	0.96282	2.83488
H	5.23285	-2.07807	1.81741
H	-4.85070	0.88337	-1.94243
H	-5.07572	-0.80032	-3.75624
H	-3.19376	-2.34941	-4.21766
H	-0.97808	-3.33624	4.37119
H	-3.24923	-4.21607	3.88459
H	0.09160	-1.76698	2.83488
H	3.37831	0.82108	4.37119
H	5.27584	-0.70588	3.88459

$[Th(C_6H_5)_6]^{2-}$ (symm. S_6)

Th	0.00000	0.00000	0.00000
C	2.06146	-0.61175	1.53118
C	0.50094	-2.09115	-1.53118
C	-1.56052	-1.47940	1.53118
C	-0.50094	2.09115	1.53118
C	1.56052	1.47940	-1.53118
C	-2.06146	0.61175	-1.53118
C	-3.36952	0.18642	-1.24516
C	-4.46372	0.51449	-2.04002
C	-4.28812	1.29589	-3.17496
C	-3.01189	1.73892	-3.49752
C	-1.93228	1.39915	-2.68765
C	1.93228	-1.39915	2.68765
C	3.01189	-1.73892	3.49752
C	4.28812	-1.29589	3.17496
C	4.46372	-0.51449	2.04002
C	3.36952	-0.18642	1.24516

C	0.24556	2.37298	2.68765
C	0.00000	3.47784	3.49752
C	-1.02179	4.36157	3.17496
C	-1.78630	4.12294	2.04002
C	-1.52332	3.01131	1.24516
C	-0.24556	-2.37298	-2.68765
C	0.00000	-3.47784	-3.49752
C	1.02179	-4.36157	-3.17496
C	1.78630	-4.12294	-2.04002
C	1.52332	-3.01131	-1.24516
C	-2.17784	-0.97383	2.68765
C	-3.01189	-1.73892	3.49752
C	-3.26633	-3.06568	3.17496
C	-2.67742	-3.60845	2.04002
C	-1.84621	-2.82488	1.24516
C	2.17784	0.97383	-2.68765
C	3.01189	1.73892	-3.49752
C	3.26633	3.06568	-3.17496
C	2.67742	3.60845	-2.04002
C	1.84621	2.82488	-1.24516
H	-5.13723	1.55722	-3.80132
H	-5.45800	0.16048	-1.77485
H	5.13723	-1.55722	3.80132
H	-2.85918	2.35223	-4.38340
H	3.54556	0.42892	0.36360
H	0.94629	-1.76589	2.97050
H	-3.54556	-0.42892	-0.36360
H	2.85918	-2.35223	4.38340
H	5.45800	-0.16048	1.77485
H	-0.94629	1.76589	-2.97050
H	1.22002	-5.22759	-3.80132
H	2.59002	-4.80700	-1.77485
H	-1.22002	5.22759	3.80132
H	-0.60750	-3.65224	-4.38340
H	-2.14423	2.85609	0.36360
H	1.05616	1.70246	2.97050
H	2.14423	-2.85609	-0.36360
H	0.60750	3.65224	4.38340
H	-2.59002	4.80700	1.77485
H	-1.05616	-1.70246	-2.97050

H	3.91721	3.67036	-3.80132
H	2.86798	4.64653	-1.77485
H	-3.91721	-3.67036	3.80132
H	3.46669	1.30001	-4.38340
H	-1.40133	-3.28500	0.36360
H	-2.00245	0.06344	2.97050
H	1.40133	3.28500	-0.36360
H	-3.46669	-1.30001	4.38340
H	-2.86798	-4.64653	1.77485
H	2.00245	-0.06344	-2.97050

$[Hf(C_6H_5)_6]^{2-}$ (symm. C_3)

Hf	0.00000	0.00000	0.00090
C	-0.47221	-1.80632	-1.45983
C	1.80042	0.49421	-1.45983
C	-1.32821	1.31211	-1.45983
C	-1.02707	-1.55831	1.46077
C	1.86307	-0.11031	1.46077
C	-0.83601	1.66862	1.46077
C	-1.51318	1.48189	2.67470
C	-1.82823	2.53190	3.53321
C	-1.45585	3.83088	3.21639
C	-0.78071	4.06061	2.02377
C	-0.49711	3.00062	1.17121
C	0.13235	-3.04267	-1.17899
C	0.05955	-4.13640	-2.03309
C	-0.66091	-4.04560	-3.21798
C	-1.29083	-2.84798	-3.52625
C	-1.18516	-1.75774	-2.66670
C	-0.92967	1.90525	-2.66670
C	-1.82101	2.54188	-3.52625
C	-3.17314	2.59517	-3.21798
C	-3.61200	2.01663	-2.03309
C	-2.70120	1.40672	-1.17899
C	2.84717	-1.06980	1.17121
C	3.90695	-1.35419	2.02377
C	4.04557	-0.65463	3.21639
C	3.10681	0.31734	3.53321
C	2.03994	0.56951	2.67470
C	-0.52677	-2.05139	2.67470

C	-1.27858	-2.84924	3.53321
C	-2.58971	-3.17625	3.21639
C	-3.12624	-2.70642	2.02377
C	-2.35006	-1.93082	1.17121
C	2.56886	1.63595	-1.17899
C	3.55245	2.11977	-2.03309
C	3.83405	1.45043	-3.21798
C	3.11184	0.30610	-3.52625
C	2.11483	-0.14751	-2.66670
H	-1.67042	-0.82873	-2.95476
H	-1.86227	-2.75793	-4.44799
H	-0.73210	-4.89809	-3.88864
H	0.55684	-5.06770	-1.76996
H	0.67513	-3.16685	-0.24258
H	0.00000	3.22793	0.22876
H	-0.48457	5.07205	1.75342
H	-1.69104	4.65389	3.88641
H	-2.36066	2.33207	4.46104
H	-1.79807	0.47524	2.96940
H	-3.08014	0.99874	-0.24258
H	-4.66717	2.05161	-1.76996
H	-3.87582	3.08306	-3.88864
H	-1.45731	2.99174	-4.44799
H	0.11751	1.86099	-2.95476
H	1.31061	1.31955	2.96940
H	3.19997	0.87836	4.46104
H	4.87591	-0.86246	3.88641
H	4.63481	-2.11638	1.75342
H	2.79547	-1.61397	0.22876
H	-2.79547	-1.61397	0.22876
H	-4.15024	-2.95567	1.75342
H	-3.18486	-3.79143	3.88641
H	-0.83931	-3.21043	4.46104
H	0.48746	-1.79480	2.96940
H	1.55291	-1.03226	-2.95476
H	3.31957	-0.23381	-4.44799
H	4.60792	1.81502	-3.88864
H	4.11033	3.01609	-1.76996
H	2.40501	2.16811	-0.24258

$[Hf(C_6H_5)_6]^{2-}$ (symm. C_3')

Hf	0.00000	0.00000	0.04266
C	0.54123	1.75469	-1.44805
C	-1.79023	-0.40863	-1.44805
C	1.98955	-0.19779	1.38514
C	-1.16607	-1.62411	1.38514
C	-0.82349	1.82190	1.38514
C	1.24899	-1.34607	-1.44805
C	1.09876	-2.73078	-1.25171
C	1.72500	-3.68421	-2.04855
C	2.54502	-3.28328	-3.09483
C	2.71791	-1.92395	-3.32536
C	2.08034	-0.98778	-2.51819
C	-0.18473	2.29551	-2.51819
C	0.30724	3.31576	-3.32536
C	1.57089	3.84569	-3.09483
C	2.32812	3.33600	-2.04855
C	1.81555	2.31695	-1.25171
C	-0.60318	3.19444	1.18113
C	-1.12234	4.18086	2.01309
C	-1.90782	3.83396	3.10451
C	-2.15971	2.49048	3.34370
C	-1.62593	1.51881	2.50181
C	-2.91431	0.41384	-1.25171
C	-4.05312	0.34821	-2.04855
C	-4.11591	-0.56241	-3.09483
C	-3.02515	-1.39180	-3.32536
C	-1.89561	-1.30774	-2.51819
C	3.06806	-1.07485	1.18113
C	4.18190	-1.11845	2.01309
C	4.27422	-0.26476	3.10451
C	3.23668	0.62512	3.34370
C	2.12830	0.64869	2.50181
C	-2.46488	-2.11959	1.18113
C	-3.05956	-3.06241	2.01309
C	-2.36640	-3.56920	3.10451
C	-1.07696	-3.11561	3.34370
C	-0.50237	-2.16751	2.50181
H	-1.17404	1.89970	-2.73383
H	-2.31868	4.59992	3.75762

H	0.46141	-3.08748	-0.44300
H	3.03909	-4.01918	-3.72414
H	0.00000	3.50761	0.33390
H	2.44314	1.94333	-0.44300
H	-0.29817	3.69919	-4.14446
H	1.57166	-4.74342	-1.85246
H	-0.91481	5.22867	1.80559
H	-4.07076	-3.40658	1.80559
H	2.23221	0.06690	-2.73383
H	-1.84570	0.47883	2.72935
H	3.32209	3.73281	-1.85246
H	1.96117	4.64152	-3.72414
H	-3.03768	-1.75381	0.33390
H	-2.90454	1.14415	-0.44300
H	3.35268	-1.59137	-4.14446
H	-2.77416	2.19469	4.19148
H	-1.05817	-1.96660	-2.73383
H	3.03768	-1.75381	0.33390
H	1.33753	1.35900	2.72935
H	4.98557	-1.82209	1.80559
H	-4.89375	1.01062	-1.85246
H	-5.00026	-0.62234	-3.72414
H	-3.05451	-2.10782	-4.14446
H	-0.51358	-3.49984	4.19148
H	-2.82431	-4.30799	3.75762
H	0.50817	-1.83783	2.72935
H	3.28773	1.30515	4.19148
H	5.14299	-0.29192	3.75762

$[Hf(C_6H_5)_6]^{2-}$ (symm. S_6)

Hf	0.00000	0.00000	0.00000
C	1.88418	-0.52765	1.38501
C	0.48514	-1.89557	-1.38501
C	-1.39904	-1.36793	1.38501
C	-0.48514	1.89557	1.38501
C	1.39904	1.36793	-1.38501
C	-1.88418	0.52765	-1.38501
C	-3.17550	0.03722	-1.12278
C	-4.27732	0.33493	-1.91845
C	-4.13311	1.15186	-3.03197

C	-2.87587	1.66039	-3.32970
C	-1.78689	1.35035	-2.52104
C	1.78689	-1.35035	2.52104
C	2.87587	-1.66039	3.32970
C	4.13311	-1.15186	3.03197
C	4.27732	-0.33493	1.91845
C	3.17550	-0.03722	1.12278
C	0.27599	2.22267	2.52104
C	0.00000	3.32077	3.32970
C	-1.06902	4.15530	3.03197
C	-1.84860	3.87173	1.91845
C	-1.55552	2.76867	1.12278
C	-0.27599	-2.22267	-2.52104
C	0.00000	-3.32077	-3.32970
C	1.06902	-4.15530	-3.03197
C	1.84860	-3.87173	-1.91845
C	1.55552	-2.76867	-1.12278
C	-2.06288	-0.87232	2.52104
C	-2.87587	-1.66039	3.32970
C	-3.06409	-3.00345	3.03197
C	-2.42871	-3.53680	1.91845
C	-1.61998	-2.73145	1.12278
C	2.06288	0.87232	-2.52104
C	2.87587	1.66039	-3.32970
C	3.06409	3.00345	-3.03197
C	2.42871	3.53680	-1.91845
C	1.61998	2.73145	-1.12278
H	-4.98895	1.38943	-3.65890
H	-5.25437	-0.07318	-1.66784
H	4.98895	-1.38943	3.65890
H	-2.74233	2.30336	-4.19734
H	3.32747	0.60550	0.25921
H	0.81877	-1.76771	2.78630
H	-3.32747	-0.60550	-0.25921
H	2.74233	-2.30336	4.19734
H	5.25437	0.07318	1.66784
H	-0.81877	1.76771	-2.78630
H	1.29119	-5.01528	-3.65890
H	2.69056	-4.51382	-1.66784
H	-1.29119	5.01528	3.65890

H	-0.62360	-3.52660	-4.19734
H	-2.18812	2.57892	0.25921
H	1.12150	1.59293	2.78630
H	2.18812	-2.57892	-0.25921
H	0.62360	3.52660	4.19734
H	-2.69056	4.51382	1.66784
H	-1.12150	-1.59293	-2.78630
H	3.69776	3.62584	-3.65890
H	2.56380	4.58701	-1.66784
H	-3.69776	-3.62584	3.65890
H	3.36593	1.22325	-4.19734
H	-1.13935	-3.18442	0.25921
H	-1.94027	0.17478	2.78630
H	1.13935	3.18442	-0.25921
H	-3.36593	-1.22325	4.19734
H	-2.56380	-4.58701	1.66784
H	1.94027	-0.17478	-2.78630

$[Th(CH_3)_6]^{2-}$ (symm. D_{3h})

Th	0.00017	0.00037	0.00000
C	-2.06774	0.00031	1.62990
C	1.03353	1.79004	1.63098
C	1.03407	-1.79030	1.62997
C	-2.06774	0.00031	-1.62990
C	1.03353	1.79004	-1.63098
C	1.03407	-1.79030	-1.62997
H	-1.72608	0.00164	2.67769
H	-2.70911	-0.88538	1.48978
H	-2.71055	0.88466	1.48797
H	0.86191	1.49433	2.67862
H	0.58888	2.78892	1.48977
H	2.12119	1.90308	1.49079
H	0.86412	-1.49454	2.67792
H	2.12143	-1.90422	1.48813
H	0.58826	-2.78871	1.48912
H	-1.72608	0.00164	-2.67769
H	-2.71055	0.88466	-1.48797
H	-2.70911	-0.88538	-1.48978
H	0.86191	1.49433	-2.67862
H	2.12119	1.90308	-1.49079

H	0.58888	2.78892	-1.48977
H	0.86412	-1.49454	-2.67792
H	0.58826	-2.78871	-1.48912
H	2.12143	-1.90422	-1.48813

$[Th(CH_3)_6]^{2-}$ (symm. S_6)

Th	0.00000	0.00000	0.00000
C	-1.18428	-1.80471	-1.54152
C	2.14927	-0.11367	-1.54815
C	-0.98583	1.92518	-1.53558
C	-2.14927	0.11367	1.54815
C	1.18428	1.80471	1.54152
C	0.98583	-1.92518	1.53558
H	-0.62652	-1.95482	-2.48068
H	-1.26487	-2.78717	-1.04804
H	-2.20515	-1.49051	-1.81463
H	3.01102	0.40705	-1.09919
H	2.45688	-1.15551	-1.73600
H	1.95855	0.35334	-2.52851
H	-1.88020	2.39182	-1.09094
H	-0.24864	2.72683	-1.70674
H	-1.27808	1.53336	-2.52383
H	-3.01102	-0.40705	1.09919
H	-1.95855	-0.35334	2.52851
H	-2.45688	1.15551	1.73600
H	0.62652	1.95482	2.48068
H	2.20515	1.49051	1.81463
H	1.26487	2.78717	1.04804
H	0.24864	-2.72683	1.70674
H	1.88020	-2.39182	1.09094
H	1.27808	-1.53336	2.52383

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