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Supporting Information

Stabilization of Classical $[B_2H_5]^-$: Structure and Bonding of $[(Cp^*Ta)_2(B_2H_5)(\mu\text{-}H)L_2]$ ($Cp^* = \eta^5\text{-}C_5Me_5$; $L = SCH_2S$)

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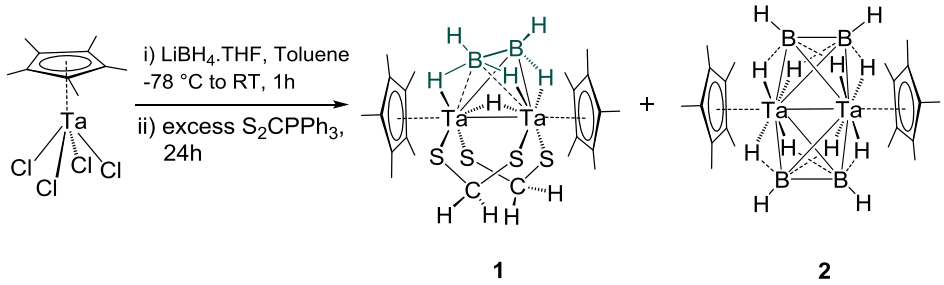
Experimental Procedures

I Experimental Details

General procedure and instrumentations

All the syntheses were carried out under an argon atmosphere with standard Schlenk line and glove box techniques. Compounds, such as, [Cp*TaCl$_4$],[1] S_2CPPh_3,[2,3] and the external reference for the $^{11}B\{^1H\}$ NMR, [Bu$_4$N][B$_3$H$_8$][4] were synthesized according to the literature methods. Thin-layer chromatography was carried out on 250 mm aluminum supported silica gel TLC plates. NMR spectra were recorded in a 500 MHz Bruker FT-NMR spectrometer. Chemical shifts are referenced to (residual) solvent signals ($^1H/^{13}C\{^1H\}$; $CDCl_3$: δ = 7.26/77.16 ppm) or external [Bu$_4$N][B$_3$H$_8$] (^{11}B: δ = 30.07 ppm). Mass spectra were recorded in a Bruker Micro TOF-II mass spectrometer in ESI ionization mode.

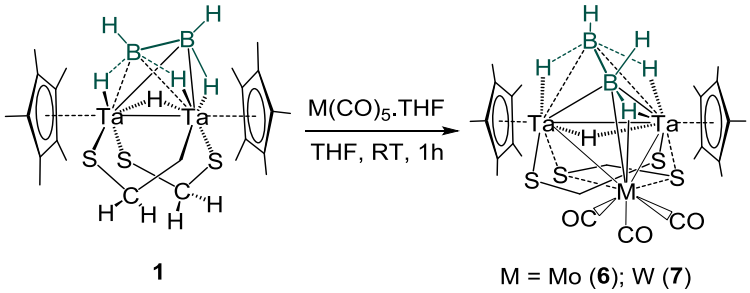
I.1 Synthesis and Characterizations



Scheme S1. Synthesis of compound **1**.

Synthesis of 1: A suspension of [Cp*TaCl$_4$] (0.100 g, 0.22 mmol) in 8 mL toluene at -78 ºC was charged dropwise with lithium borohydride solution 2.0 M in THF (0.7 mL) in toluene (10 mL) over 15 min and kept under constant stirring for 1 hour. Then freshly prepared solution of excess S_2CPPh_3 (0.075 g of PPh_3 dissolved in 6 mL of CS_2) was added in the reaction mixture over 5 min and kept under constant stirring for 24h at room temperature. The colour of the reaction mixture changed from yellow to brown. The solvent was evaporated in vacuum; residue was extracted into hexane/CH_2Cl_2 (60:40 v/v) and passed through Celite. After the removal of the solvent from the filtrate, the residue was subjected to chromatographic workup using silica-gel TLC plates. Elution with hexane/CH_2Cl_2 (60:40 v/v) yielded orange [(Cp*Ta)$_2$(μ,η^2:η^2-B$_2$H$_5$)(μ-H)(κ^2,μ-S$_2$CH$_2$)$_2$], **1** (0.0125g, 14.02 %) along with known compound **2** (0.025 g, 33.30 %).

1: HR-MS (ESI$^+$) calcd for $C_{22}H_{40}B_2S_4Ta_2Na^+$ $[M+Na]^+$ *m/z* 839.1051, found 839.1048; $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, 22 ºC): δ = 35.0 (br, 1B), -11.7 ppm (br, 1B); ^1H NMR (500 MHz, $CDCl_3$, 22 ºC): δ = 9.25 (br, 1H; Ta-H-Ta), 6.72, 6.33, 3.51 (d, J_{HH} = 9.7 Hz, 4H; 2×CH_2S_2), 4.05, 1.68 (br, 2H; BH_t), 2.21 (s, 30H; 2×Cp*), -2.36 (br, 1H; Ta-H-B), -6.61 ppm (br, 2H; Ta-H-B); $^1H\{^{11}B\}$ NMR (500 MHz, $CDCl_3$, 22 ºC): δ = 9.25 (br, 1H; Ta-H-B), 6.72, 6.33, 3.51 (d, J_{HH} = 9.7 Hz, 4H; 2×CH_2S_2), 4.37, 1.68 (br, 2H; BH_t), 2.21 (s, 30H; 2×Cp*), -2.36(br, 1H; Ta-H-B), -6.61 ppm (br, 2H; Ta-H-B); $^{13}C\{^1H\}$ NMR (125, MHz, $CDCl_3$, 22 ºC): δ = 116.9 (s, C_5Me_5), 49.7, 46.2 (s, CH_2S_2), 12.4 ppm (s, C_5Me_5).



Scheme S2. Synthesis of compounds **6** and **7**.

Synthesis of 6 and **7**: In a flame-dried schlenk tube, freshly prepared $Mo(CO)_5$·THF solution in THF (0.015 g $Mo(CO)_6$ dissolved in 10 mL of THF, 0.11 mmol) was added to $[(Cp^*Ta)_2(\mu,\eta^2{:}\eta^2\text{-}B_2H_5)(\mu\text{-}H)(\kappa^2,\mu\text{-}S_2CH_2)_2]$, **1** (0.040 g, 0.048 mmol) in THF (8 ml) and allowed to react at room temperature for 1h. The solvent was removed under vacuum and the solid was extracted into n-hexane-CH_2Cl_2 (80:20v/v) and passed through Celite. After the removal of solvent the resultant residue was chromatographed on silica gel TLC plates. Elution with hexane/CH_2Cl_2 (80:20 v/v) mixture yielded air and moisture sensitive violet complex $[\{(Cp^*Ta)(CH_2S_2)\}_2\text{-}(B_2H_5)(H)\{Mo(CO)_3\}]$, (0.004 g, 8.18%). Similarly, complex **7** $[\{(Cp^*Ta)(CH_2S_2)\}_2(B_2H_5)(H)\{W(CO)_3\}]$, (0.0034 g, 6.40 %) was also prepared from the reaction of **1** and $W(CO)_5$·THF.

6: HR-MS (ESI^+) calcd for $C_{25}H_{41}B_2S_4O_3MoTa_2$ $[M+H]^+$ *m/z* 999.0139, found 999.0159; $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, 22 ºC): δ = 36.4 (br, 1B), 16.9 ppm (br, 1B); ^1H NMR (500 MHz, $CDCl_3$, 22 ºC): δ = 9.25 (br, 1H; Ta-H-Ta), 7.46, 6.29, 4.18 (d, J_{HH} = 10.2 Hz, 4H; 2×CH_2S_2), 4.87, 1.72 (br, 2H; BH_t), 2.14 (s, 30H; 2×Cp*), -6.55 (br, 2H; Ta-H-B), -12.99 ppm (br, 1H; Ta-H-B); $^1H\{^{11}B\}$ NMR (500 MHz, $CDCl_3$, 22 ºC): δ = 7.46, 6.29, 4.19 (d, J_{HH} = 10.2 Hz, 4H; 2×CH_2S_2), 4.87, 1.72 (br, 2H; BH_t), 2.12 (s, 30H; 2×Cp*), -6.51 (br, 2H; Ta-H-B), -12.98 ppm (br, 1H; Ta-H-B); $^{13}C\{^1H\}$ NMR (125, MHz, $CDCl_3$, 22 ºC): δ = 115.4 (s, C_5Me_5), 59.7, 38.3 (s, 2×CH_2S_2), 12.4 ppm (s, $C_5\mathit{Me}_5$); IR (CH_2Cl_2): $\tilde{\nu}$ = 2372.98 cm^{-1} (BH_t), 1969.93 cm^{-1}, 1890.86 cm^{-1}, 1845.54 cm^{-1} (Mo-CO).

7: HR-MS (ESI^+) calcd for $C_{25}H_{41}B_2S_4O_3WTa_2$ $[M+H]^+$ *m/z* 1085.0594, found 1085.0567; $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$, 22 ºC): δ = 36.4 (br, 1B), 18.0 ppm (br, 1B); ^1H NMR (500 MHz, $CDCl_3$, 22 ºC): δ = 7.58, 6.20, 5.06 (d, J_{HH} = 11.1 Hz, 4H; 2×CH_2S_2), 2.12 (s, 30H; 2×Cp*), -6.49, -12.71 ppm (br, 3H; Ta-H-B); $^1H\{^{11}B\}$ NMR (500 MHz, $CDCl_3$, 22 ºC): δ = 7.58, 6.20, 5.06 (d, J_{HH} = 11.1 Hz, 4H; 2×CH_2S_2), 2.12 (s, 30H; 2×Cp*), -6.47 (br, 2H; Ta-H-B), -12.66 ppm (br, 1H; Ta-H-B); $^{13}C\{^1H\}$ NMR (125, MHz, $CDCl_3$, 22 ºC): δ = 114.9 (s, C_5Me_5), 12.2 ppm (s, $C_5\mathit{Me}_5$); IR (CH_2Cl_2): $\tilde{\nu}$ = 2346.94 cm^{-1} (BH_t), 1968.96 cm^{-1}, 1896.04 cm^{-1}, 1850.36 cm^{-1} (W-CO).

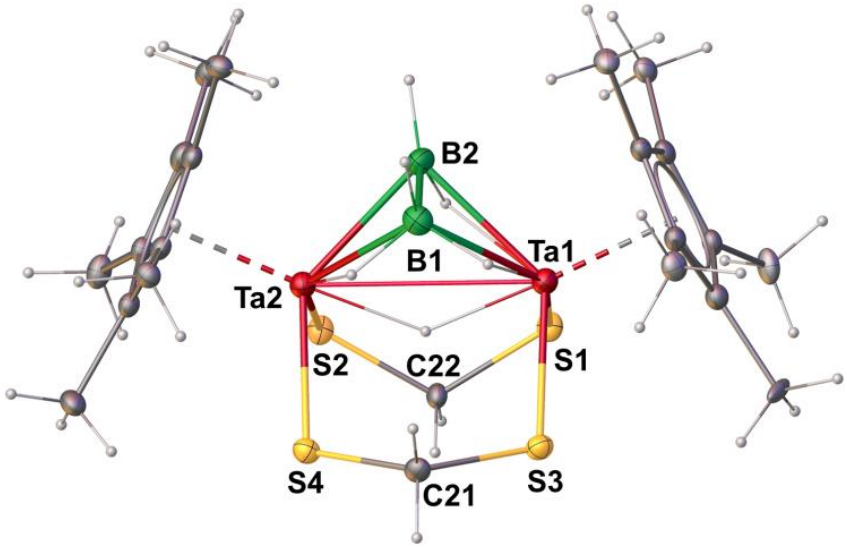


Figure S1. Full molecular structure and labeling diagram of **1**. Selected bond lengths (Å) and angles (deg): B1-B2 1.74(2), Ta1-B1 2.440(18), Ta1-B2 2.343(15), Ta2-B1 2.479(18), Ta2-B2 2.318(17), Ta1-Ta2 3.2903(8), Ta1-S1 2.418(4), Ta2-S2 2.412(4), C22-S1 1.829(15), C22-S2 1.819(15), C21-S4 1.797(16), C21-S3 1.843(16); Ta1-B1-Ta2 84.0(5), Ta1-B2-Ta2 89.8(5), S1-C22-S2 117.3(8), S4-C21-S3 121.0(8), B2-Ta2-S4 128.7(4).

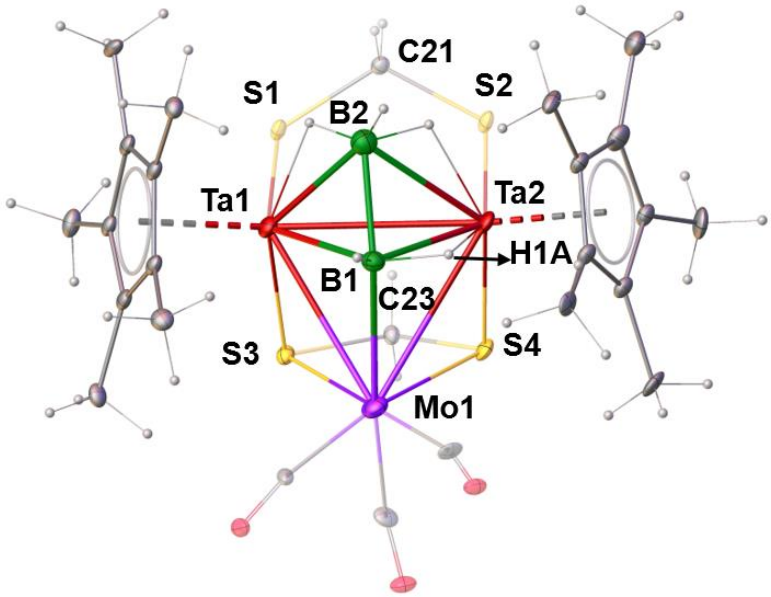


Figure S2. Full molecular structure and labeling diagram of **6**. The hydrogen atom (Ta-H-Ta) could not be located in the refinement. Selected bond lengths (Å) and angles (deg): B1-B2 1.84(5), B1-Ta1 2.42(4), B1-Ta2 2.37(3), B2-Ta1 2.37(4), B2-Ta2 2.48(4), B1-Mo1 2.56(3), Mo1-Ta1 3.182(3), Mo1-Ta2 3.245(3), Ta1-Ta2 3.281(2), S3-Mo1 2.542(9), S4-Mo1 2.565(9); B2-B1-Mo1 137(2), Ta1-Mo1-Ta2 61.38(6), S3-Mo1-S4 72.1(3), S3-C22-S4 109.2(17).

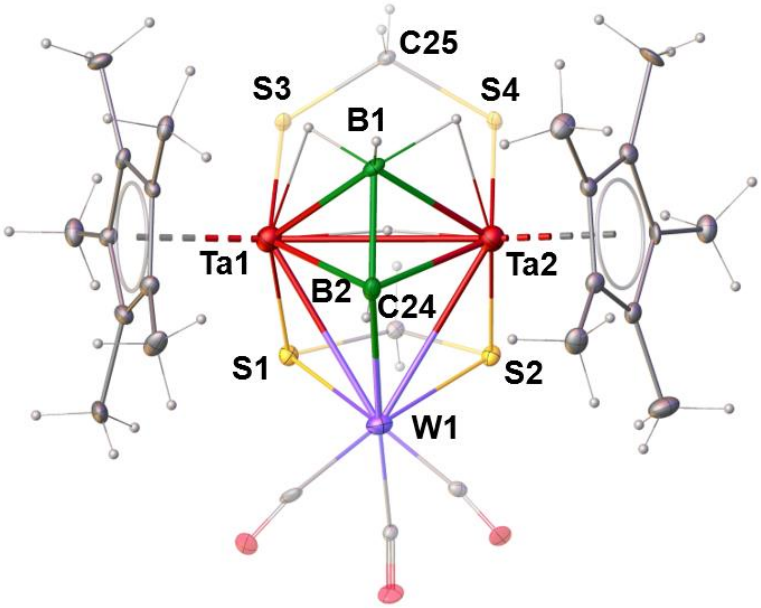


Figure S3. Full molecular structure and labeling diagram of **7**. The hydrogen atoms (B2-H-W) could not be located in the refinement. Selected bond lengths (Å) and angles (deg): B1-B2 1.79(2), B1-Ta1 2.416(14), B1-Ta2 2.390(12), B2-Ta1 2.365(13), B2-Ta2 2.371(13), B2-W1 2.515(13), Ta1-Ta2 3.2765(6), Ta1-W1 3.1692(6), Ta2-W1 3.1882(7); B1-B2-Ta1 69.5(6), B1-B2-Ta2 68.5(6), B1-B2-W1 138.0(8).

I.2 Spectroscopic Details

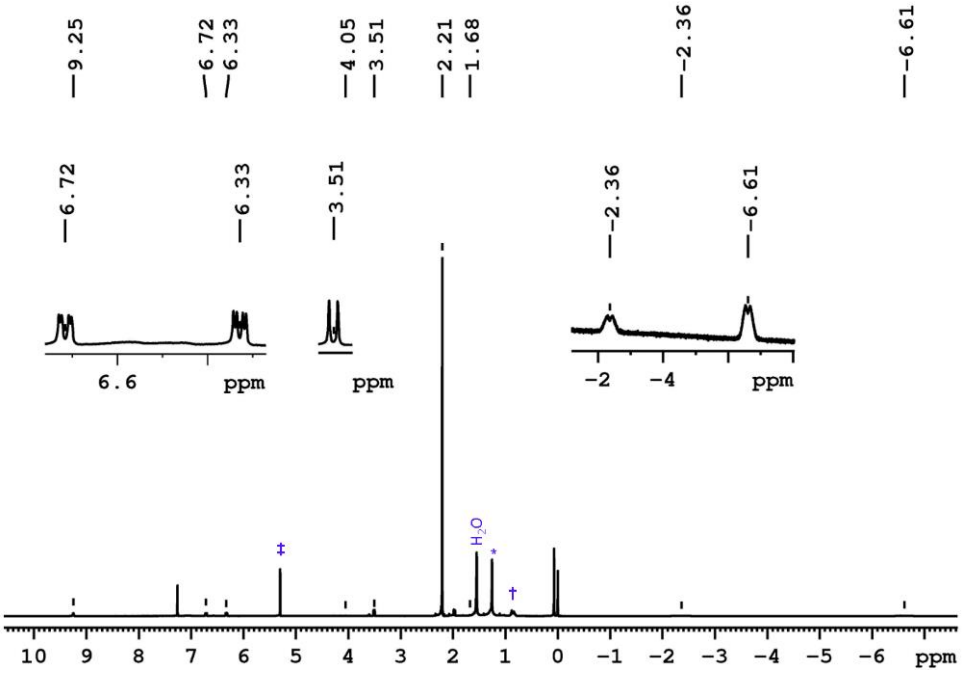


Figure S4. ^{1}H NMR spectrum of compound **1** in $CDCl_3$. (‡ CH_2Cl_2; * Hexane; † Grease)

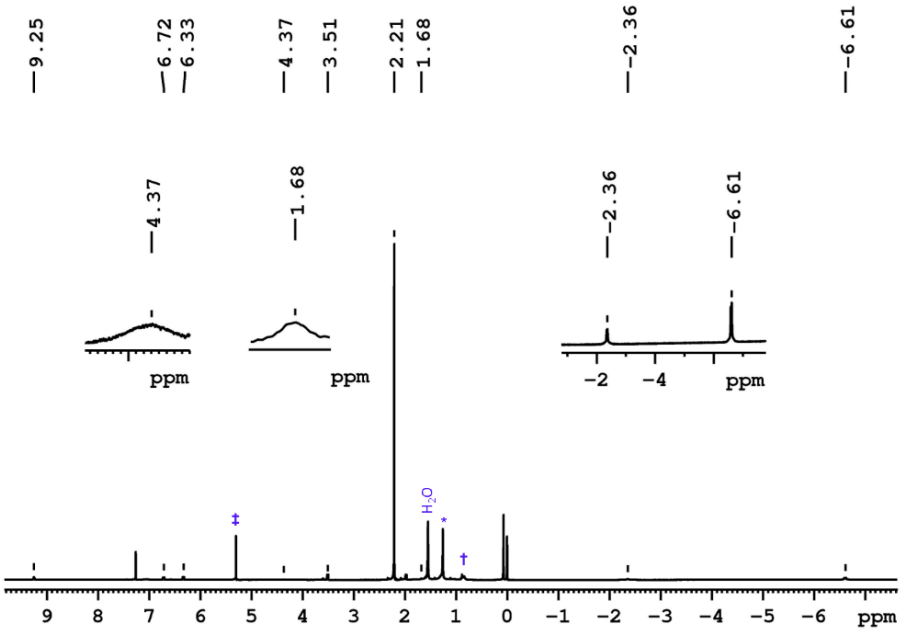


Figure S5. $^{1}H\{^{11}B\}$ NMR spectrum of compound **1** in $CDCl_3$. (‡ CH_2Cl_2; * Hexane; † Grease)

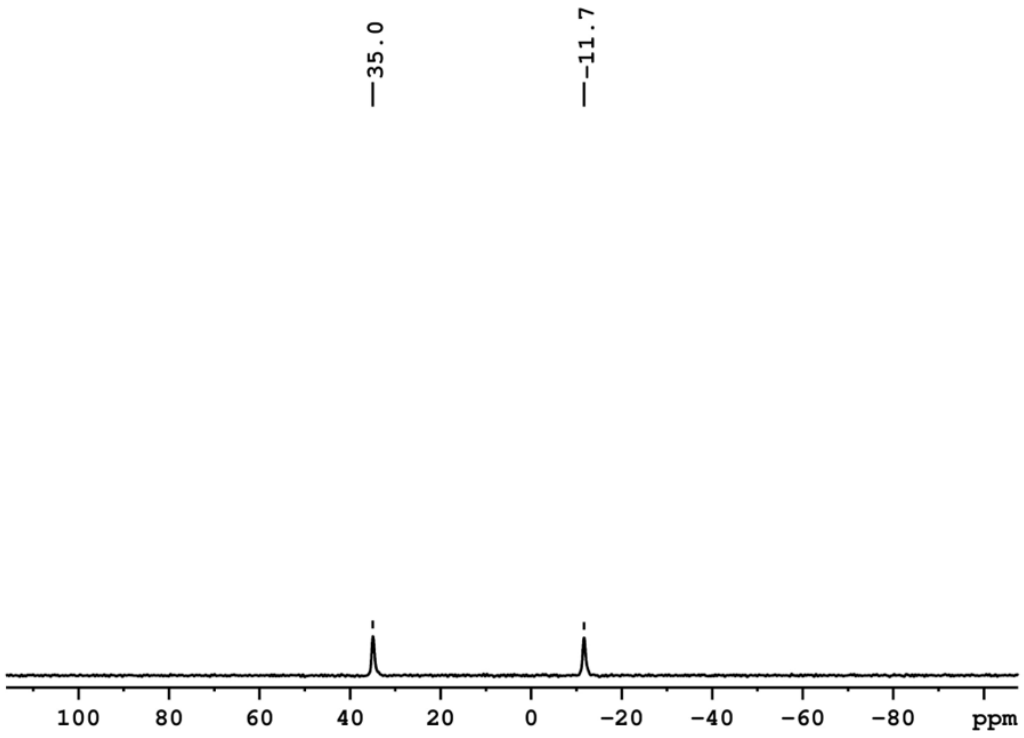


Figure S6. $^{11}B\{^{1}H\}$ NMR spectrum of compound **1** in $CDCl_3$.

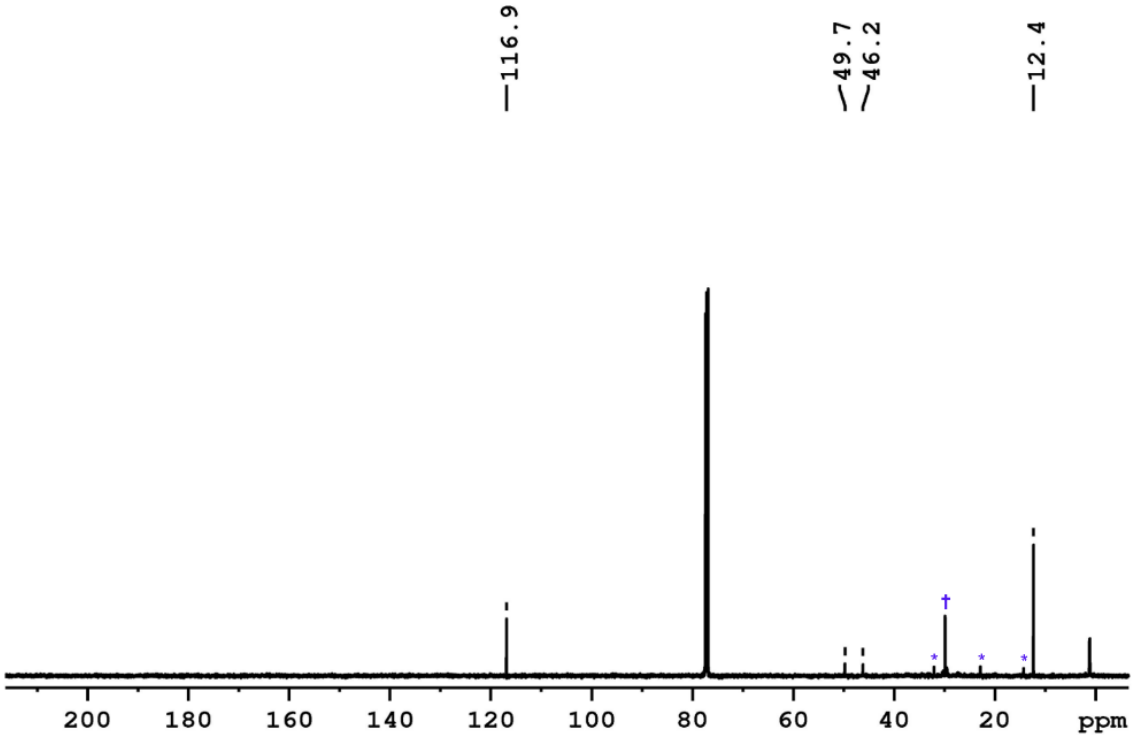


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of compound **1** in $CDCl_3$. (* Hexane; † Grease)

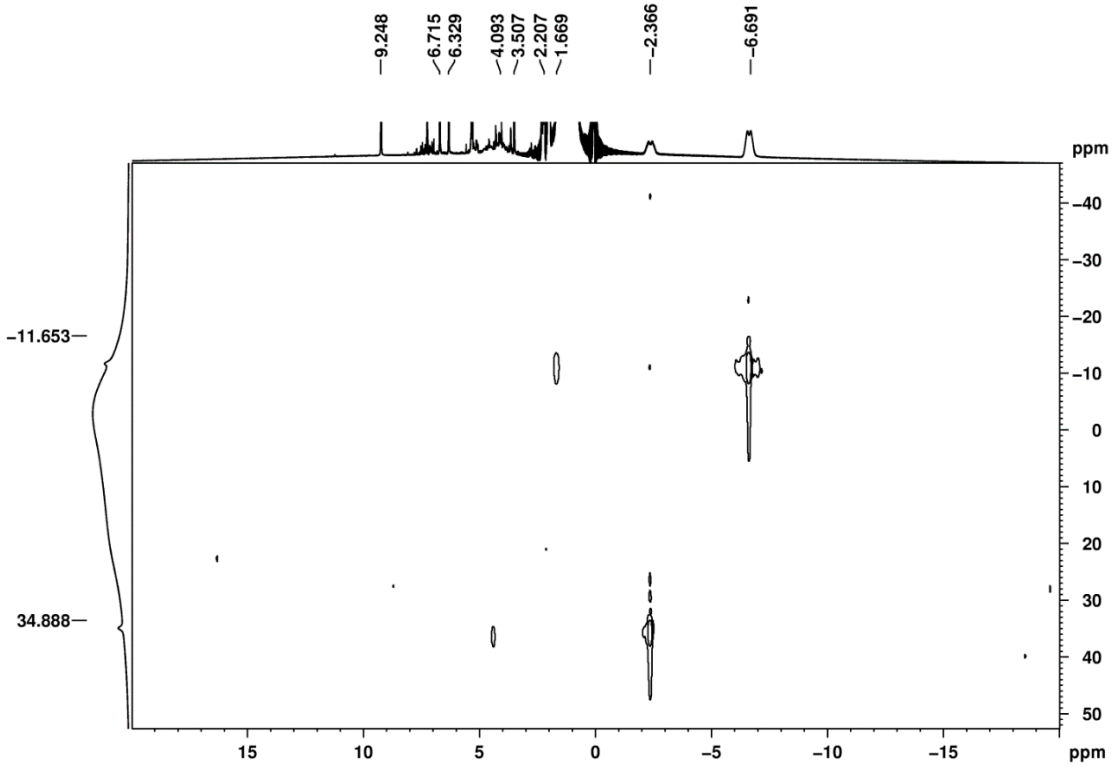


Figure S8. ^{1}H-$^{11}B\{^{1}H\}$ HSQC spectrum of compound **1**.

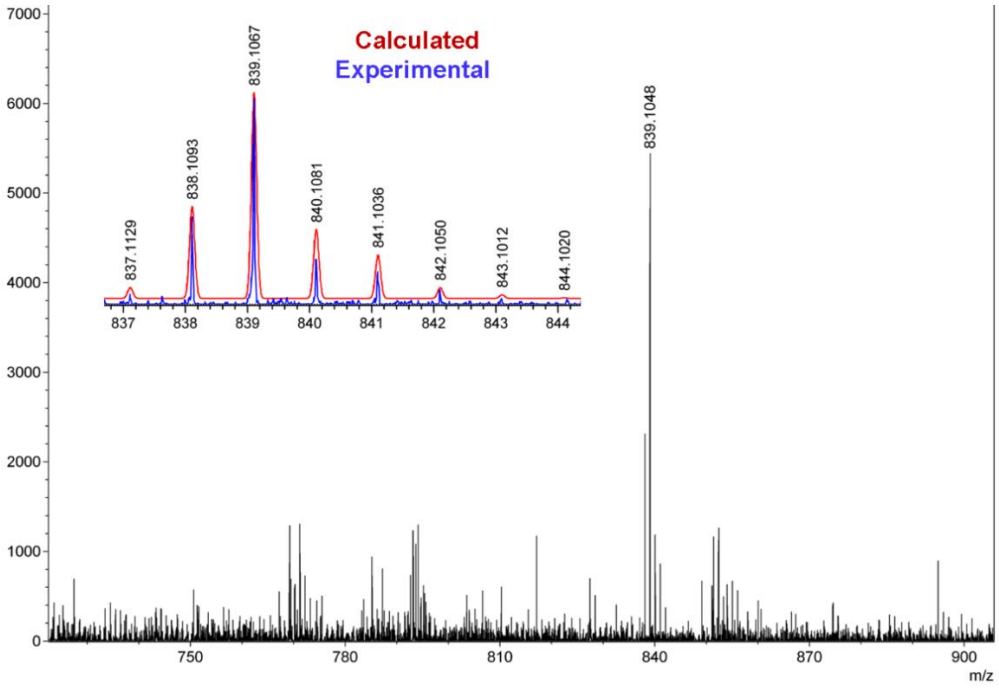


Figure S9. ESI(MS) spectrum of compound **1**.

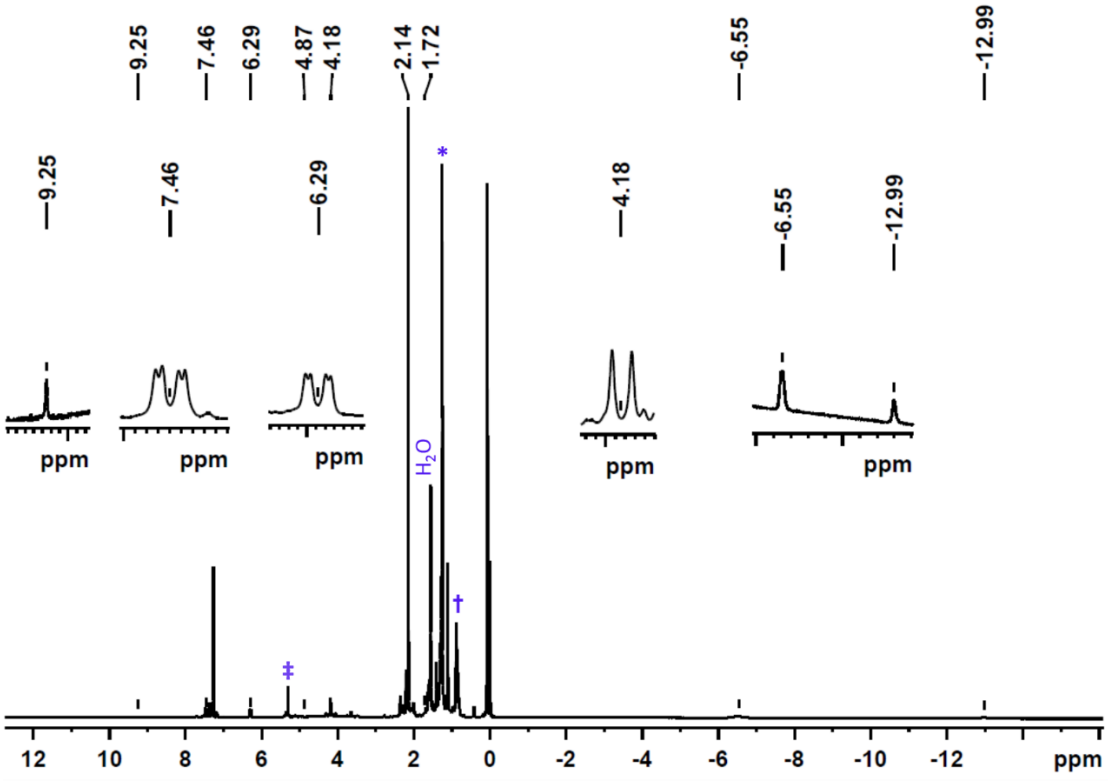


Figure S10. ^{1}H NMR spectrum of compound **6** in $CDCl_3$. (‡ CH_2Cl_2; * Hexane; † Grease)

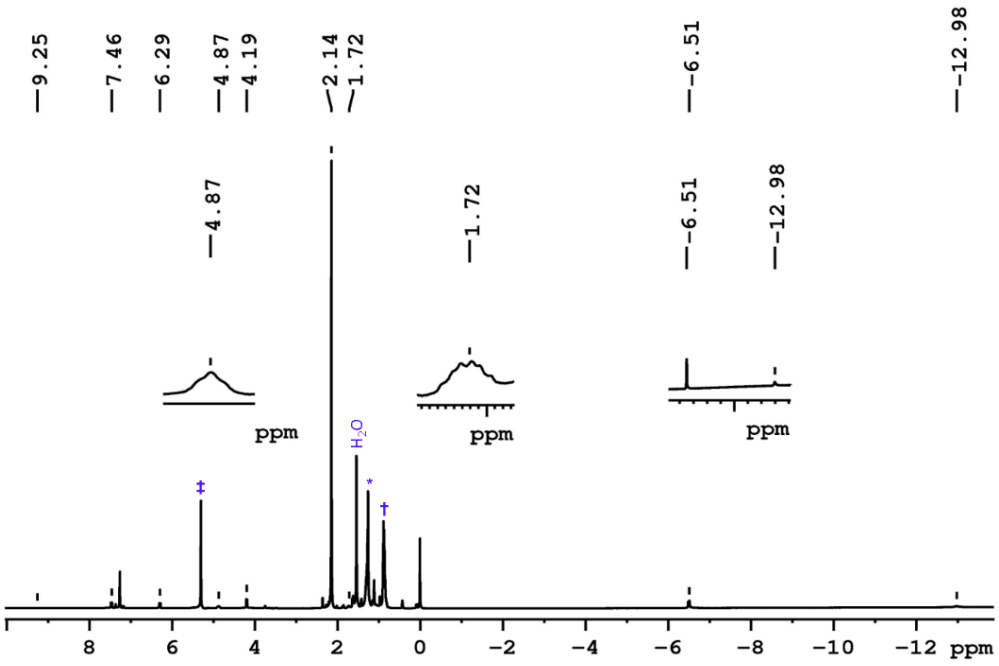


Figure S11. $^{1}H\{^{11}B\}$ NMR spectrum of compound **6** in $CDCl_3$. (‡ CH_2Cl_2; * Hexane; † Grease)

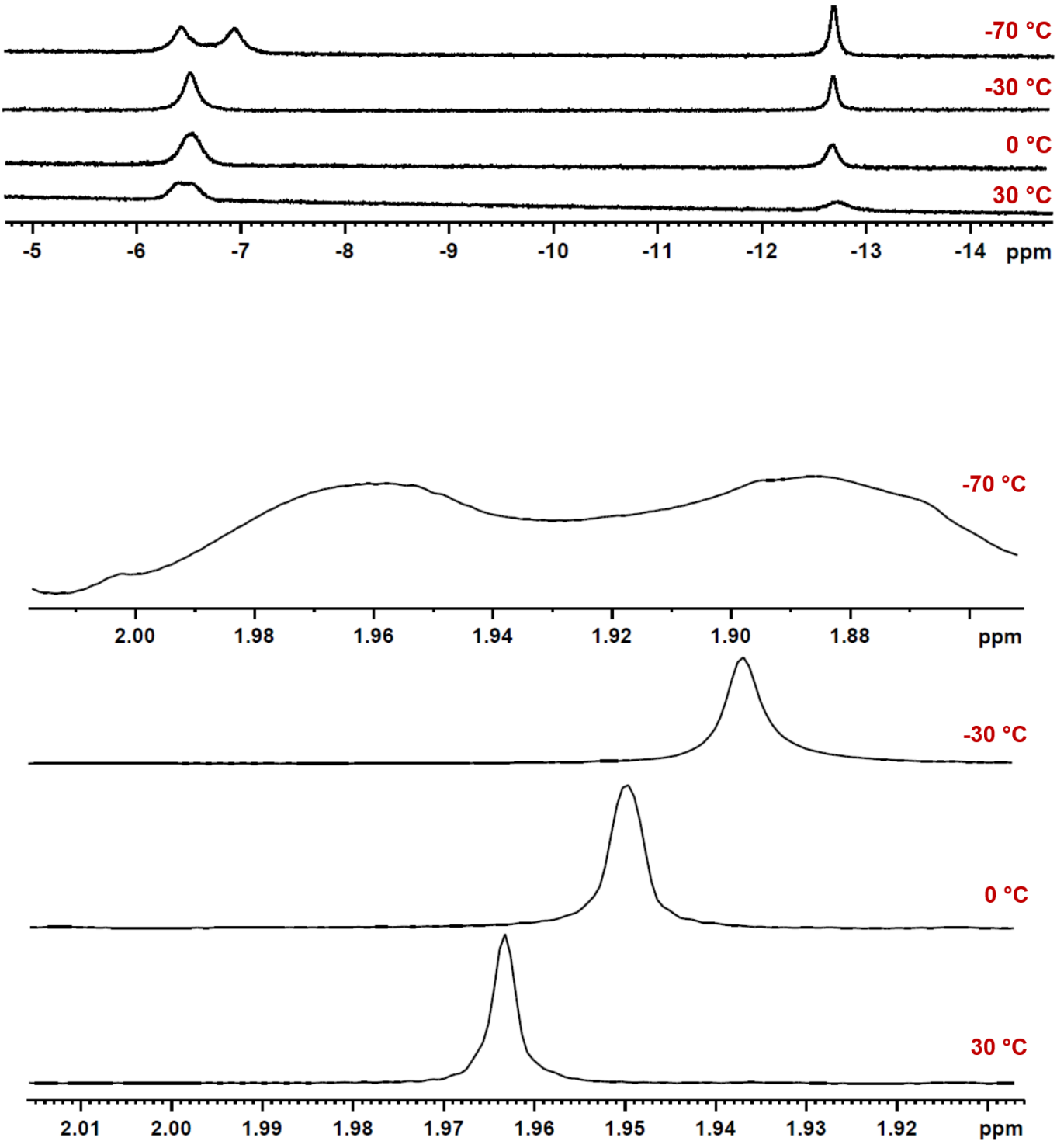


Figure S12. Variable temperature ^{1}H NMR spectrum of **6** in d^{8}-toluene.

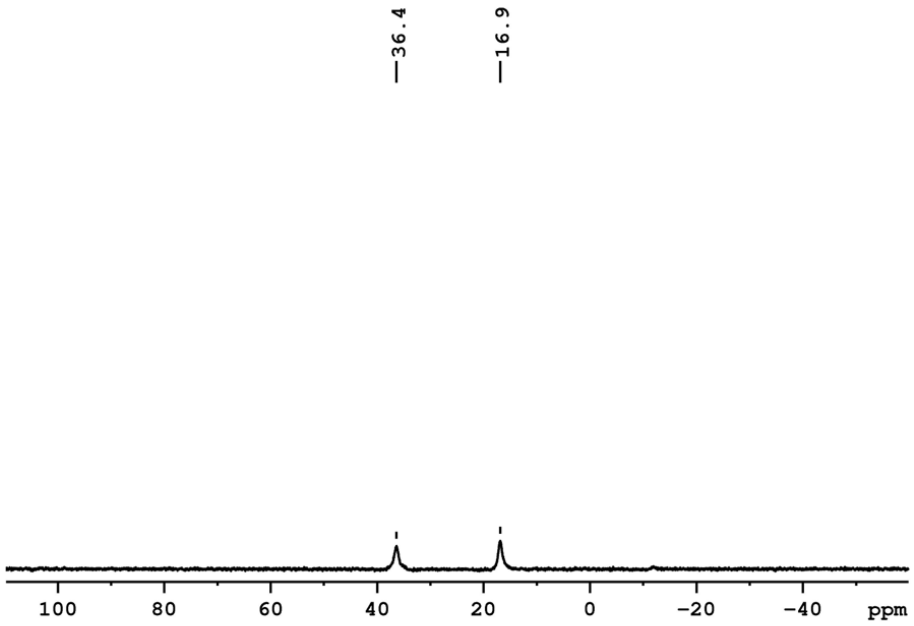


Figure S13. $^{11}B\{^{1}H\}$ NMR spectrum of compound **6** in $CDCl_3$.

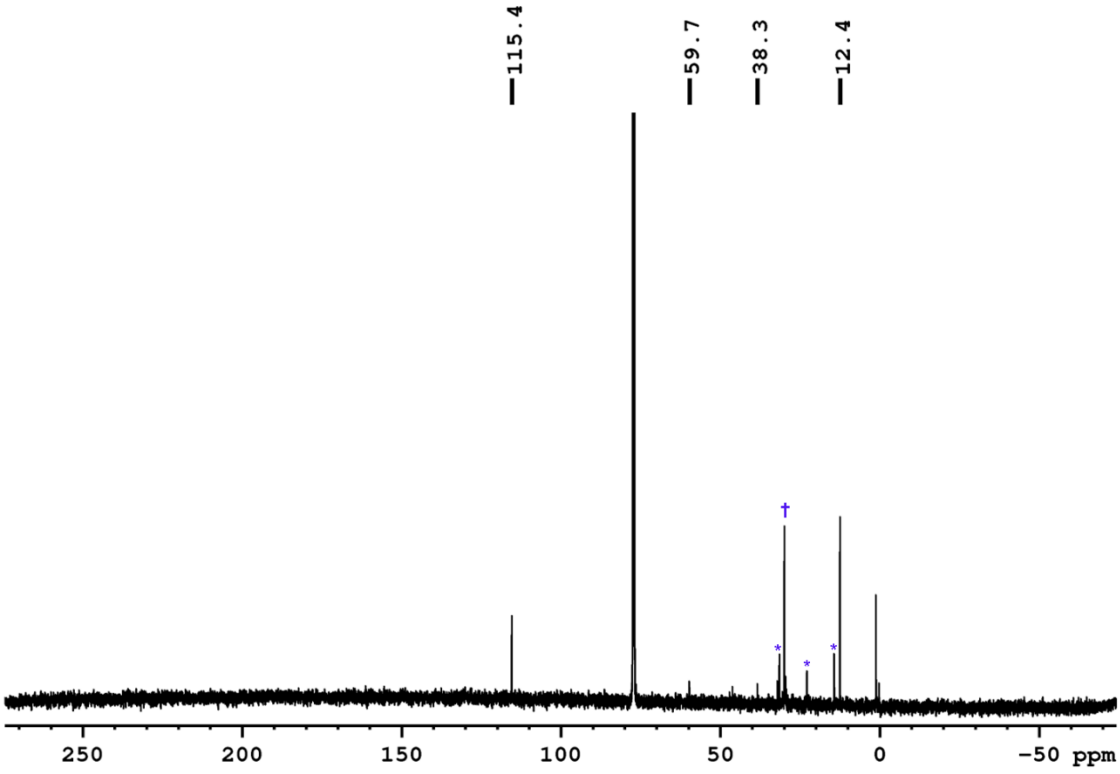


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of compound **6** in $CDCl_3$. (* Hexane; † Grease)

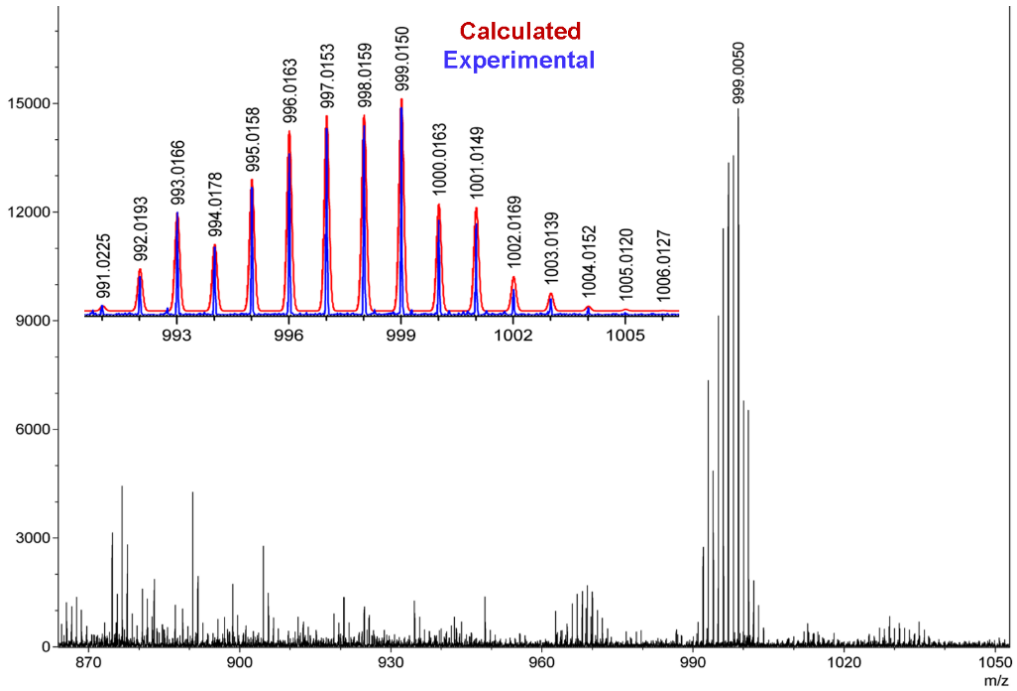


Figure S15. ESI(MS) spectrum of compound **6**.

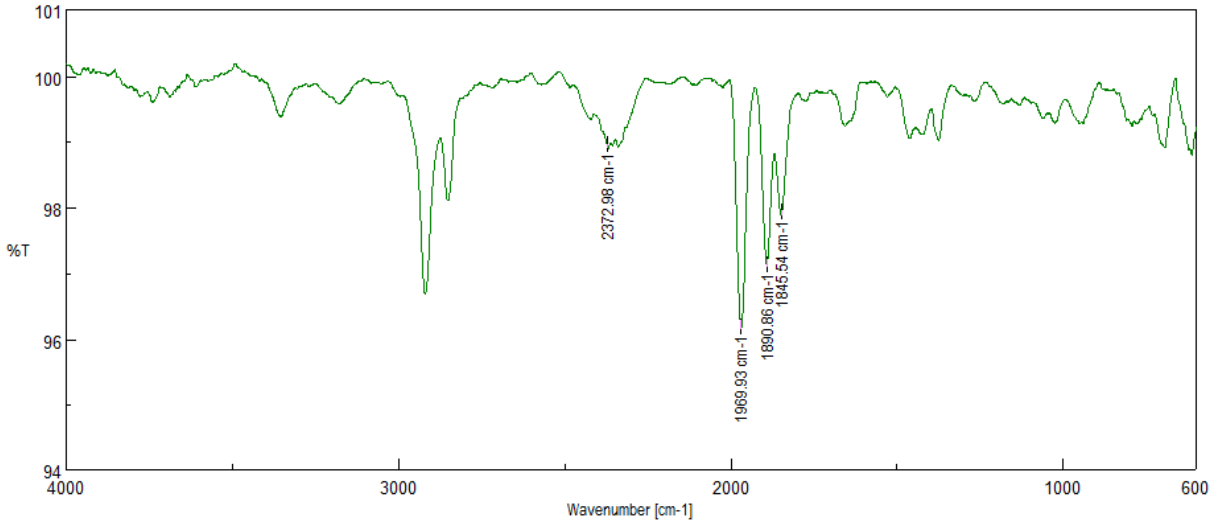


Figure S16. IR spectrum of compound **6**.

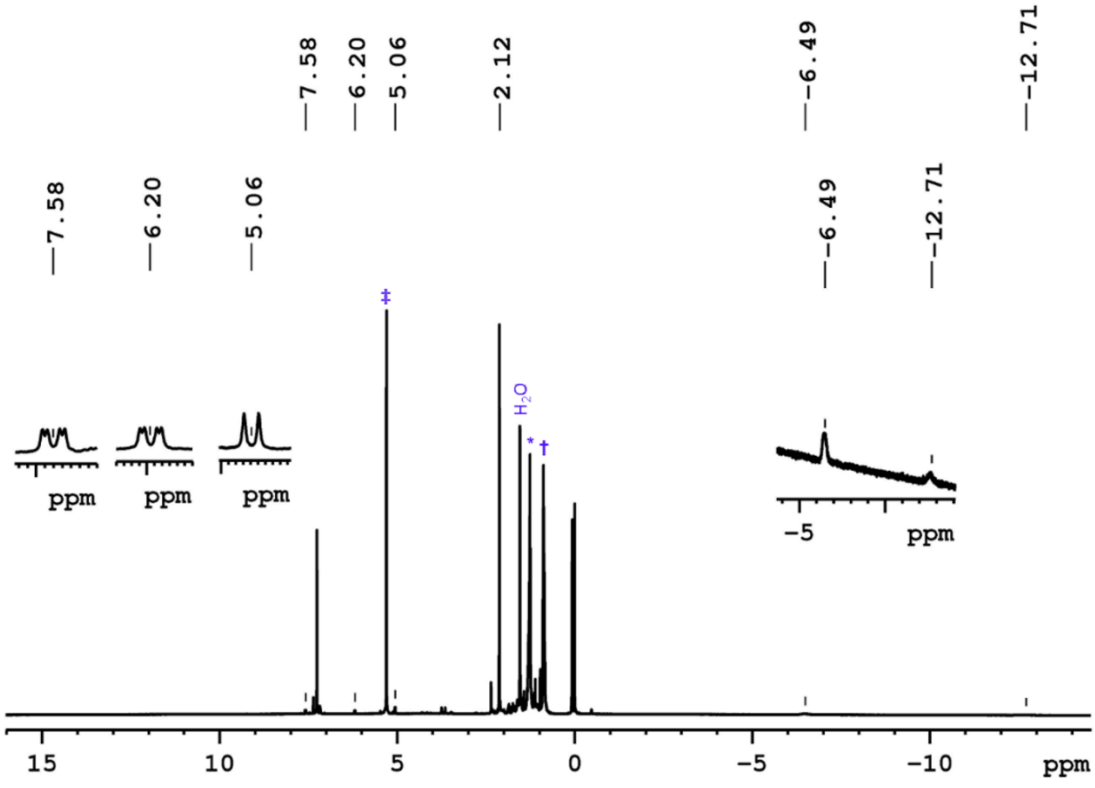


Figure S17. ^{1}H NMR spectrum of compound **7** in $CDCl_3$. (‡ CH_2Cl_2; * Hexane; † Grease)

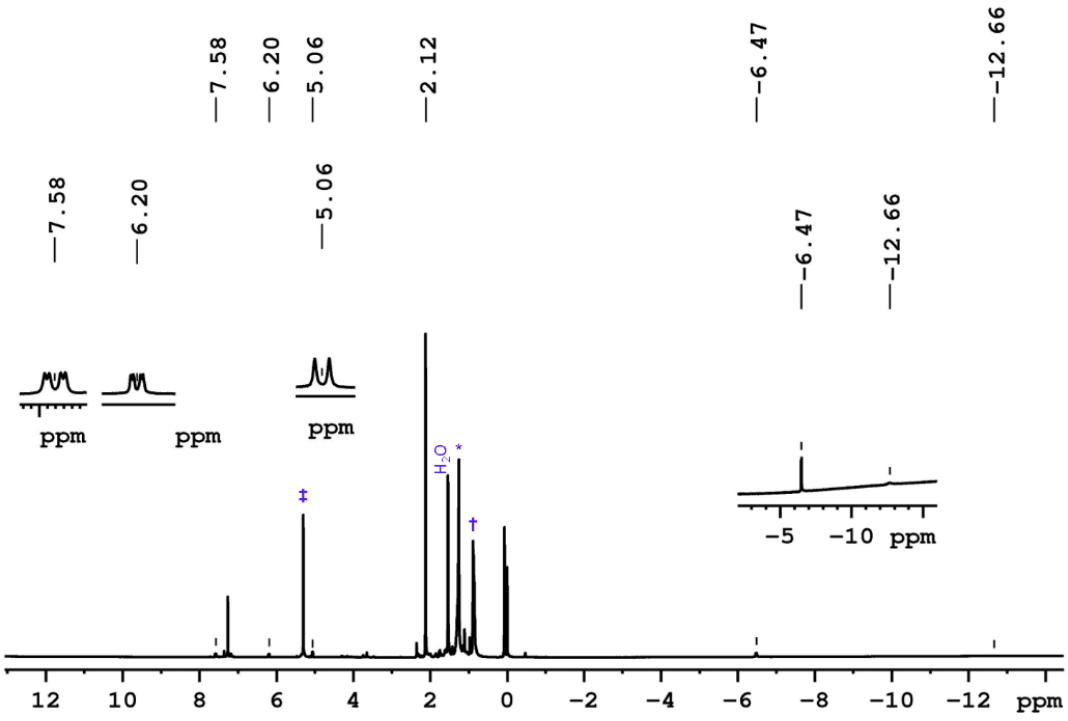


Figure S18. $^{1}H\{^{11}B\}$ NMR spectrum of compound **7** in $CDCl_3$. (‡ CH_2Cl_2; * Hexane; † Grease)

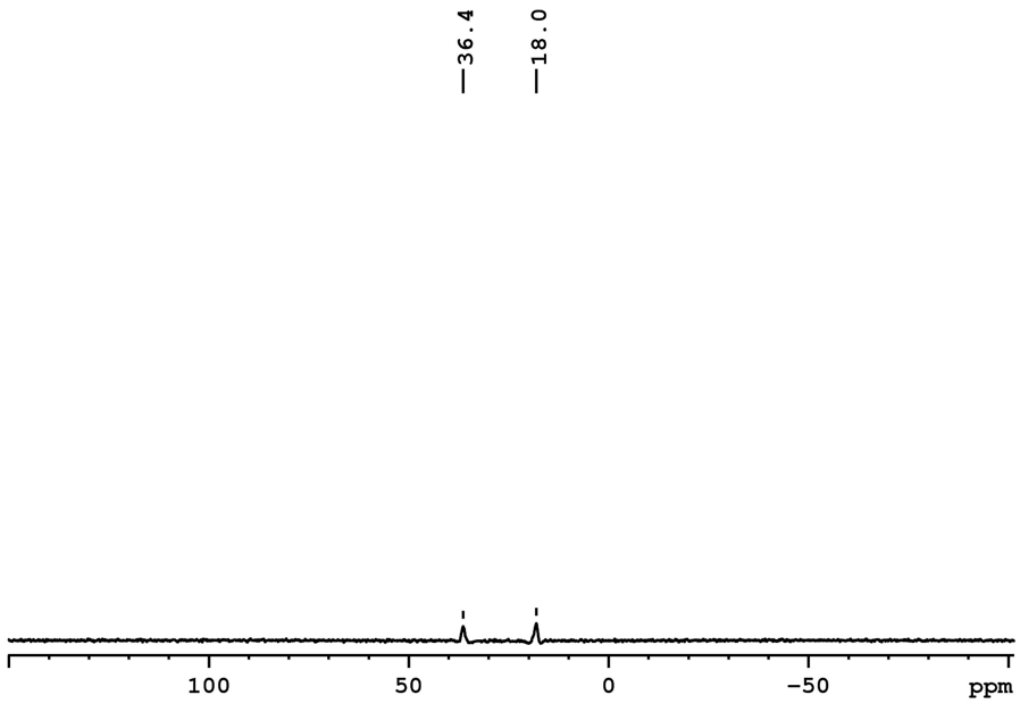


Figure S19. $^{11}B\{^{1}H\}$ NMR spectrum of compound **7** in $CDCl_3$.

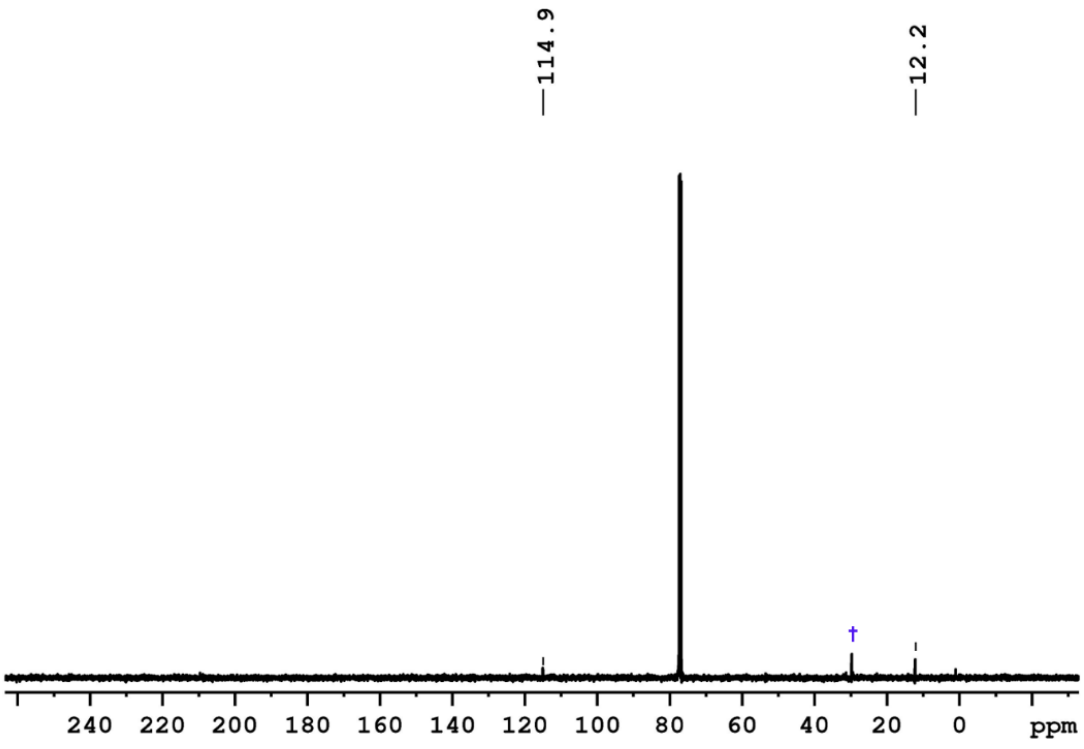


Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of compound **7** in $CDCl_3$. († Grease)

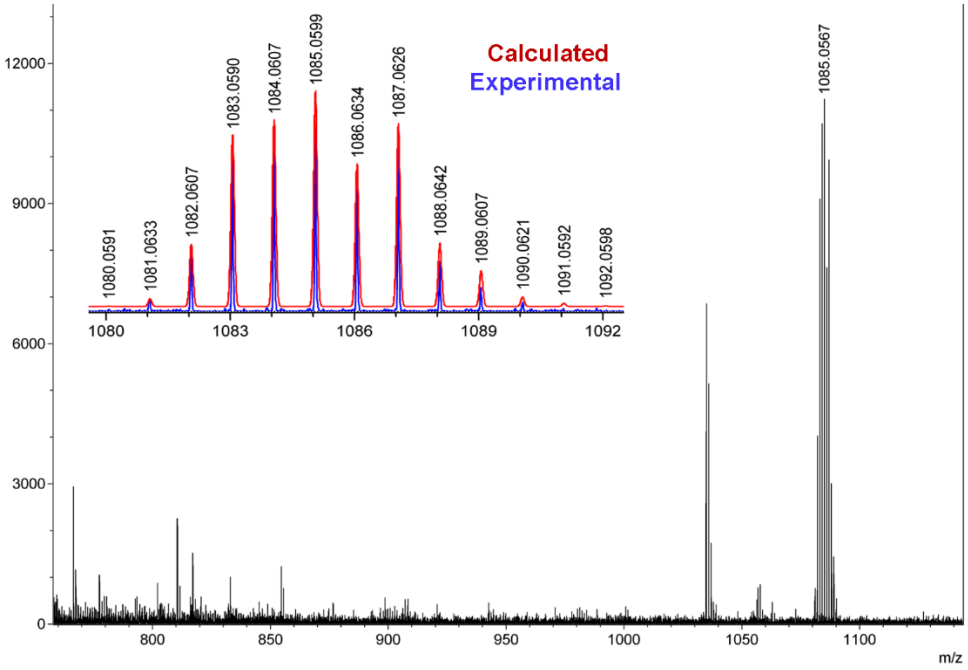


Figure S21. ESI(MS) spectrum of compound **7**.

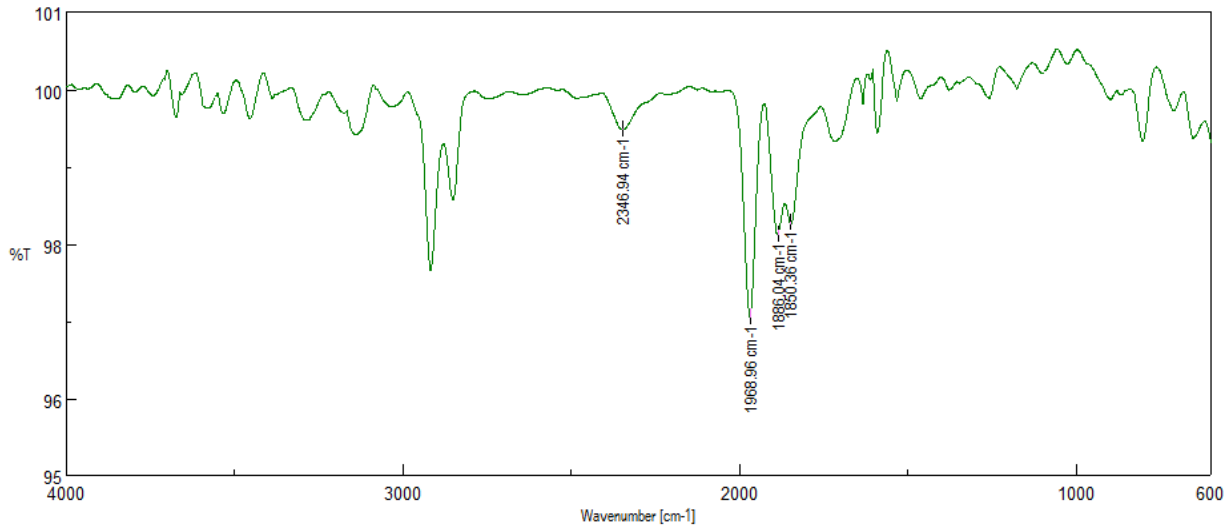


Figure S22. IR spectrum of compound **7**.

I.3 X-ray Analysis Details

The crystal data for compounds **1**, **6** and **7** were collected and integrated using a Bruker AXS kappa APEX II CCD diffractometer, with graphite monochromated Mo Kα (λ = 0.71073 Å) radiation at 296 K. The structures were solved by heavy atom methods using SHELXS-97 or SIR92 and refined using SHELXL-2014.[5] The molecular structures were drawn using Olex^2 software.[6] Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1828324 (**1**), CCDC-1921750 (**6**) and CCDC-1921751 (**7**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

*Crystal data for **1***: $C_{22}H_{40}B_2S_4Ta_2$, M_r = 816.30 g/mol, monoclinic, space group $P2_1/c$, a = 11.9818(5) Å, b = 14.7212(6) Å, c = 15.9129(6) Å, α = 90°, β = 107.354(2)°, γ = 90°, V = 2679.05(19) Å^3, Z = 4, ρ_{calcd} = 2.024 g/cm^3, μ = 8.483 mm^{-1}, GOF = 1.091, F(000) = 1568, R_1 = 0.0505, wR_2 = 0.1591, reflections collected 4722, independent reflections 4701 ($2\theta \leq 50.00°$) and 295 parameters.

*Crystal data for **6***: $C_{25}H_{39}B_2S_4O_3MoTa_2$, M_r = 995.26 g/mol, monoclinic, space group $P2_1/n$, a = 8.195(4) Å, b = 17.593(8) Å, c = 22.053(11) Å, α = 90°, β = 98.497(19)°, γ = 90°, V = 3145(3) Å^3, Z = 4, ρ_{calcd} = 2.102 g/cm^3, μ = 7.626 mm^{-1}, GOF = 1.002, F(000) = 1900, R_1 = 0.0984, wR_2 = 0.2582, reflections collected 6523 independent reflections 4100 ($2\theta \leq 45.35°$) and 365 parameters.

*Crystal data for **7***: $C_{25}H_{39}B_2S_4O_3WTa_2$, M_r = 1080.15 g/mol, orthorhombic, space group $P2_1$, a = 8.3877(2) Å, b = 19.8088(8) Å, c = 21.4750(9) Å, α = 90°, β = 90°, γ = 90°, V = 3568.1(2) Å^3, Z = 4, ρ_{calcd} = 2.011 g/cm^3, μ = 9.590 mm^{-1}, GOF = 1.096, F(000) = 2016, R_1 = 0.0280, wR_2 = 0.0627, reflections collected 24868, independent reflections 6064 ($2\theta \leq 49.51°$) and 344 parameters.

I.4 Computational Details

I.4 Computational Details

All the calculations are carried out using Gaussian 09 program package, Version-D.[7] Geometry optimization are carried out using B3LYP functional with LANL2DZ basis set for metal atoms (Ta, Mo and W) and 6-31G(d) basis set for all the other elements (B, C, H and S). The nature of stationary points is examined by vibrational frequency calculations at the same level of theory. The connection between transition states and intermediates in each case is confirmed by following the transition state imaginary frequency in either direction and then optimizing both the structures. Natural Bond Orbital (NBO) analysis is performed to get the Natural Population Analysis (NPA) charges and Wiberg bond order with the NBO6 method at the same level of theory.[8]

In order to understand the electron flow on going from non-classical to classical structure, the orbital evolution was analyzed by invoking the intrinsic bond orbital (IBO) representation of the wavefunction.[9] In the case of free $[B_2H_5]^-$, the structural transformation from non-classical to the classical one was followed by forcing B-B-H angle to vary from 54.3° to 114.3° with step size 3°. IBOs at each points are computed using PBE/def2tzvp level of theory and IboView program package. In the case of metal supported $[B_2H_5]^-$ complex, transition state connecting classical and non-classical structure was further computed considering the model complex $[(CpTa)_2(\mu,\eta^2{:}\eta^2\text{-}B_2H_5)(\mu\text{-}H)(\kappa^2,\mu\text{-}S_2CH_2)_2]$ at B3LYP/def2-TZVP level of theory using Gaussian 09 program package, Version-D. Intrinsic reaction coordinate (IRC) calculations are carried out at the same level of theory. Orbital coefficients are generated at each points of the IRC using Gaussian 09 program package. Intrinsic bond orbitals (IBOs) (*iboexp* = 2) are generated using IboView by taking the orbital information generated from Gaussian 09 program package. Further, IBO evolution for the IRC path are used for the analysis of the electron flow. QTAIM analysis is carried out using AIMALL package with the wave function files generated at B3LYP functional with LANL2DZ basis set for metal atoms (Ta, Mo and W) and 6-31G(d) basis set for all the other elements (B, C, H and S).[10]

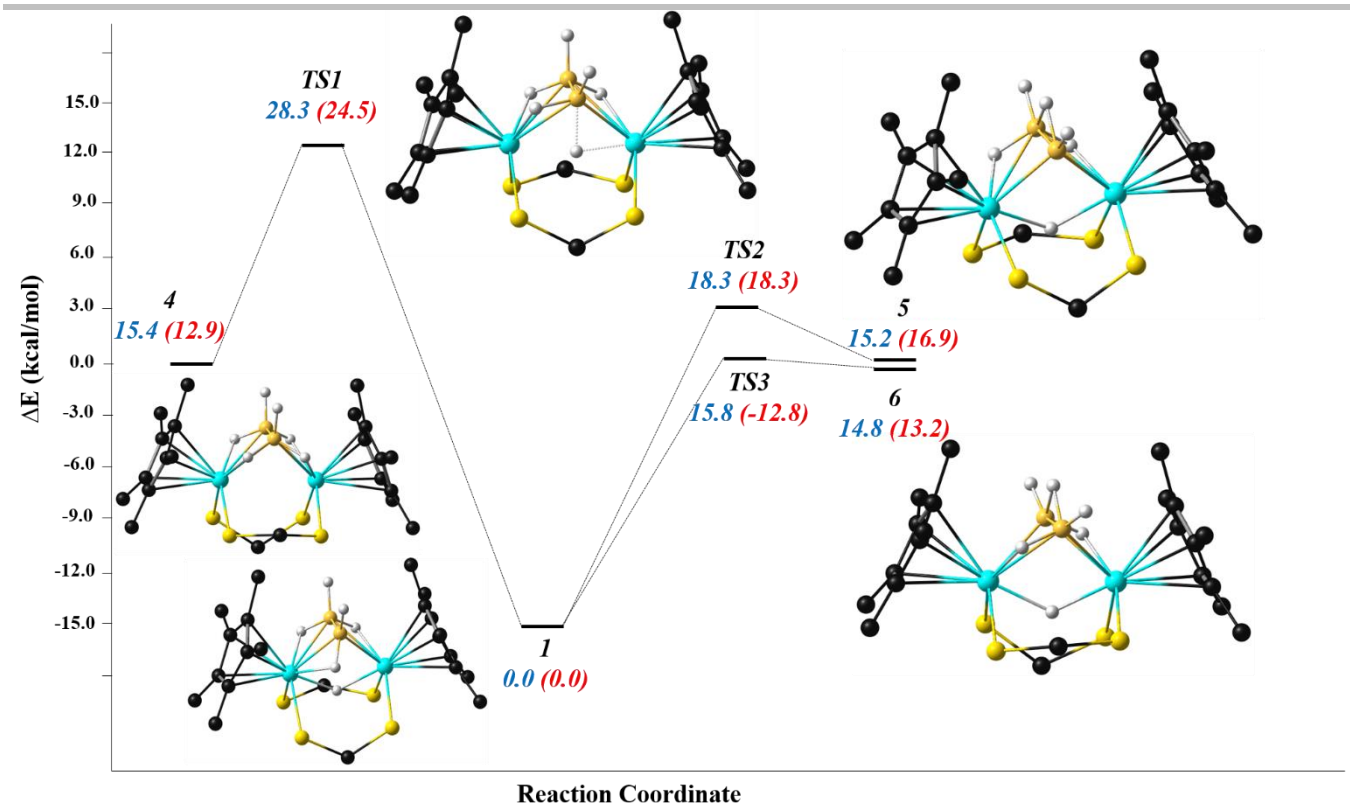


Figure S23. Energy landscape of the molecular formula $[(Cp^*Ta)_2(B_2H_6)(\kappa^2,\mu\text{-}S_2CH_2)_2]$ at B3LYP level of theory with the LANL2DZ basis set for Ta and 6-31G(d,p) basis set for other atoms. Color code: Blue (ΔE) and Red (ΔG).

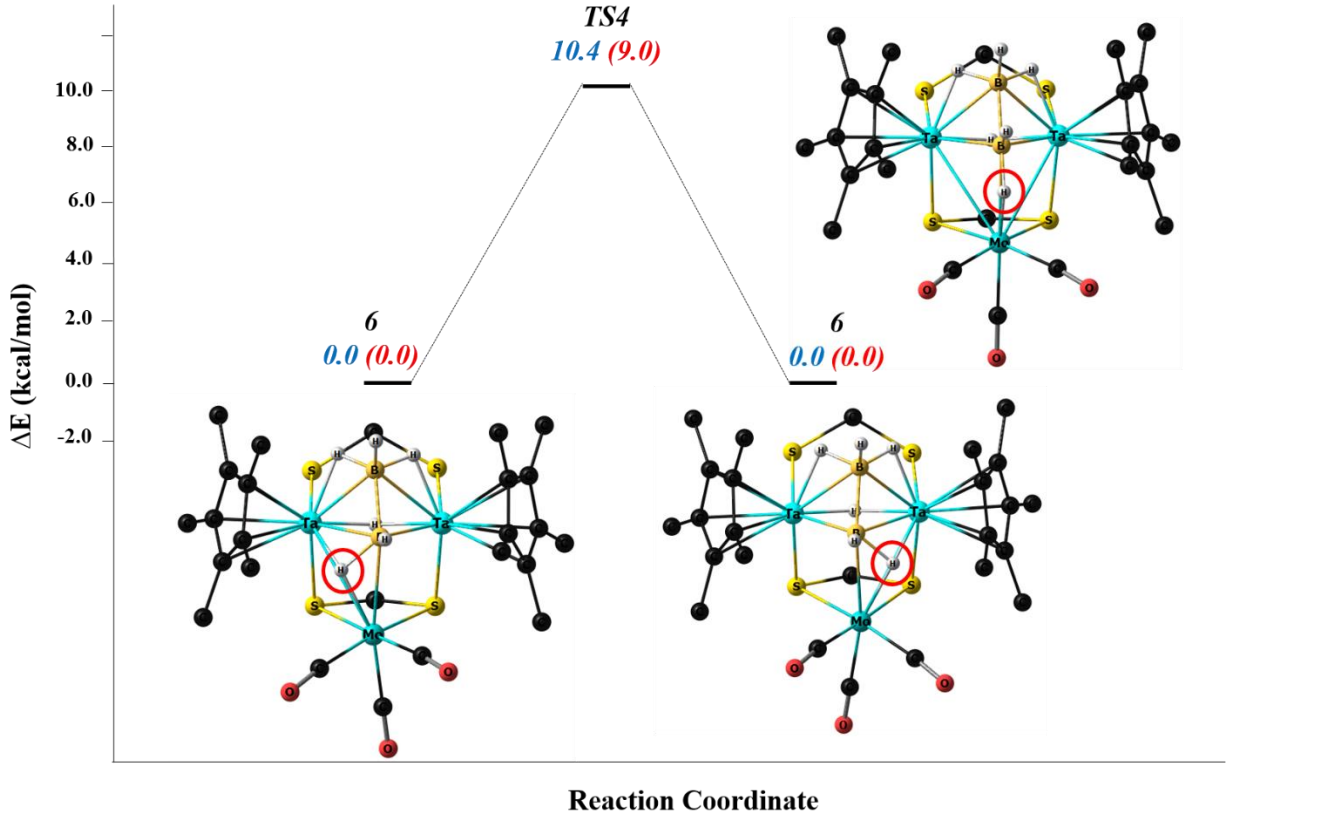


Figure S24. Energy landscape of the molecular formula $[\{(Cp^*Ta)(CH_2S_2)\}_2(B_2H_5)(H)\{Mo(CO)_3\}]$ (**6**) at B3LYP level of theory with the LANL2DZ basis set for Ta, Mo and 6-31G(d,p) basis set for other atoms. Color code: Blue (ΔE) and Red (ΔG).

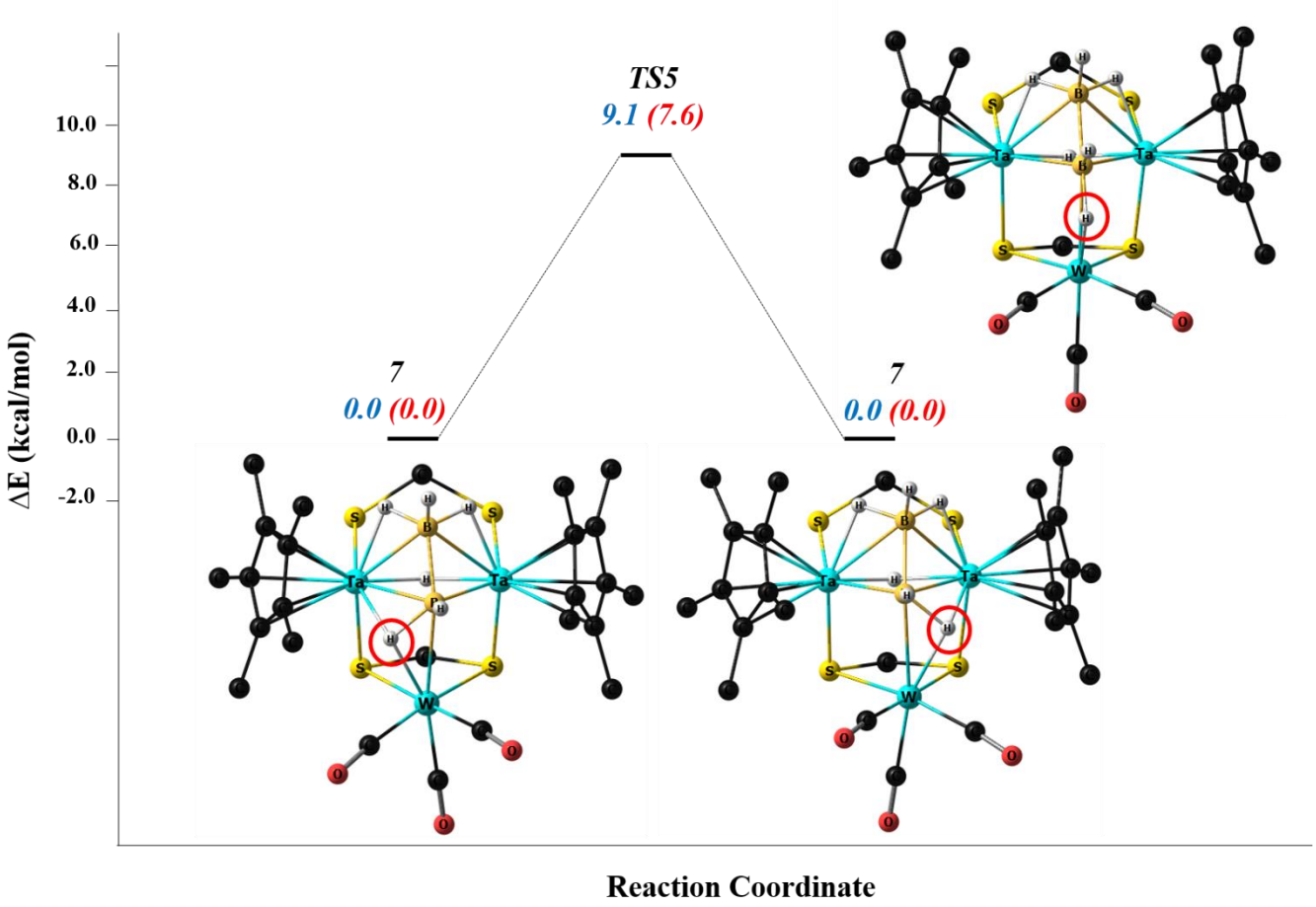


Figure S25. Energy landscape of the molecular formula [{(Cp*Ta)(CH_2S_2)}$_2$(B_2H_5)(H){W(CO)$_3$}] (**7**) at B3LYP level of theory with the LANL2DZ basis set for Ta, W and 6-31G(d,p) basis set for other atoms. Color code: Blue (ΔE) and Red (ΔG).

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Cartesian coordinates of all the optimized geometries using B3LYP functional with LANL2DZ basis set for Ta, Mo and 6-31G(d,p) basis set for other atoms.

1

Total energy: -2620.7485 a. u.
Total energy including ZPVE: -2620.1718 a. u.
Total free energy including ZPVE: -2620.2386 a. u.

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1	-5.649643000	0.625096000	2.102613000
1	-4.629801000	-0.797828000	2.381475000
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1	-4.433282000	-2.294963000	-1.183473000
1	-4.794019000	-2.167796000	0.538072000
1	-5.898121000	-1.452694000	-0.647777000
6	-3.617944000	-0.077712000	-2.909735000
1	-3.488465000	-1.160379000	-2.986218000
1	-4.593672000	0.179176000	-3.344529000
1	-2.845818000	0.396693000	-3.520950000
6	-2.668549000	2.802926000	-1.900568000
1	-2.125392000	2.455960000	-2.782257000
1	-3.554078000	3.354070000	-2.247180000
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1	-2.832153000	2.613604000	2.291458000
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1	2.078630000	2.473629000	-2.733110000
6	3.585182000	-0.065722000	-2.922250000
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3

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1	-4.730037000	-1.161751000	2.130490000
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4

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1	-4.305781000	-2.091137000	-2.009415000
1	-5.804860000	-1.398195000	-1.371680000
1	-4.719271000	-0.417079000	-2.372181000
6	-4.821448000	1.758418000	-0.405380000
1	-4.335311000	2.704970000	-0.156316000
1	-4.866826000	1.691847000	-1.495950000
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6	-3.476367000	1.697488000	2.468750000
1	-3.355635000	2.660085000	1.964017000
1	-4.427279000	1.725025000	3.018634000
1	-2.673049000	1.603373000	3.204458000
6	-2.620787000	-1.326484000	3.091041000
1	-2.057121000	-0.581069000	3.659181000
1	-3.493763000	-1.605727000	3.697650000
1	-1.991967000	-2.213808000	2.984912000
6	-3.254763000	-3.079006000	0.515321000
1	-3.171085000	-3.403314000	-0.524600000
1	-2.356921000	-3.420358000	1.037354000
1	-4.119636000	-3.589374000	0.961683000
6	3.072067000	-0.798397000	1.758430000
6	3.478597000	0.557344000	1.486263000
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1	4.119682000	-3.589358000	0.961580000
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1	1.992185000	-2.213724000	2.985062000
1	3.493835000	-1.605275000	3.697803000
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6	3.476321000	1.697636000	2.468653000
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1	1.001006000	1.231377000	1.317253000
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1	-0.000042000	-2.129016000	1.414133000
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16	1.552164000	-1.356994000	-2.044395000
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16	1.605487000	2.339696000	-1.042367000
73	-1.677163000	0.080273000	-0.095745000
73	1.677150000	0.080202000	-0.095739000
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1	-1.000916000	1.231468000	1.317378000

5

Total energy: -2620.7251 a. u.
Total energy including ZPVE: -2620.1493 a. u.
Total free energy including ZPVE: -2620.2175 a. u.

$N_{Img} = 0$

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6	-4.114896000	-0.485939000	0.179959000
6	-4.000814000	0.927381000	-0.016077000
6	-4.621906000	1.985082000	0.851451000
1	-4.083766000	2.933791000	0.790239000
1	-5.656263000	2.162461000	0.525461000
1	-4.647283000	1.690075000	1.903083000
6	-4.838926000	-1.156893000	1.314606000
1	-4.421465000	-2.142434000	1.535825000
1	-4.789379000	-0.563171000	2.231320000
1	-5.899186000	-1.290772000	1.059335000
6	-3.690574000	-2.610268000	-1.280992000
1	-3.606973000	-3.199759000	-0.365258000
1	-4.651905000	-2.850475000	-1.756493000
1	-2.894128000	-2.932150000	-1.957212000
6	-2.730863000	-0.353524000	-3.323025000
1	-2.242548000	-1.321279000	-3.461398000
1	-3.610480000	-0.327582000	-3.980938000
1	-2.041247000	0.421804000	-3.668227000
6	-3.192488000	2.489833000	-1.939480000
1	-2.944032000	3.261913000	-1.205786000
1	-2.389956000	2.469568000	-2.681908000
1	-4.113597000	2.797693000	-2.453354000
6	3.133685000	-0.116366000	-1.915304000
6	3.532929000	-1.167240000	-1.019466000
6	4.095888000	-0.563509000	0.148790000
6	4.035650000	0.854633000	-0.018687000
6	3.433944000	1.131089000	-1.289891000
6	3.293321000	2.494028000	-1.906250000
1	2.495927000	2.517996000	-2.652603000
1	3.063055000	3.253532000	-1.153996000
1	4.228548000	2.786123000	-2.403856000
6	2.708114000	-0.314905000	-3.342007000
1	2.142786000	0.538702000	-3.722523000
1	3.593986000	-0.437841000	-3.980278000
1	2.090394000	-1.209171000	-3.465047000
6	3.533954000	-2.639804000	-1.325725000
1	3.386832000	-3.233305000	-0.419297000
1	2.744119000	-2.909062000	-2.032756000
1	4.493607000	-2.936372000	-1.771457000
6	4.799566000	-1.284663000	1.263136000

1	4.772535000	-0.713280000	2.195451000
1	4.347036000	-2.259173000	1.462099000
1	5.854463000	-1.446469000	1.001743000
6	4.704855000	1.861299000	0.873870000
1	4.258922000	2.853830000	0.780988000
1	4.648815000	1.573478000	1.926599000
1	5.766237000	1.942941000	0.600676000
6	0.043985000	-2.770419000	1.600485000
1	-0.006456000	-3.446357000	2.457725000
1	0.159414000	-3.368716000	0.693692000
6	0.083018000	1.997356000	2.453029000
1	0.100578000	2.921637000	3.035701000
1	0.192783000	1.143671000	3.126288000
5	-0.149993000	-1.074157000	-1.334702000
1	0.475139000	1.442256000	-2.352620000
1	0.921716000	-1.563877000	-0.869633000
1	0.035407000	-0.376234000	-2.410574000
5	0.145687000	0.642500000	-1.518833000
1	-0.874293000	1.276440000	-1.069140000
16	-1.574984000	1.896970000	1.671856000
16	1.566264000	2.049133000	1.369703000
16	-1.610688000	-1.969721000	1.504154000
16	1.567519000	-1.770672000	1.806818000
73	-1.664400000	0.024789000	0.099642000
73	1.667859000	-0.017913000	0.109785000
1	-0.011207000	0.016822000	0.902607000
1	-0.671199000	-2.026285000	-1.844598000

TS1

Total energy: -2620.7033 a. u.
Total energy including ZPVE: -2620.1302 a. u.
Total free energy including ZPVE: -2620.1995 a. u.

N_{Img} = 720.3

6	-3.485006000	1.657168000	0.543758000
6	-3.304914000	1.642784000	-0.881789000
6	-3.747415000	0.368927000	-1.372269000
6	-4.170305000	-0.411724000	-0.250642000
6	-4.026353000	0.392091000	0.929191000
6	-4.568610000	0.053534000	2.287897000
1	-4.017606000	0.556896000	3.085943000
1	-5.618000000	0.373369000	2.349433000
1	-4.530391000	-1.019561000	2.487865000
6	-4.815880000	-1.766383000	-0.316754000
1	-4.380847000	-2.378967000	-1.110875000
1	-4.700378000	-2.311969000	0.623701000
1	-5.891158000	-1.664799000	-0.517525000
6	-3.864348000	-0.036992000	-2.813733000
1	-3.660480000	-1.102667000	-2.942349000
1	-4.880637000	0.164271000	-3.179670000
1	-3.166916000	0.517147000	-3.447506000
6	-2.907336000	2.824662000	-1.721403000
1	-2.448422000	2.517877000	-2.663637000
1	-3.792581000	3.430642000	-1.958198000
1	-2.189884000	3.466529000	-1.203782000
6	-3.308346000	2.845205000	1.449527000
1	-2.989680000	2.543514000	2.451328000
1	-2.562660000	3.543815000	1.060613000
1	-4.255921000	3.391962000	1.549922000
6	3.213684000	1.801645000	-0.702856000
6	3.625857000	0.605267000	-1.390596000
6	4.166848000	-0.306098000	-0.426768000
6	4.057435000	0.314142000	0.857331000
6	3.463236000	1.612007000	0.685379000
6	3.259554000	2.630285000	1.772585000
1	2.444457000	3.316558000	1.529034000
1	3.016725000	2.155120000	2.727393000
1	4.169778000	3.228762000	1.918615000
6	2.785604000	3.082090000	-1.361165000
1	2.137969000	3.676229000	-0.712109000

1	3.667728000	3.691070000	-1.603443000
1	2.241079000	2.900156000	-2.291263000
6	3.667970000	0.422884000	-2.884098000
1	3.579535000	-0.630773000	-3.161536000
1	2.862131000	0.968264000	-3.383192000
1	4.620068000	0.797583000	-3.285401000
6	4.875495000	-1.595795000	-0.730570000
1	4.855939000	-2.276345000	0.125360000
1	4.414673000	-2.118149000	-1.573280000
1	5.928075000	-1.406130000	-0.983238000
6	4.683345000	-0.197774000	2.124578000
1	4.185959000	0.191141000	3.016261000
1	4.655078000	-1.288620000	2.181968000
1	5.735506000	0.116857000	2.165643000
6	-0.011677000	-2.421343000	-1.986498000
1	-0.038236000	-3.417935000	-2.435941000
1	-0.004145000	-1.673225000	-2.784212000
6	0.019287000	-1.771516000	2.429694000
1	0.001946000	-2.228661000	3.422678000
1	0.014784000	-2.548089000	1.660597000
5	-0.011192000	0.967751000	-1.577238000
1	-0.002128000	1.930980000	-2.295451000
1	0.913190000	0.199973000	-1.894780000
1	-1.007680000	0.276251000	-1.908393000
5	0.122323000	1.541754000	0.066688000
1	0.420417000	2.664139000	0.375871000
16	-1.570309000	-0.838200000	2.290171000
16	1.597230000	-0.837391000	2.332164000
16	-1.543124000	-2.228750000	-1.017328000
16	1.555852000	-2.254566000	-1.036937000
73	-1.715509000	0.000463000	0.011752000
73	1.748542000	-0.095192000	-0.008132000
1	-1.055372000	1.645927000	0.609814000
1	0.077878000	0.240664000	0.748335000

TS2

Total energy: -2620.7194 a. u.
Total energy including ZPVE: -2620.1450 a. u.
Total free energy including ZPVE: -2620.2133 a. u.

N_{img} = 565.1

6	-3.417645000	-1.646254000	0.530367000
6	-3.130936000	-0.899090000	1.707790000
6	-3.535985000	0.463593000	1.476699000
6	-4.104801000	0.541876000	0.165160000
6	-4.029814000	-0.759837000	-0.419994000
6	-4.693141000	-1.174409000	-1.703228000
1	-4.235618000	-2.068674000	-2.131800000
1	-5.751654000	-1.398655000	-1.511044000
1	-4.646044000	-0.387039000	-2.459562000
6	-4.818854000	1.730651000	-0.413643000
1	-4.330299000	2.669212000	-0.138236000
1	-4.855214000	1.687043000	-1.505689000
1	-5.853735000	1.766893000	-0.046263000
6	-3.557948000	1.567561000	2.499334000
1	-3.405905000	2.544361000	2.032152000
1	-4.526902000	1.587965000	3.017322000
1	-2.781106000	1.435924000	3.257807000
6	-2.703831000	-1.461302000	3.033459000
1	-2.081732000	-0.760102000	3.596972000
1	-3.589967000	-1.678961000	3.646038000
1	-2.141863000	-2.391235000	2.919949000
6	-3.228692000	-3.126497000	0.349825000
1	-2.976371000	-3.374322000	-0.684473000
1	-2.422817000	-3.506226000	0.983047000
1	-4.148269000	-3.667526000	0.613023000
6	3.089166000	-1.028950000	1.642143000
6	3.476182000	0.354602000	1.571257000
6	4.088842000	0.581989000	0.295475000
6	4.060881000	-0.646057000	-0.429469000

6	3.434318000	-1.639205000	0.397712000
6	3.314650000	-3.103303000	0.076983000
1	2.481108000	-3.564075000	0.613555000
1	3.152518000	-3.272609000	-0.990064000
1	4.232936000	-3.631681000	0.368767000
6	2.636593000	-1.755841000	2.876755000
1	1.973345000	-2.590654000	2.637885000
1	3.506825000	-2.162379000	3.410899000
1	2.105089000	-1.095362000	3.565840000
6	3.444660000	1.343923000	2.704369000
1	3.319877000	2.366503000	2.336967000
1	2.629384000	1.137366000	3.402387000
1	4.385989000	1.303461000	3.269471000
6	4.805410000	1.833150000	-0.123936000
1	4.827973000	1.942213000	-1.211685000
1	4.329141000	2.727920000	0.283459000
1	5.844934000	1.806518000	0.231172000
6	4.755954000	-0.898453000	-1.737929000
1	4.323103000	-1.744583000	-2.275236000
1	4.705834000	-0.029029000	-2.398341000
1	5.815976000	-1.122537000	-1.553632000
6	0.068044000	3.190591000	-0.228194000
1	0.068288000	4.197815000	-0.650791000
1	0.110073000	3.267236000	0.860908000
6	-0.007055000	-0.519069000	-3.032013000
1	-0.013178000	-0.968660000	-4.027803000
1	0.001239000	0.569834000	-3.123231000
5	0.095025000	0.300854000	1.818050000
1	-0.179934000	-1.250161000	2.185503000
1	0.987145000	1.113749000	1.339194000
1	0.204054000	0.508273000	3.001356000
5	-0.048623000	-1.185453000	0.964594000
1	0.301214000	-2.282483000	0.666711000
16	-1.571761000	-1.038223000	-2.222737000
16	1.545554000	-1.060843000	-2.224420000
16	-1.563930000	2.456152000	-0.687613000
16	1.641647000	2.410292000	-0.802672000
73	-1.687009000	0.084556000	-0.078613000
73	1.671366000	0.069414000	-0.068015000
1	0.000091000	0.564072000	-0.697413000
1	-0.955781000	0.957753000	1.521013000

TS3

Total energy: -2620.7245 a. u.
Total energy including ZPVE: -2620.1502 a. u.
Total free energy including ZPVE: -2620.2181 a. u.

N_{Img} = 367.1

6	-3.350803000	-1.234745000	1.239298000
6	-3.140388000	0.023486000	1.905429000
6	-3.627329000	1.057526000	1.048696000
6	-4.123690000	0.447591000	-0.150796000
6	-3.983663000	-0.970534000	-0.014246000
6	-4.592954000	-2.000193000	-0.922493000
1	-4.036437000	-2.940036000	-0.909898000
1	-5.620002000	-2.211702000	-0.593870000
1	-4.635748000	-1.657721000	-1.959001000
6	-4.856737000	1.156108000	-1.256498000
1	-4.452777000	2.156330000	-1.433131000
1	-4.797193000	0.604325000	-2.198424000
1	-5.919224000	1.264211000	-0.998278000
6	-3.741381000	2.512713000	1.400996000
1	-3.652246000	3.147695000	0.516755000
1	-4.717609000	2.708875000	1.866219000
1	-2.967706000	2.818770000	2.110001000
6	-2.713665000	0.194280000	3.336051000
1	-2.193162000	1.141609000	3.497276000
1	-3.593774000	0.181522000	3.993723000
1	-2.048176000	-0.610374000	3.659003000
6	-3.122143000	-2.598896000	1.830805000
1	-2.888257000	-3.335254000	1.056743000

1	-2.294247000	-2.596753000	2.544993000
1	-4.020517000	-2.942412000	2.361918000
6	3.138435000	0.024930000	1.918694000
6	3.561303000	1.091993000	1.054201000
6	4.103854000	0.510354000	-0.135488000
6	4.011919000	-0.911088000	-0.007964000
6	3.403961000	-1.210083000	1.254876000
6	3.220396000	-2.585906000	1.830035000
1	2.403806000	-2.611450000	2.555326000
1	2.992421000	-3.319598000	1.051924000
1	4.136390000	-2.912662000	2.341804000
6	2.720199000	0.188037000	3.351649000
1	2.126515000	-0.659234000	3.702562000
1	3.610388000	0.258732000	3.991928000
1	2.132775000	1.097340000	3.506270000
6	3.599603000	2.554182000	1.404968000
1	3.470970000	3.178292000	0.516584000
1	2.814109000	2.822293000	2.117242000
1	4.565059000	2.811693000	1.862361000
6	4.817084000	1.249027000	-1.232507000
1	4.785414000	0.698162000	-2.176961000
1	4.374193000	2.232377000	-1.410016000
1	5.873191000	1.395614000	-0.967137000
6	4.658964000	-1.908043000	-0.927316000
1	4.182907000	-2.889418000	-0.871035000
1	4.622793000	-1.584924000	-1.970430000
1	5.714389000	-2.030618000	-0.646552000
6	0.044966000	2.862526000	-1.421317000
1	-0.003804000	3.607048000	-2.219408000
1	0.158245000	3.381096000	-0.466383000
6	0.064464000	-1.784597000	-2.581956000
1	0.078243000	-2.648476000	-3.251103000
1	0.177193000	-0.869756000	-3.168452000
5	-0.121757000	1.041365000	1.407448000
1	0.351801000	-1.465633000	2.342237000
1	0.928266000	1.559076000	0.932579000
1	0.112196000	0.444725000	2.474290000
5	0.119754000	-0.673477000	1.468443000
1	-0.804911000	-1.347380000	0.860976000
16	-1.595680000	-1.761734000	-1.796000000
16	1.544520000	-1.948855000	-1.505284000
16	-1.612614000	2.058253000	-1.395321000
16	1.567403000	1.878375000	-1.705858000
73	-1.663387000	-0.005751000	-0.095097000
73	1.674786000	0.027795000	-0.110084000
1	-0.011913000	0.072751000	-0.891009000
1	-0.788087000	1.973546000	1.755848000

6

Total energy: -3028.4161 a. u.

Total energy including ZPVE: -3027.8144 a. u.

Total free energy including ZPVE: -3027.8904 a. u.

N_{Img} = 0.0

5	-0.083056000	0.206470000	1.493985000
1	0.903830000	0.927344000	1.047679000
5	0.012369000	-1.557676000	1.505789000
1	0.005164000	-1.981434000	2.622741000
6	-3.782521000	0.655389000	0.431483000
6	-3.308044000	0.219527000	1.711514000
6	-3.339762000	-1.211984000	1.717957000
6	-3.884938000	-1.661699000	0.471272000
6	-4.129935000	-0.512829000	-0.336892000
6	-4.808035000	-0.505581000	-1.678917000
1	-4.497564000	0.350511000	-2.281165000
1	-5.897048000	-0.448941000	-1.552527000
1	-4.585483000	-1.411098000	-2.248184000
6	-4.149350000	2.059873000	0.035240000
1	-3.678867000	2.803754000	0.675824000
1	-5.236629000	2.184318000	0.119145000

1	-3.877348000	2.284430000	-0.999614000
6	-3.102431000	1.052387000	2.943689000
1	-2.253323000	0.701309000	3.533822000
1	-3.997521000	0.983244000	3.576426000
1	-2.935515000	2.102725000	2.716234000
6	-3.081090000	-2.073984000	2.920970000
1	-3.985329000	-2.130028000	3.540727000
1	-2.278349000	-1.672111000	3.542220000
1	-2.807853000	-3.093631000	2.640206000
6	-4.308306000	-3.069317000	0.167562000
1	-5.303684000	-3.247577000	0.595959000
1	-3.621667000	-3.803647000	0.594017000
1	-4.361259000	-3.257207000	-0.904861000
6	3.880364000	0.437492000	0.260149000
6	4.064279000	-0.867197000	-0.317280000
6	3.693922000	-1.840147000	0.665304000
6	3.243860000	-1.137196000	1.832144000
6	3.387806000	0.264012000	1.593902000
6	3.222561000	1.309564000	2.660021000
1	3.374627000	2.317039000	2.278262000
1	3.961376000	1.135563000	3.452056000
1	2.231638000	1.270286000	3.121796000
6	4.378502000	1.713928000	-0.358394000
1	5.470165000	1.761254000	-0.256650000
1	3.960090000	2.597616000	0.120825000
1	4.147610000	1.769302000	-1.425029000
6	4.714967000	-1.149109000	-1.642367000
1	4.496047000	-0.364280000	-2.369735000
1	4.375139000	-2.098156000	-2.062499000
1	5.804811000	-1.204114000	-1.524366000
6	3.919336000	-3.321617000	0.580496000
1	4.911027000	-3.563280000	0.984998000
1	3.869144000	-3.677474000	-0.448088000
1	3.179296000	-3.878207000	1.160756000
6	2.911232000	-1.752074000	3.160540000
1	2.486160000	-2.751990000	3.053411000
1	2.194438000	-1.143236000	3.714775000
1	3.821392000	-1.839113000	3.768134000
6	-0.027278000	-3.405046000	-1.389935000
1	-0.040963000	-4.215387000	-2.120758000
1	-0.011056000	-3.833410000	-0.383724000
6	-0.016539000	0.574783000	-2.872394000
1	-0.022655000	1.202358000	-3.765855000
1	-0.051115000	-0.484338000	-3.140051000
6	-1.093465000	3.214250000	1.070723000
6	-0.136287000	3.801962000	-1.449394000
6	1.488591000	3.390980000	0.667701000
42	0.102261000	2.269136000	-0.180192000
8	-1.730245000	3.861793000	1.805568000
8	-0.268226000	4.684458000	-2.187203000
8	2.252414000	4.140440000	1.135716000
16	-1.618459000	-2.506046000	-1.600687000
16	-1.512394000	1.043254000	-1.884833000
16	1.530192000	0.976043000	-1.950529000
16	1.543509000	-2.501671000	-1.669935000
73	-1.681033000	-0.586182000	-0.026380000
73	1.640068000	-0.635065000	0.000839000
1	-0.180379000	0.600370000	2.616832000
1	-0.978897000	-2.108420000	0.931055000
1	-0.017477000	-0.798111000	-0.784939000
1	0.935150000	-2.179881000	0.886338000

7

Total energy: -3028.70760 a. u.

Total energy including ZPVE: -3028.1059 a. u.

Total free energy including ZPVE: -3028.1821 a. u.

N_{Img} = 0.0

5	0.097415000	0.079869000	1.500373000
1	-0.926947000	0.796814000	1.082173000
5	0.011050000	-1.689585000	1.500714000

1	0.018873000	-2.121453000	2.614312000
6	-3.878978000	0.269027000	0.278314000
6	-3.386730000	0.085658000	1.610738000
6	-3.224247000	-1.316071000	1.831715000
6	-3.663403000	-2.010866000	0.655835000
6	-4.045942000	-1.030672000	-0.315288000
6	-4.695327000	-1.304757000	-1.642711000
1	-4.489664000	-0.507552000	-2.360545000
1	-5.784066000	-1.376675000	-1.523447000
1	-4.342786000	-2.243312000	-2.075656000
6	-4.389517000	1.547258000	-0.326889000
1	-3.980800000	2.430251000	0.162093000
1	-5.481755000	1.582701000	-0.226348000
1	-4.158615000	1.616231000	-1.392842000
6	-3.235364000	1.120237000	2.689810000
1	-2.239263000	1.099625000	3.141884000
1	-3.961051000	0.917239000	3.486989000
1	-3.415527000	2.128958000	2.323768000
6	-2.884094000	-1.942215000	3.152933000
1	-3.791661000	-2.039630000	3.762841000
1	-2.168123000	-1.335529000	3.710716000
1	-2.454768000	-2.938983000	3.034225000
6	-3.871492000	-3.493866000	0.554062000
1	-4.858303000	-3.752478000	0.960047000
1	-3.122074000	-4.048542000	1.124122000
1	-3.821362000	-3.836548000	-0.478960000
6	3.781864000	0.546452000	0.455957000
6	4.133494000	-0.603135000	-0.338591000
6	3.903885000	-1.770259000	0.447899000
6	3.361188000	-1.350863000	1.705877000
6	3.317756000	0.080263000	1.728927000
6	3.107961000	0.885218000	2.978964000
1	2.929545000	1.938401000	2.774381000
1	4.005502000	0.810945000	3.607579000
1	2.264078000	0.513202000	3.563865000
6	4.137565000	1.961394000	0.087404000
1	5.224501000	2.090752000	0.168464000
1	3.665659000	2.688391000	0.745967000
1	3.860095000	2.206302000	-0.941486000
6	4.805029000	-0.564275000	-1.683427000
1	4.489092000	0.303648000	-2.265677000
1	4.581877000	-1.458034000	-2.270710000
1	5.894509000	-0.506885000	-1.561708000
6	4.341441000	-3.166977000	0.115623000
1	5.337712000	-3.343707000	0.542657000
1	4.398578000	-3.332124000	-0.960283000
1	3.661204000	-3.916856000	0.524737000
6	3.115930000	-2.239742000	2.891908000
1	2.852867000	-3.256338000	2.590990000
1	2.311058000	-1.859422000	3.523895000
1	4.022736000	-2.298664000	3.507610000
6	0.060198000	-3.516967000	-1.423538000
1	0.080416000	-4.320235000	-2.162073000
1	0.045300000	-3.955233000	-0.421579000
6	0.021523000	0.456657000	-2.874214000
1	0.025108000	1.086654000	-3.766039000
1	0.062644000	-0.602246000	-3.141691000
6	-1.502969000	3.194094000	0.712766000
6	0.120968000	3.645430000	-1.390630000
6	1.071453000	3.026931000	1.119610000
74	-0.111866000	2.090469000	-0.144926000
8	-2.279055000	3.928473000	1.190514000
8	0.245906000	4.543029000	-2.113079000
8	1.708019000	3.663650000	1.867978000
16	-1.515692000	-2.620065000	-1.698132000
16	-1.519222000	0.853982000	-1.938185000
16	1.502365000	0.938836000	-1.869059000
16	1.644720000	-2.605364000	-1.624778000
73	-1.626558000	-0.776308000	0.004459000
73	1.688018000	-0.702703000	-0.017445000
1	0.185108000	0.448598000	2.632381000

1	-0.911103000	-2.315002000	0.876025000
1	0.031211000	-0.940287000	-0.785071000
1	1.002542000	-2.238476000	0.920299000

TS4

Total energy: -3028.3995 a. u.
Total energy including ZPVE: -3027.8001 a. u.
Total free energy including ZPVE: -3027.8760 a. u.

N_{img} = 353.2

5	0.000001000	0.181811000	1.495191000
1	-0.000004000	1.472070000	1.521221000
5	0.000000000	-1.564002000	1.462339000
1	0.000000000	-2.081464000	2.537297000
6	-3.848730000	0.512843000	0.328865000
6	-3.337240000	0.259805000	1.644103000
6	-3.254662000	-1.155856000	1.813806000
6	-3.756134000	-1.785767000	0.627382000
6	-4.099663000	-0.757264000	-0.302379000
6	-4.775234000	-0.956218000	-1.630752000
1	-4.545938000	-0.142845000	-2.322781000
1	-5.864921000	-0.990669000	-1.502918000
1	-4.464669000	-1.891400000	-2.102123000
6	-4.321292000	1.832306000	-0.218280000
1	-3.883492000	2.679676000	0.307218000
1	-5.411267000	1.899248000	-0.109472000
1	-4.093751000	1.942609000	-1.281758000
6	-3.147306000	1.241052000	2.765863000
1	-2.172594000	1.126801000	3.247798000
1	-3.915211000	1.068956000	3.530976000
1	-3.237837000	2.272554000	2.432718000
6	-2.917782000	-1.846006000	3.103749000
1	-3.807976000	-1.893585000	3.744513000
1	-2.139301000	-1.312371000	3.652835000
1	-2.571100000	-2.868584000	2.940995000
6	-4.041561000	-3.252323000	0.479064000
1	-5.024608000	-3.478931000	0.912579000
1	-3.299887000	-3.865567000	0.996538000
1	-4.047715000	-3.559028000	-0.566638000
6	3.848730000	0.512844000	0.328866000
6	4.099663000	-0.757261000	-0.302380000
6	3.756136000	-1.785765000	0.627381000
6	3.254662000	-1.155857000	1.813806000
6	3.337240000	0.259805000	1.644103000
6	3.147306000	1.241051000	2.765865000
1	3.237833000	2.272553000	2.432721000
1	3.915215000	1.068957000	3.530975000
1	2.172597000	1.126795000	3.247804000
6	4.321290000	1.832309000	-0.218278000
1	5.411265000	1.899251000	-0.109474000
1	3.883491000	2.679677000	0.307225000
1	4.093745000	1.942614000	-1.281755000
6	4.775235000	-0.956214000	-1.630753000
1	4.545939000	-0.142840000	-2.322781000
1	4.464669000	-1.891395000	-2.102125000
1	5.864922000	-0.990665000	-1.502919000
6	4.041564000	-3.252321000	0.479062000
1	5.024611000	-3.478928000	0.912579000
1	4.047722000	-3.559025000	-0.566641000
1	3.299890000	-3.865566000	0.996534000
6	2.917782000	-1.846007000	3.103748000
1	2.571106000	-2.868587000	2.940993000
1	2.139296000	-1.312376000	3.652831000
1	3.807974000	-1.893580000	3.744515000
6	0.000000000	-3.393911000	-1.447974000
1	0.000000000	-4.185487000	-2.199216000
1	0.000000000	-3.847698000	-0.452955000
6	0.000000000	0.623982000	-2.854054000
1	0.000001000	1.267065000	-3.736426000
1	0.000001000	-0.430875000	-3.140612000
6	-1.360229000	3.344604000	0.826255000

6	0.000001000	3.803266000	-1.451385000
6	1.360224000	3.344603000	0.826259000
42	-0.000001000	2.268245000	-0.129490000
8	-2.104057000	4.073554000	1.350239000
8	0.000004000	4.706603000	-2.171714000
8	2.104051000	4.073552000	1.350246000
16	-1.584574000	-2.488377000	-1.672871000
16	-1.519007000	1.040265000	-1.887183000
16	1.519007000	1.040266000	-1.887182000
16	1.584574000	-2.488376000	-1.672871000
73	-1.663734000	-0.613929000	-0.029017000
73	1.663734000	-0.613929000	-0.029018000
1	0.000002000	0.247262000	2.704012000
1	-0.960036000	-2.135082000	0.830465000
1	0.000000000	-0.802467000	-0.807847000
1	0.960035000	-2.135082000	0.830465000

TS5

Total energy: -3028.69314 a. u.

Total energy including ZPVE: -3028.09404 a. u.

Total free energy including ZPVE: -3028.1700 a. u.

N_{Img} = 269.9

5	0.000003000	0.067155000	1.470634000
1	0.000004000	1.401137000	1.566632000
5	-0.000006000	-1.693246000	1.459502000
1	-0.000008000	-2.190303000	2.543605000
6	-3.846201000	0.378275000	0.349062000
6	-3.335791000	0.108855000	1.661076000
6	-3.249500000	-1.308764000	1.811067000
6	-3.749392000	-1.923953000	0.616087000
6	-4.093522000	-0.883853000	-0.299817000
6	-4.769558000	-1.064876000	-1.630585000
1	-4.544580000	-0.239719000	-2.310078000
1	-5.859069000	-1.105365000	-1.502634000
1	-4.455879000	-1.991249000	-2.117100000
6	-4.324964000	1.702140000	-0.182660000
1	-3.914752000	2.544553000	0.371894000
1	-5.418311000	1.749918000	-0.101446000
1	-4.073123000	1.839624000	-1.237711000
6	-3.148880000	1.072859000	2.798294000
1	-2.171337000	0.957471000	3.274446000
1	-3.911777000	0.881607000	3.563796000
1	-3.248349000	2.109364000	2.483563000
6	-2.914581000	-2.016385000	3.092110000
1	-3.806811000	-2.076475000	3.729025000
1	-2.139582000	-1.488786000	3.651923000
1	-2.563980000	-3.035351000	2.915400000
6	-4.034008000	-3.388778000	0.449689000
1	-5.013080000	-3.622815000	0.888347000
1	-3.286968000	-4.008131000	0.951978000
1	-4.048340000	-3.680808000	-0.600049000
6	3.846211000	0.378246000	0.349045000
6	4.093514000	-0.883895000	-0.299814000
6	3.749369000	-1.923976000	0.616105000
6	3.249486000	-1.308762000	1.811076000
6	3.335800000	0.108853000	1.661064000
6	3.148899000	1.072877000	2.798267000
1	3.248485000	2.109372000	2.483537000
1	3.911726000	0.881558000	3.563822000
1	2.171312000	0.957584000	3.274355000
6	4.324998000	1.702095000	-0.182696000
1	5.418346000	1.749855000	-0.101476000
1	3.914798000	2.544524000	0.371842000
1	4.073167000	1.839565000	-1.237750000
6	4.769551000	-1.064943000	-1.630578000
1	4.544564000	-0.239804000	-2.310091000
1	4.455880000	-1.991330000	-2.117072000
1	5.859062000	-1.105418000	-1.502627000
6	4.033960000	-3.388807000	0.449727000
1	5.013040000	-3.622851000	0.888365000

1	4.048261000	-3.680857000	-0.600006000
1	3.286924000	-4.008140000	0.952047000
6	2.914559000	-2.016358000	3.092131000
1	2.563924000	-3.035315000	2.915436000
1	2.139584000	-1.488728000	3.651947000
1	3.806795000	-2.076469000	3.729035000
6	-0.000013000	-3.512841000	-1.474552000
1	-0.000015000	-4.301420000	-2.228958000
1	-0.000016000	-3.970272000	-0.480962000
6	-0.000003000	0.492870000	-2.862818000
1	-0.000003000	1.133521000	-3.746945000
1	-0.000008000	-0.563474000	-3.143408000
6	-1.370506000	3.153078000	0.844736000
6	0.000004000	3.658867000	-1.387641000
6	1.370546000	3.153064000	0.844714000
74	0.000007000	2.085927000	-0.103516000
8	-2.123920000	3.875002000	1.369034000
8	0.000003000	4.587712000	-2.076011000
8	2.123979000	3.874981000	1.368994000
16	-1.582856000	-2.604410000	-1.694801000
16	-1.508470000	0.918539000	-1.882458000
16	1.508471000	0.918529000	-1.882465000
16	1.582837000	-2.604423000	-1.694798000
73	-1.657326000	-0.743728000	-0.024212000
73	1.657320000	-0.743735000	-0.024213000
1	0.000010000	0.148951000	2.678814000
1	-0.959714000	-2.272204000	0.831361000
1	-0.000004000	-0.953128000	-0.812045000
1	0.959704000	-2.272206000	0.831364000