UCLA
UCLA Previously Published Works

Title
Bimetallic Cleavage of Aromatic C–H Bonds by Rare-Earth-Metal Complexes

Permalink
https://escholarship.org/uc/item/1703p12x

Journal
Journal of the American Chemical Society, 136(50)

ISSN
0002-7863

Authors
Huang, Wenliang
Dulong, Florian
Khan, Saeed I
et al.

Publication Date
2014-12-17

DOI
10.1021/ja510761j

Peer reviewed

eScholarship.org Powered by the California Digital Library
University of California

Supporting Information for

Bimetallic Cleavage of Aromatic C-H Bonds by Rare Earth Metal Complexes

Wenliang Huang[1†], Florian Dulong[2], Saeed I. Khan[1], Thibault Cantat[2*], Paula L. Diaconescu[1*]

Affiliations:

[1]Department of Chemistry & Biochemistry, University of California, Los Angeles, California 90095

[2]CEA, IRAMIS, NIMBE, CNRS UMR 3299 91191 Gif-sur-Yvette, France

*Correspondence to: thibault.cantat@cea.fr (TC) and pld@chem.ucla.edu (PLD)

†Current address: Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139, United States

Table of Contents

1. Experimental details S2

2. DFT calculations S9

3. NMR spectra S15

4. X-ray crystallography data S46

5. Optimized coordinates S55

6. References S87

1. Experimental Details

General considerations: All experiments were performed under a dry nitrogen atmosphere using standard Schlenk techniques or an MBraun nitrogen glove box unless

otherwise specified. Solvents, including toluene, hexanes, diethyl ether (Et_2O), tetrahydrofuran (THF), and dichloromethane, were purified using a two-column solid-state purification system and transferred to the glove box without exposure to air. *n*-Pentane was distilled over calcium hydride under dinitrogen atmosphere. Methanol was distilled over calcium oxide under a dinitrogen atmosphere. All solvents were stored on activated molecular sieves for at least a day prior to use. NMR solvents, benzene-d_6 and toluene-d_8, were obtained from Cambridge Isotope Laboratories, degassed three times, and stored over activated molecular sieves for one week prior to use. Rare earth metal oxides (scandium, yttrium, lanthanum, and lutetium) were purchased from Stanford Materials Corporation, 4 Meadowpoint, Aliso Viejo, CA 92656, and used as received. Trimethylsilyl iodide (Me_3SiI) was purchased from Alfa Aesar, directly brought into glove box, and stored over activated molecular sieves in a -35 °C freezer prior to use. KO^{t}Bu was purchased from Strem Chemicals Inc. and directly brought into glove box without exposure to air or moisture. 1,3,5-trideuterobenzene was purchased from Sigma-Aldrich in a sealed ampule and used as received. Potassium graphite (KC_8) was synthesized by Professor Richard B. Kaner's group (UCLA). Other solid chemicals were purified by crystallization; liquid chemicals were degassed three times and stored over activated molecular sieves for one week prior to use. $(NN^{fc})MI(THF)_2$, **1** (NN^{fc} = 1,1'-$(NSi^tBuMe_2)_2fc$; M = Sc, **1a**; M = Y, **1b**; M = Lu, **1c**), alternative label NN^{TBS} may also be used in the supporting information) were synthesized according to published protocols.[1] Organic lithium reagents were synthesized by lithium-halogen exchange reaction from the corresponding bromo or iodo-organic substrates and *n*-butyl lithium (*n*BuLi). Nuclear magnetic resonance (NMR) spectra were recorded on Bruker AV300, Bruker DRX500, Bruker AV500 (work supported by the NSF grants CHE-1048804), or Bruker AV600 spectrometers at 25 °C in C_6D_6 or C_7D_8 unless otherwise specified. Chemical shifts are reported with respect to internal solvent (C_6D_6 at 7.16 ppm or C_7D_8 at 2.08 ppm). CHN analyses were performed in house on a CE-440 Elemental Analyzer manufactured by EXETER ANALYTICAL, INC.

C-H activation of benzene by 1/KC_8 and product characterization: Standard procedure (using **1a** as an example): 0.3000 g of **1a** (0.395 mmol) was dissolved in 6.0 mL of benzene. 0.0840 g KC_8 (0.621 mmol) was added to the solution of **1a**. The mixture was allowed to stir at 25 °C. Aliquots were taken at 1.50 h, 3.75 h, and 4.50 h to monitor the reaction by ^{1}H NMR spectroscopy (Figures S1-S3). The reaction went to completion after stirring at 25 °C for 4.5 h. The ^{1}H NMR spectra of the aliquots showed a 1:1 scandium molar ratio formation of $[(NN^{fc})Sc(THF)_x]_2(\mu\text{-}H)_2$ (**2a**, x is solvent dependent and could be either 0 or 1) and $(NN^{fc})ScPh(THF)$ (**3a**). After completion, the mixture was filtered through Celite to remove graphite and KI. The volatiles were removed under reduced pressure. 5 mL of hexanes was added to the resulting oily film to make a slurry and the volatiles removed again under reduced pressure. The same procedure was repeated using *n*-pentane. The resulting orange solid was extracted by *n*-pentane and then toluene. The *n*-pentane extraction (0.1450 g after removing volatiles) contained mainly **3a** and a small amount of **2a**, while the toluene extraction (0.0540 g) contained almost exclusively **2a**. Pure **3a** could not be obtained from this reaction due to its high solubility in common organic solvents. Therefore, an independent synthesis of **3a** from **1a** and phenyl lithium was employed to obtain the pure compound, which is described below. **2a** could be obtained analytically pure with the molecular formula of $[(NN^{fc})Sc]_2(\mu\text{-}H)_2$ after recrystallization of the toluene extraction in toluene layered with *n*-pentane. Single crystals of **2a** were grown from a concentrated hexanes solution. The molecular formula was determined to be $[(NN^{fc})Sc(THF)](\mu\text{-}H)_2[Sc(NN^{fc})]$; however, crystals of **2a** grown from toluene layered with

hexanes had no coordinating THF molecule based on the corresponding ^{1}H NMR spectrum. Yield: 0.0400 g, 20.7% (maximum 50%, same for the other **2** and **3**). Characterization of **2a**: ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 5.73 (br s, 1H, *hydride*), 4.30, 3.96, 3.91, and 3.77 (s, 2H each, all belong to C*H* on Cp), 1.10 (s, 18H, C(C*H*$_3$)$_3$), and 0.50 and 0.35 (s, 6H each, SiC*H*$_3$). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 107.5 (*C*N), 71.7, 70.0, 69.2, and 66.6 (*C*H on Cp), 27.6 (C(*C*H$_3$)$_3$), 21.4 (*C*(CH$_3$)$_3$), and -1.2 and -2.1 (Si*C*H$_3$). Anal. (%): Calcd. for $C_{44}H_{78}N_4Fe_2Sc_2Si_4$, M_w = 977.082: C, 54.09; H, 8.05; N, 5.73. Found: C, 52.68; H, 7.64; N, 5.13.

M = Y: Scale: 0.3000 g of **1b** (0.374 mmol), 0.0910 g of KC_8 (0.673 mmol, 1.8 equiv), and 5.0 mL of benzene. The reaction went to completion after stirring at 25 °C for 3 h as indicated by the disappearance of **1b**. The ^{1}H NMR of the crude reaction mixture (after filtering through Celite and removing volatiles) showed the formation of **2b** and **3b** in a 1:1 yttrium molar ratio. The crude product was then extracted by *n*-pentane and toluene. **3b** precipitated out from the *n*-pentane extraction, yield: 0.0580 g, 20.6%. However, the contamination of **3b** with **2b** could not be resolved due to their relative solubility. Single crystals of **3b** were obtained from an independent synthesis. **2b** precipitated out from the toluene extraction, yield: 0.0282 g, 12.5%. Single crystals of **2b** were grown from a toluene solution layered with hexanes. Characterization of **2b**: ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 7.71 (t, 1H, *hydride*), 4.14 (OC*H*$_2$CH$_2$), 4.05, and 3.74 (br s, 4H each, both belong to C*H* on Cp), 1.47 (OCH$_2$C*H*$_2$), 1.07 (s, 18H, C(C*H*$_3$)$_3$), and 0.32 (s, 12H, SiC*H*$_3$). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 107.0 (*C*N), 71.8 and 67.1 (*C*H on Cp), 67.1 (O*C*H$_2$CH$_2$), 28.1 (C(*C*H$_3$)$_3$), 25.5 (OCH$_2$*C*H$_2$), 20.5 (*C*(CH$_3$)$_3$), and -1.2 (Si*C*H$_3$). Anal. (%): Calcd. for $C_{52}H_{94}N_4Fe_2O_2Si_4Y_2$, M_w = 1209.196: C, 51.65; H, 7.84; N, 4.63. Found: C, 51.78; H, 7.73; N, 4.67.

M = Lu: Scale: 0.3000 g of **1c** (0.338 mmol), 0.0820 g KC_8 (0.607 mmol, 1.8 equiv), and 5.0 mL of benzene. The reaction went to completion after stirring at 25 °C for 3 h as indicated by the disappearance of **1c**. The ^{1}H NMR of the crude reaction mixture (after filtering through Celite and removing volatiles) showed the formation of **2c** and **3c** in a 1:1 lutetium molar ratio. The crude product was then extracted by *n*-pentane and toluene. **3c** precipitated out from the *n*-pentane extraction, yield: 0.0630 g, 22.2%. However, the contamination of **3c** with **2c** could not be resolved due to their relative solubility. Single crystals of **3c** were obtained from an independent synthesis. **2c** precipitated out from the toluene extraction, yield: 0.0444 g, 19.0%. Single crystals of **2c** were grown from a toluene solution layered with hexanes. Characterization of **2b**: ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 12.49 (s, 1H, *hydride*), 4.16 (OC*H*$_2$CH$_2$), 4.01, and 3.82 (br s, 4H each, both belong to C*H* on Cp), 1.47 (OCH$_2$C*H*$_2$), 1.07 (s, 18H, C(C*H*$_3$)$_3$), and 0.32 (s, 12H, SiC*H*$_3$). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 106.3 (*C*N), 72.1, 68.7, and 65.9 (*C*H on Cp), 67.4 (O*C*H$_2$CH$_2$), 28.2 (C(*C*H$_3$)$_3$), 25.6 (OCH$_2$*C*H$_2$), 20.6 (*C*(CH$_3$)$_3$), and -1.2 (Si*C*H$_3$). Anal. (%): Calcd. for $C_{52}H_{94}N_4Fe_2$ $Lu_2O_2Si_4$, M_w = 1381.318: C, 45.22; H, 6.86; N, 4.06. Found: C, 45.03; H, 6.87; N, 4.02.

Synthesis of phenyl lithium (PhLi): 0.5000 g of iodobenzene (2.451 mmol) was dissolved in Et_2O and placed in an ice bath. 0.94 mL of 2.6 M *n*BuLi (1 equiv) was added dropwise. The mixture was allowed to stir at 0 °C for 30 min. Volatiles were removed under reduced pressure. The remaining solid was first washed with hexanes and then extracted with Et_2O. The volatiles were removed again and the remaining solid was dried under reduced pressure for two hours. Due to the low solubility of PhLi in C_6D_6, the empirical molecular formula was determined from the reaction with **1c** (see below) to be $C_6H_5Li(OEt_2)_{0.31}$ (M_w = 106.9 g/mol). Yield: 0.2266 g, 86.5%.

Synthesis of *o*-tolylLi: Scale: 0.5670 g of 2-iodotoluene (2.600 mmol) and 1.00 mL of 2.6 M *n*BuLi (1 equiv). A similar procedure to that for obtaining PhLi was followed. The empirical molecular formula was determined to be $C_7H_7Li(OEt_2)_{0.115}$ (Mw = 106.6 g/mol). Yield: 0.2641 g, 95.3%.

Synthesis of *m*-tolylLi: Scale: 0.5670 g of 3-iodotoluene (2.600 mmol) and 1.00 mL of 2.6 M *n*BuLi (1 equiv). A similar procedure to that for obtaining PhLi was followed. The empirical molecular formula was determined to be $C_7H_7Li(OEt_2)_{0.285}$ (Mw = 119.2 g/mol). Yield: 0.2389 g, 77.1%.

Synthesis of *p*-tolylLi: Scale: 0.2541 g of 4-iodotoluene (1.165 mmol) and 0.45 mL of 2.6 M *n*BuLi (1 equiv). A similar procedure to that for obtaining PhLi was followed. The empirical molecular formula was determined to be $C_7H_7Li(OEt_2)_{0.616}$ (Mw = 143.7 g/mol). Yield: 0.1675 g, 76.5%.

Synthesis of α-naphthylLi: Scale: 0.5000 g of α-bromonaphthalene (2.415 mmol) and 0.97 mL of 2.5 M *n*BuLi (1 equiv). A similar procedure to that for obtaining PhLi was followed. The empirical molecular formula was determined to be $C_{10}H_7Li(OEt_2)_{0.185}$ (Mw = 147.84 g/mol). Yield: 0.334.5 g, 93.7%.

Synthesis of β-naphthylLi: Scale: 0.5000 g of β-bromonaphthalene (2.415 mmol) and 0.97 mL of 2.5 M *n*BuLi (1 equiv). A similar procedure to that for obtaining PhLi was followed. The empirical molecular formula was determined to be $C_{10}H_7Li(OEt_2)_{0.688}$ (Mw = 185.14 g/mol). Yield: 0.4130 g, 92.4%.

Synthesis of (NN^{fc})MAr(THF), MAr (M = Sc, Y, and Lu; Ar = Ph, tolyl, or naphthalenyl). Synthesis of 3a: 0.1000 g of **1a** (0.1318 mmol) was dissolved in 4 mL of Et_2O. 0.0141 g of PhLi (0.132 mmol) was dissolved in 1 mL of Et_2O and added dropwise to **1a** solution at 25 °C. The reaction mixture was allowed to stir at 25 °C for one hour. The volatiles were removed under reduced pressure. The remaining yellow solid was extracted into hexanes and then the volatiles were removed under reduced pressure. The same procedure was repeated with *n*-pentane to drive the equilibrium (NN^{fc})Sc(μ-Ph)$_2$Li + (NN^{fc})ScI ↔ 2 (NN^{fc})ScPh + LiI to the left based on different solubility of the compounds involved (a similar equilibrium exists for the other metal phenyl, metal tolyl, and metal naphthalenyl complexes and was overcome by a similar work-up protocol). The remaining solid was dissolved in a minimum amount of *n*-pentane and stored in a -35 °C freezer. An orange solid precipitated out after several days. Yield: 0.0726 g, 86.5%. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 8.15 (m, 2H, *ortho*-C*H*), 7.44 (t, 2H, *meta*-C*H*), 7.32 (t, 1H, *para*-C*H*), 3.99 (br s, 4H) and 3.53 (br s, 4H), both belong to C*H* on Cp, 3.86 (m, 4H, OCH_2CH$_2$), 1.29 (m, 4H, OCH$_2$CH_2), 1.02 (s, 18H, C(CH_3)$_3$), and 0.22 (s, 12H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 182.4 (*ipso*-*C*), 137.0 (*ortho*-*C*H), 126.9 and 126.8 (*meta*- and *para*-*C*H), 105.3 (*C*N), 71.5 and 68.7 (*C*H on Cp), 68.3 (O*C*H$_2$CH$_2$), 27.8 (C(*C*H$_3$)$_3$), 25.2 (OCH$_2$*C*H$_2$), 20.4 (*C*(CH$_3$)$_3$) and -2.4 (Si*C*H$_3$). Anal. (%): Calcd. for $C_{32}H_{51}N_2OFeScSi_2$, M_w = 636.746: C, 60.36; H, 8.07; N, 4.40. Found: C, 58.51; H, 7.86; N, 3.95.

Synthesis of 3b: Scale: 0.1000 g of **1b** (0.1246 mmol) and 0.0133 g (0.124 mmol) of PhLi. A similar procedure to that for obtaining **3a** was followed. However, due to the previously mentioned equilibrium between metal phenyl and metal iodide, **3b** synthesized by this method co-crystallized with 15% **1b** with a formula of (NN^{fc})YPh(THF)$_2$. Single-crystal X-ray diffraction of **3b** confirmed the co-crystallization. Yield: 0.0437 g, 46.6%. ^{1}H NMR (with 15% **1b**) (500 MHz, C_6D_6, 25 °C) δ, ppm: 8.12 (d, 2H, *ortho*-C*H*), 7.48 (t, 2H, *meta*-C*H*), 7.36 (m, 1H, *para*-C*H*), 4.07 (t, 4H) and 3.22 (t, 4H), both belong to C*H* on Cp, 3.94 (br s, 8H, OCH_2CH$_2$), 1.33 (br s, 8H, OCH$_2$CH_2), 1.04 (s, 18H, C(CH_3)$_3$), and 0.30 (s, 12H, SiCH_3). ^{13}C

NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 186.1 (d, *ipso*-*C*, J_{YC} = 59 Hz), 138.4 (*ortho*-*C*H), 126.3 and 125.7 (*meta*- and *para*-*C*H), 104.4 (*C*N), 71.6 (O*C*H_2CH_2), 66.8 and 66.2 (*C*H on Cp), 28.0 (C(*C*H_3)$_3$), 25.0 (OCH_2*C*H_2), 20.7 (*C*(CH_3)$_3$) and -1.4 (Si*C*H_3). Anal. (%): Calcd. for $C_{36}H_{59}N_2O_2FeYSi_2$ with 15% of **1b**, M_w = 752.803: C, 55.45; H, 7.72; N, 3.68. Found: C, 55.67; H, 7.85; N, 3.87.

Synthesis of 3c: Scale: 0.1000 g of **1c** (0.1125 mmol) and 0.0120 g (0.112 mmol) of PhLi. A similar procedure to that for obtaining **1c** was followed. However, due to the previously mentioned equilibrium between metal phenyl and metal iodide, **3c** synthesized by this method co-crystallized with 15% **1c** with a formula of (NN^{fc})LuPh(THF)$_2$. Single X-ray diffraction of **3c** confirmed the co-crystallization.Yield: 0.0401 g, 42.5%. ^{1}H NMR (with 15% **1c**) (500 MHz, C_6D_6, 25 °C) δ, ppm: 8.08 (d, 2H, *ortho*-C*H*), 7.52 (t, 2H, *meta*-C*H*), 7.35 (t, 1H, *para*-C*H*), 4.03 (t, 4H) and 3.30 (t, 4H), both belong to C*H* on Cp, 4.00 (br s, 8H, OCH_2CH_2), 1.35 (br s, 8H, OCH$_2$CH_2), 1.03 (s, 18H, C(CH_3)$_3$), and 0.27 (s, 12H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 193.6 (*ipso*-*C*), 139.6 (*ortho*-*C*H), 126.6 and 126.1 (*meta*- and *para*-*C*H), 104.3 (*C*N), 71.9 (O*C*H_2CH_2), 67.2 and 66.4 (*C*H on Cp), 28.2 (C(*C*H_3)$_3$), 25.1 (OCH_2*C*H_2), 21.0 (*C*(CH_3)$_3$) and -1.3 (Si*C*H_3). Anal. (%): Calcd. for $C_{36}H_{59}N_2O_2FeLuSi_2$ with 15% **1c**, M_w = 838.864: C, 49.81; H, 6.96; N, 3.31. Found: C, 49.94; H, 7.01; N, 3.50.

Synthesis of (NN^{fc})Sc(*o*-tolyl)(THF) (4o): Scale: 0.1000 g **1a** (0.1318 mmol) and 0.0141 g (0.132 mmol) *o*-tolylLi. A similar procedure to that for obtaining **3a** was followed. Yield: 0.0556 g, 64.8%. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 7.81 (m, 1H, *ortho*-C*H*), 7.30 (m, 2H, *meta*-C*H*), 7.23 (m, 1H, *para*-C*H*), 4.12, 4.04, 3.60, and 2.97 (br s, 2H each, all belong to C*H* on Cp), 4.04 (br s, 4H, OCH_2CH_2), 2.65 (s, 3H, benzylic CH_3), 1.29 (m, 4H, OCH$_2$CH_2), 0.92 (s, 18H, C(CH_3)$_3$), and 0.12 and 0.06 (br s, 6H each, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 184.3 (*ipso*-*C*), 143.0, 135.1, 127.5, 127.1, and 123.8 (aromatic-*C*H), 102.2 (*C*N), 73.1 (O*C*H_2CH_2), 69.1, 68.2, 67.7, and 67.2 (*C*H on Cp), 27.8 (C(*C*H_3)$_3$), 26.3 (benzylic *C*H_3), 25.0 (OCH$_2$*C*H_2), 20.3 (*C*(CH_3)$_3$) and -2.4 (Si*C*H_3). Anal. (%): Calcd. for $C_{33}H_{53}N_2OFeScSi_2$, M_w = 650.733: C, 60.91; H, 8.21; N, 4.30. Found: C, 60.52; H, 8.17; N, 3.85.

Synthesis of (NN^{fc})Sc(*m*-tolyl)(THF) (4m): Scale: 0.1000 g of **1a** (0.1318 mmol) and 0.0157 g (0.132 mmol) *m*-tolylLi. A similar procedure to that for obtaining **3a** was followed. Yield: 0.0676 g, 78.8%. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 8.04 (s, 1H, *ortho*-C*H*), 7.98 (d, 1H, *ortho*-CH), 7.39 (t, 1H, *meta*-C*H*), 7.17 (1H, *para*-C*H*), 4.01, 3.99, and 3.56 (br, 8H total, all belong to C*H* on Cp), 3.90 (m, 4H, OCH_2CH_2), 2.46 (s, 3H, benzylic CH_3), 1.29 (m, 4H, OCH$_2$CH_2), 1.03 (s, 18H, C(CH_3)$_3$), and 0.24 (s, 12H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 182.2 (*ipso*-*C*), 138.0, 134.9, 134.0, 127.6, and 126.7 (aromatic-*C*H), 103.0 (*C*N), 68.4 (O*C*H_2CH_2), 71.7, 69.2, and 68.7 (*C*H on Cp), 27.8 (C(*C*H_3)$_3$), 22.1 (benzylic *C*H_3), 25.2 (OCH$_2$*C*H_2), 20.4 (*C*(CH_3)$_3$) and -2.3 (Si*C*H_3). Anal. (%): Calcd. for $C_{33}H_{53}N_2OFeScSi_2$, M_w = 650.773: C, 60.91; H, 8.21; N, 4.30. Found: C, 60.88; H, 8.23; N, 4.17.

Synthesis of (NN^{fc})Sc(*p*-tolyl)(THF) (4p): Scale: 0.1000 g **1a** (0.1318 mmol) and 0.0189 g (0.131 mmol) *p*-tolylLi. A similar procedure to that for obtaining **3a** was followed. Yield: 0.0601 g, 70.0%. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 8.09 (d, 2H, *ortho*-C*H*), 7.27 (t, 2H, *meta*-CH), 3.99 and 3.55 (br s, 4H each, both belong to C*H* on Cp), 3.91 (m, 4H, OCH_2CH_2), 2.31 (s, 3H, benzylic CH_3), 1.30 (m, 4H, OCH$_2$CH_2), 1.03 (s, 18H, C(CH_3)$_3$), and 0.24 (s, 12H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 178.6 (*ipso*-*C*), 137.2, 135.6, and 127.5 (aromatic-*C*H), 105.4 (*C*N), 68.3 (O*C*H_2CH_2), 71.6, and 68.3 (*C*H on Cp), 27.8 (C(*C*H_3)$_3$), 21.9 (benzylic *C*H_3), 25.2 (OCH$_2$*C*H_2), 20.4 (*C*(CH_3)$_3$) and -2.4 (Si*C*H_3). Anal. (%): Calcd. for $C_{33}H_{53}N_2OFeScSi_2$, M_w = 650.773: C, 60.91; H, 8.21; N, 4.30. Found: C, 60.53; H, 8.26; N, 4.07.

Synthesis of (NN^{fc})Lu(α-naphthyl)(THF) (6c-α): Scale: 0.2000 g of **1c** (0.225 mmol) and 0.0333 g *α*-naphthylLi (0.225 mmol). A similar procedure to that for obtaining **3a** was followed. However, the aforementioned equilibrium among the ate complex, **6c-α**, (NN^{fc})Lu(α-naphthyl)$_2$Li, **1c**, and LiI could not be overcome even after three extraction/trituration procedures using either hexanes or *n*-pentane. Although neither analytical nor NMR pure samples could be obtained, single crystals of **6c-α** with the formula of (NN^{fc})Lu(α-naphthyl)(THF)$_2$ were grown from a hexanes solution of the mixture and characterized by X-ray crystallography. In addition, the proton chemical shifts for **6c-α** and (NN^{fc})Lu(α-naphthyl)$_2$Li could be assigned based on integration (Figure S51); a relatively pure sample of (NN^{fc})Lu(α-naphthyl)$_2$Li could be obtained by fractional crystallization to confirm the assignment of its ^{1}H NMR spectrum (Figure S52). However, due to the dynamic equilibrium in solution of **6c-α**, **1c**, LiI, and ate complex (NN^{fc})Lu(α-naphthyl)$_2$Li, the proton chemical shifts of **6c-α** could not be definitively determined.

Synthesis of (NN^{fc})Lu(β-naphthyl)(THF) (6c-β): Scale: 0.2000 g of **1c** (0.225 mmol) and 0.0417 g β-naphthylLi (0.225 mmol). A similar procedure to that for obtaining **3a** was followed. Same as **6c-α**, **6c-β** could not be isolated from the equilibrium mixture. Crystallization from hexanes resulted in the growth of single crystals of the ate complex, (NN^{fc})Lu(β-naphthyl)$_2$Li(THF), which was characterized by X-ray crystallography. Though no analytically or spectroscopically pure samples could be obtained, the proton chemical shifts for **6c-β** and ate complex (NN^{fc})Lu(β-naphthyl)$_2$Li could be assigned based on integration (Figure S53). However, due to the dynamic equilibrium, the proton chemical shifts of **6c-β** could not be definitively determined.

Synthesis of (NN^{fc})ScBn(THF) (7, Bn = CH_2Ph): 0.2500 g of $ScBr_3(THF)_{2.5}$ (0.538 mmol) was dispersed in 50 mL of THF in a 100 mL round bottom flask and chilled with a dry ice/acetone bath for 15 min. KBn (2.4 equiv, 0.1680 g, 1.29 mmol) was dissolved in 5 mL of THF and chilled with a dry ice/acetone bath for 5 min before it was added dropwise to the $ScBr_3(THF)_{2.5}$ dispersion. The red color of KBn immediately disappeared upon addition and the mixture turned off-white. The mixture was allowed to stir for 1 h at 0 °C with an ice bath. The solution was filtered through Celite. The filtration was transferred to a 100 mL round bottom flask and chilled with an ice bath for 15 min. 0.8 equiv of $H_2(NN^{fc})$ (0.1910 g, 0.430 mmol) was dissolved in 5 mL of THF and chilled with the ice bath before it was added to the filtrate of *in situ* formed $ScBn_3(THF)_3$. The mixture was then allowed to stir at 0 °C for 1 h. The volatiles were removed under reduced pressure to yield an orange solid which was extracted into ca. 5 mL of toluene. 10 mL of hexanes was layered on top of the toluene solution. After storing at -35 °C for 1 d, orange crystals formed. Yield: 0.2100 g, 75.0%. ^{1}H NMR (500 MHz, C_6D_6, 25 °C) δ, ppm: 7.33 (m, 2H, *ortho*-C*H*), 7.23 (m, 2H, *meta*-CH), 6.83 (m, 1H, *para*-C*H*), 3.97, and 3.23 (br, 8H total, C*H* on Cp), 3.74 (m, 4H, OCH_2CH$_2$), 2.52 (s, 2H, ScCH_2), 1.31 (m, 4H, OCH$_2$CH_2), 1.02 (s, 18H, C(CH_3)$_3$), and 0.25 (s, 12H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6, 25 °C) δ, ppm: 150.1 (*ipso*-*C*), 129.0, 126.2, and 119.5 (aromatic-*C*H), 103.8 (*C*N), 70.9 (O*C*H$_2$CH$_2$), 69.4, and 68.1 (*C*H on Cp), 55.4 (Sc*C*H$_2$), 27.8 (C(*C*H$_3$)$_3$), 25.2 (OCH$_2$*C*H$_2$), 20.4 (*C*(CH$_3$)$_3$) and -2.4 (Si*C*H$_3$). Anal. (%): Calcd. for $C_{33}H_{53}N_2OFeScSi_2$, M_w = 650.773: C, 60.91; H, 8.21; N, 4.30. Found: C, 60.14; H, 8.17; N, 4.46.

C-H activation of toluene by 1a/KC_8 system and product identification: 0.1500 g of **1a** (0.198 mmol) was dissolved in 3.0 mL of toluene. 0.0440 g of KC_8 (0.325 mmol) was added to the solution of **1a**. The mixture was allowed to stir at 25 °C. Aliquots were taken at 1.00, 2.33,

3.00, 4.00, and 5.00 h to monitor the reaction by ^{1}H NMR spectroscopy. The reaction went to completion after 5 h. The ^{1}H NMR spectra of the aliquots showed the formation of two scandium tolyl isomers accompanied by the formation of **2a**. By comparison with independently synthesized **4o**, **4m**, and **4p**, the two isomers were identified as **4o** and **4m** with an average ratio of 1 : 4.5(1) throughout the duration of the reaction (ratio of **4o** *vs*. **4m** based on integration of benzylic CH_3 peaks (**4o** at 2.66 ppm and **4m** at 2.46 ppm): 1.00 h, 1.00 : 4.72; 2.33 h, 1.00 : 4.72; 3.00 h, 1.00 : 4.62; 4.00 h, 1.00 : 4.62; 5.00 h, 1.00 : 4.79, Figures S34-S38). No peaks corresponding to **4o** or the benzylic C-H activation product, **8**, appeared in any ^{1}H NMR spectra.

Determination of *inter*molecular kinetic isotope effect: 0.1500 g of **1a** (0.198 mmol) was dissolved in 1.50 mL of benzene and 1.50 mL of benzene-d_6. 0.0455 g of KC_8 (0.329 mmol) was added to the solution of **1a**. The mixture was allowed to stir at 25 °C. Aliquots were taken at 1.00, 2.08, and 3.00 h to monitor the reaction by ^{1}H NMR spectroscopy. The reaction went to completion after 3 h. Integration of the *o*-C*H* of the phenyl group against SiCH_3 of **3a** (for both -H_5 and -D_5) showed an average ratio of 2.28(4) throughout the reaction time (1.00 h, 2.34 : 24.00; 2.00 h, 2.22 : 24.00; 3.08 h, 2.29 : 24.00, Figures S39-S41). This consistency confirmed that the experimental observed k_H/k_D is a genuine kinetic isotope effect. The *inter*molecular KIE was calculated based on the following equation: (2.28*11.6/2.0)/[24.00-(2.28*11.6/2.0)] = 1.2(1). The factor 11.6/2.0 is derived from the relative integration of the ^{1}H NMR spectrum of pure **ScPh** (Figure S4).

Determination of *intra*molecular kinetic isotope effect: 0.0320 g of **1a** (0.042 mmol) was dissolved in 0.500 g of 1,3,5-$C_6H_3D_3$ (ca. 0.6 mL) and the solution was transferred into a J-Young tube equipped with an air-tight Teflon cap (see Figure S42 for ^{1}H NMR spectrum prior to KC_8 addition). 0.0200 g of KC_8 (0.148 mmol) was added to the solution. The reaction was monitored by ^{1}H NMR spectroscopy. After 3.0 h at 25 °C with occasional shaking, the reaction went to completion as indicated by the disappearance of proton signals for **1a**. The J-Young tube was then brought back to the glove-box and the solution was filtered through Celite to remove KI, graphite and excessive KC_8. The volatiles were removed under reduced pressure. The crude product (ca. 0.030 g) was dissolved in 0.6 mL of C_6D_6 and examined by ^{1}H NMR spectroscopy. Integration of the *o*-CH peak at 8.16 ppm (only present in the C-D activation product) against the *m*-CH peak at 7.45 ppm (only present in the C-H activation product) showed a 1.00 : 4.51 ratio (Figure S43). In addition, the fact that both peaks were singlets is consistent with the formation of 3,5-dideuterophenyl and 2,6-dideuterophenyl species from C-H and C-D bond activation, respectively.

C-H activation of benzene by 1a/KC_8 system under various atmospheres (H_2, argon, and vacuum): Standard procedure (using H_2 as an example): 0.0508 g of **1a** (0.067 mmol) was dissolved in 1.20 mL of benzene in a 20 mL Schlenk tube placed in a cold well chilled with an external dry ice / isopropanol bath. After the solution was frozen, 0.0180 g of KC_8 (0.133 mmol, 2 equiv) was added on top of the frozen solution. The Schlenk tube was then evacuated under reduced pressure to remove N_2, after which was taken out of the glove-box and connected to a Schlenk line with an H_2 gas flow. The tube was evacuated again on the line and then filled with H_2 for 1 min. During these operations, the tube was kept in a dry ice / isopropanol bath and the solution was always frozen. After filling with H_2, the tube was sealed, the solution thawed and stirred at 25 °C for 30 min before it was brought back into the glove-box for work-up. The reaction mixture was filtered through Celite and the volatiles were removed under reduced pressure. The ^{1}H NMR spectrum of the crude product showed a 74% conversion to **2a** and **3a** in a 1:1 scandium molar ratio with 26% **1a** left unreacted (Figure S44).

Reaction under argon: Scale: 0.0534 g of **1a** (0.070 mmol) and 0.0280 g (0.207 mmol) KC_8 in 1.20 mL of benzene. The procedure was similar to the reaction under H_2 except argon was used instead of H_2. After 1.0 h stirring at 25 °C, the reaction mixture was worked up in a similar way. The ^{1}H NMR spectrum of the crude product showed a 73% conversion to **2a** and **3a** in 1:1 scandium molar ratio with 27% **1a** left (Figure S45).

Reaction under vacuum: Scale: 0.0507 g of **1a** (0.067 mmol) and 0.0360 g (0.266 mol) KC_8 in 1.20 mL of benzene. The procedure was similar to the reaction under H_2 except there was no gas filling after evacuating N_2. After 2.0 h of stirring at 25 °C, the reaction mixture was worked up in a similar way. The ^{1}H NMR spectrum of the crude product showed a complete conversion of **1a** and the formation of **2a** and **3a** (Figure S46).

C-H activation of benzene by 1a/Na system: 0.0506 g of **1a** (0.0667 mmol) was dissolved in 1.5 mL of C_6H_6. 0.0100 g sodium (0.435 mmol, 6.5 equiv) was pressed on the bottom and the sides of a 20 mL scintillation vial to achieve a sodium mirror. The solution of **1a** was added to the sodium mirror and the mixture was allowed to stir at 25 °C for 3 h. Small, shiny metallic particles were observed while stirring. The reaction mixture was filtered through Celite and the volatiles were removed under reduced pressure. The ^{1}H NMR spectrum of the crude product showed the formation of **2a** and **3a** with a 1 : 1 scandium molar ratio (Figure S47).

Attempt of C-H activation of benzene by 1a/Na(Hg) system: 0.8960 g of mercury was weighed in a 20 mL scintillation vial. 0.0101 g of sodium was added to mercury and was immediately absorbed. 0.0500 g of **1a** was dissolved in 3.0 mL of C_6H_6 and added to sodium amalgam (1.1% sodium weight). The reaction mixture was allowed to stir at 25 °C for 2 h before taking an aliquot. The ^{1}H NMR spectrum of the aliquot showed no formation of **2a** and **3a** and intact **1a** (Figure S48). An additional 0.0133 g of sodium was then added and resulted in a solid alloy (2.5% sodium weight). The reaction mixture was allowed to stir at 25 °C for two more hours before taking another aliquot. The ^{1}H NMR spectrum of the second aliquot still showed no formation of **2a** and **3a** and intact **1a** (Figure S49).

C-H activation of [(NN^{fc})M(THF)$_x$]$_2$(μ-C$_{10}$H$_8$), 5 (M = Sc, x = 0, 6a; M = Lu, x = 1, 6c). C-H activation from 5a: 0.0120 g of **5a** was dissolved in 0.6 mL of C_6D_6 and transferred into a J-Young tube equipped with an air-tight Teflon cap (Figure S54). The J-Young tube was kept in an 85 °C bath and the reaction was monitored by ^{1}H NMR spectroscopy. After two days of heating at 85 °C, small peaks in the aromatic region corresponding to a C-H activated naphthalene fragment appeared slightly above the baseline together with peaks indicating significant free naphthalene formation (Figure S55). Longer heating did not result in the accumulation of this product but rather decomposition to free naphthalene and other unidentified species (Figure S56). Since the products, scandium hydride and scandium aryl complexes, were not stable in solution at temperatures higher than 50 °C, it is likely that though C-H activation of the naphthalene fragment occurred, the products decomposed faster than the C-H activation reaction occurred.

C-H activation from 5c: 0.0060 g of **5c** was dissolved in 0.6 mL of C_6D_6 and transferred into a J-Young tube equipped with an air-tight Teflon cap (Figure S57). The J-Young tube was kept in a 50 °C bath and the reaction was monitored by ^{1}H NMR spectroscopy. After heating at 50 °C for two days, the reaction went to completion (Figure S59). The ratio of **6c** to **2c** (per lutetium) was close to 1 : 1 after 8.5 h at 50 °C (Figure S58) but changed after prolonged heating (Figure S59) due to the fast decomposition of **2c**. The C-H activation of **5c** could also be carried out at a higher temperature in a shorter time to reach completion (Figures S60-S62). **2c** was identified by the characteristic hydride peak at 12.5 ppm (Figure S17), while **6c** could not be

definitely determined to be either the α-naphthyl or β-naphthyl species because of the equilibrium in the **1c**/naphthyl lithium system. However, it is clear that only one isomer is formed in the reaction.

2. DFT Calculations

Computational Details. The B3LYP hybrid density functional[2-3] was employed to optimize the equilibrium molecular structure of the model complexes. In the model structures, the Si^{t}BuMe$_2$ substituents on the nitrogen atoms were replaced by SiMe$_3$ groups. The ECP28MWB small core relativistic effective core potential developed by the Stuttgart-Dresden group was used for lutetium, it incorporates scalar relativistic effect.[4-5] The RECP was used in combination with its ECP28MWB_SEG optimized basis set, which treats the 4f electrons are as part of the valence shell. ECP10MDF RECP[6] and associated basis set were used for scandium. 6-31G* basis sets were used for carbon, hydrogen, nitrogen, phosphorus and sulfur. The LANL2DZ effective core potential[7] and valence double zeta basis set was used for iron. Harmonic vibrational analyses were performed to confirm to characterize the structures as minima or transition states. All calculations were carried out using the Gaussian09[8] suite of codes and NBO _ENREF_9[9] analysis was employed for charge determination.

Full citation for reference 8 in SI:

M. J. T. Frisch, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H.P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. (Gaussian Inc., Wallingford, CT, 2009).

Scheme S1. Free energy surface for the activation of benzene mediated by scandium(III).

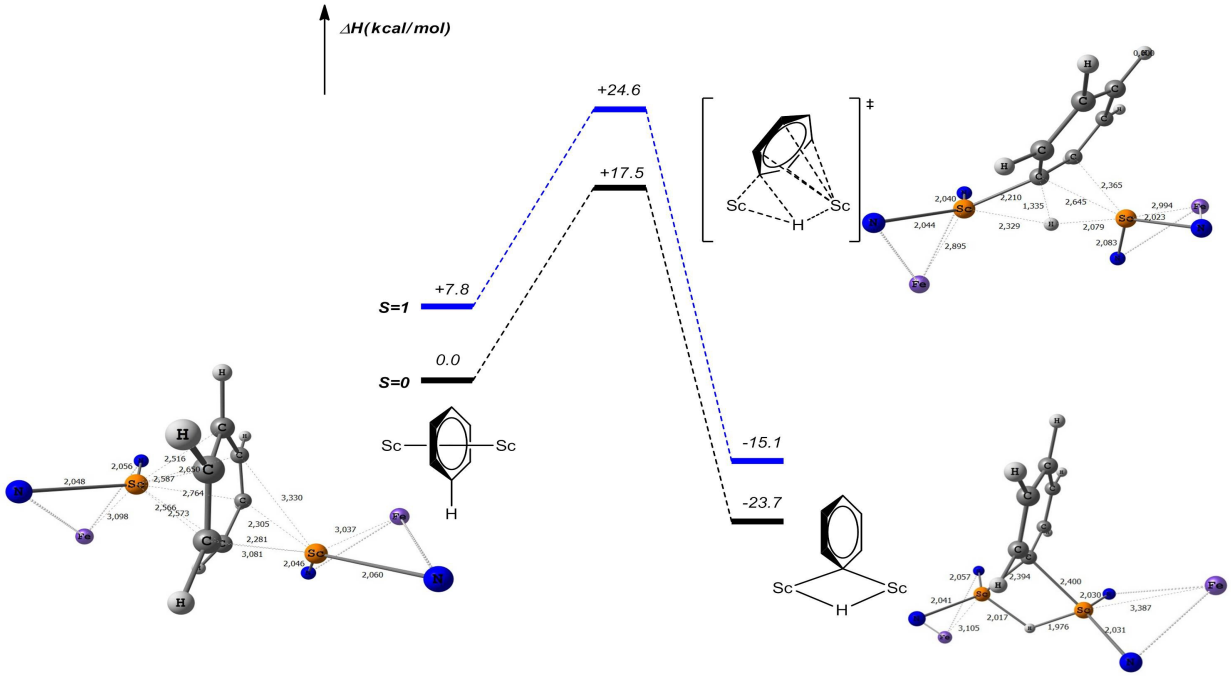
Scheme S2. Free energy surface for the activation of naphthalene mediated by scandium(III).

Scheme S3. Free energy surface for the activation of naphthalene mediated by lutetium(III).

Comments on Scheme S2 and S3:

The isomerization of **5c** enables the coordination of the lutetium ions on the same ring at a low energy cost of 0.3 kcal/mol. This step precedes the C-H activation step, which proceeds with a low barrier of 15.0 kcal/mol. In contrast, the C-H activation reaction from **5a** requires an activation energy of 22.9 kcal/mol, including a 5.9 kcal/mol cost to promote the isomerization of **5a**.

Scheme S4. Free energy surface for toluene activation by **1a** and KC_8. Activation barriers and the free energies of dinuclear products for three aromatic C-H bonds (*ortho*, **VI**; *meta*, **IV**; *para*, **V**) and the benzylic C-H bond (**VII**) are listed. The activation barrier was calculated to be 14.5, 14.6, 17.6, and 50.4 kcal/mol for *ortho*, *meta*, *para*, and benzylic C-H activation, respectively.



(The optimized structures are given for the lowest energy (singlet) surface)

Scheme S5. Comparison of the free energy surfaces for benzene activation by **1a** and KC_8 for a singlet (black) and triplet (blue) reaction coordinate; the optimized structures are given for the lowest energy (singlet) surface.

3. NMR spectra

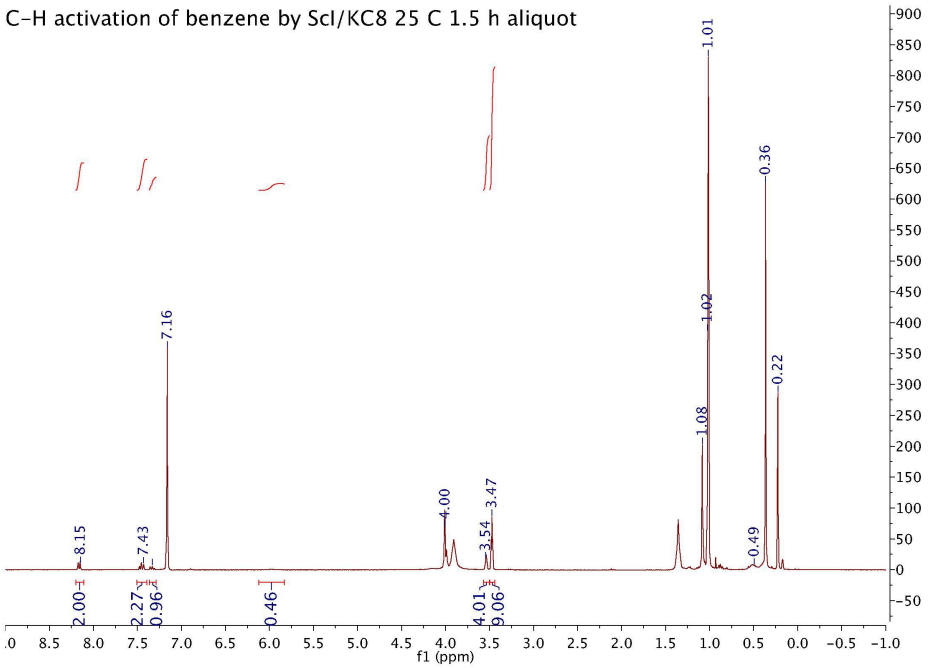


Figure S1. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation by **1a**/KC_8 at 25 °C after 1.5 h (aliquot). Note: peaks at 8.15, 7.43, and 3.54 ppm belong to **3a**; peak at 3.47 ppm belongs to **2a** (similar assignment for Figure S2 and S3).

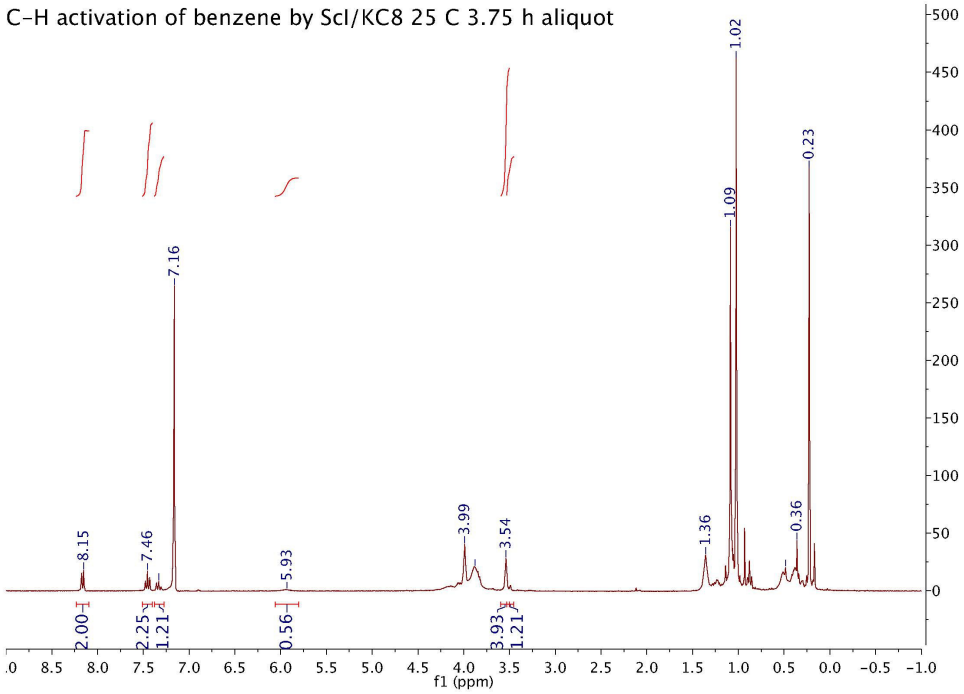


Figure S2. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation by **1a**/KC_8 at 25 °C after 3.75 h (aliquot).

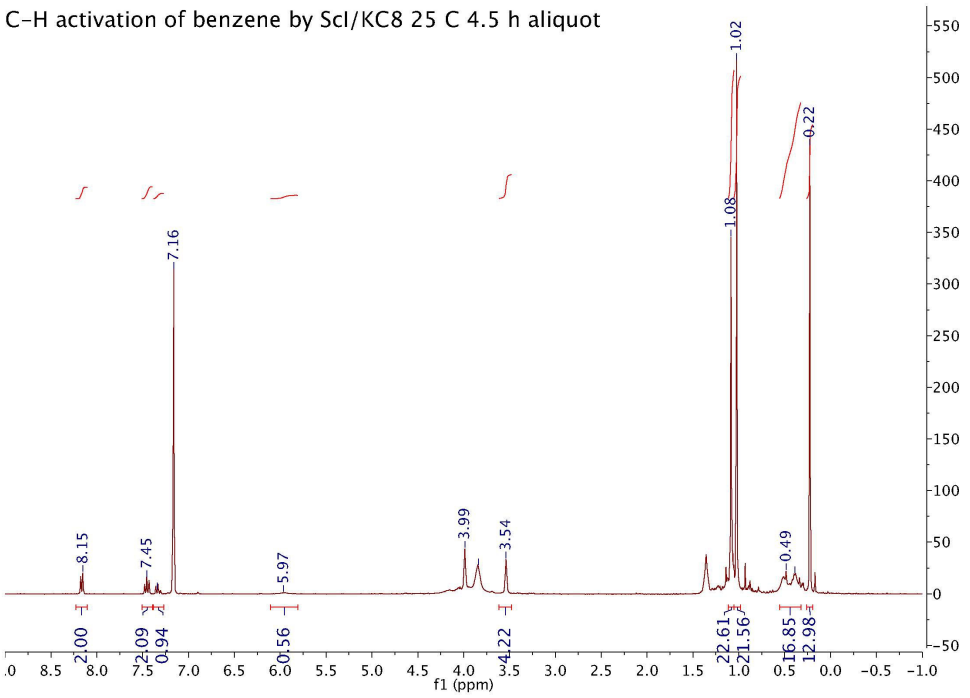


Figure S3. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation by **1a**/KC_8 at 25 °C after 4.5 h (aliquot). Note: peaks at 8.15, 7.45, 3.54, 1.02, and 0.22 ppm belong to **3a**; peaks at 5.95, 1.08, and 0.49 ppm belong to **2a**. The integration indicated that **3a** and **2a** were generated in an approximately 1:1 scandium molar ratio.

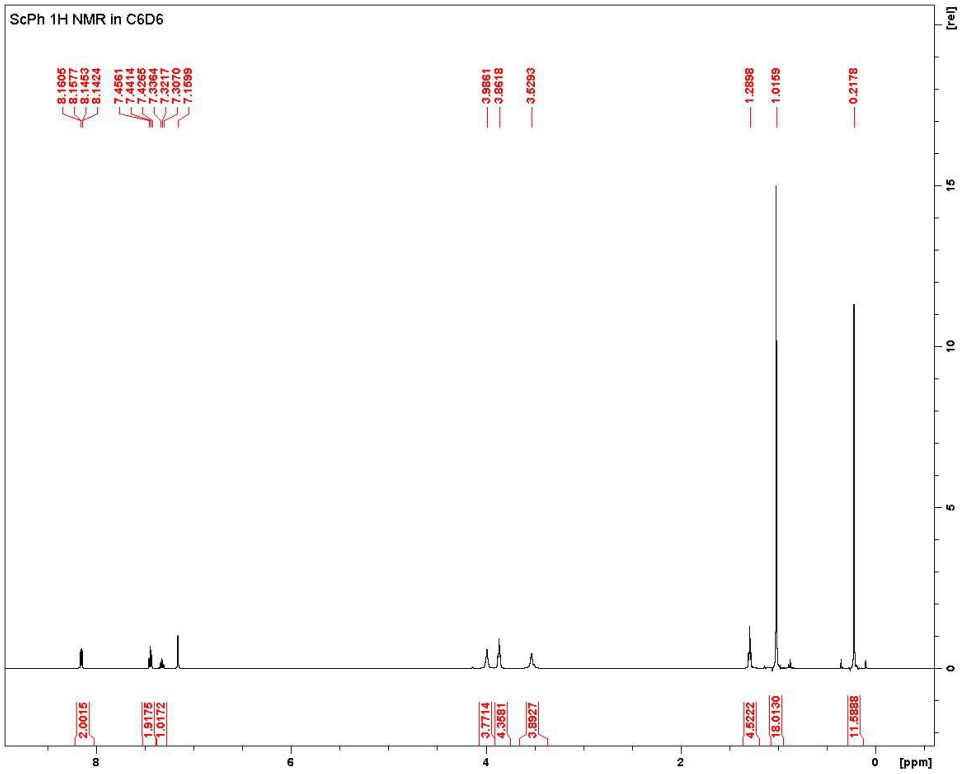


Figure S4. ^{1}H NMR spectrum of **3a** (C_6D_6, 500 MHz, 298 K).

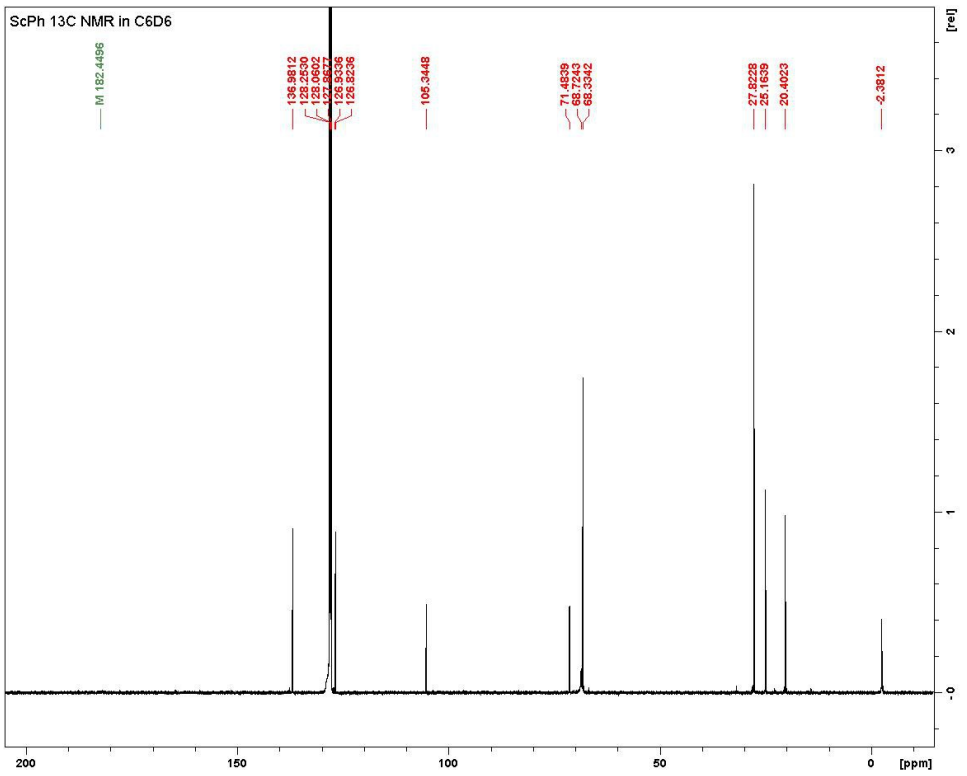


Figure S5. ^{13}C NMR spectrum of **3a** (C_6D_6, 126 MHz, 298 K).

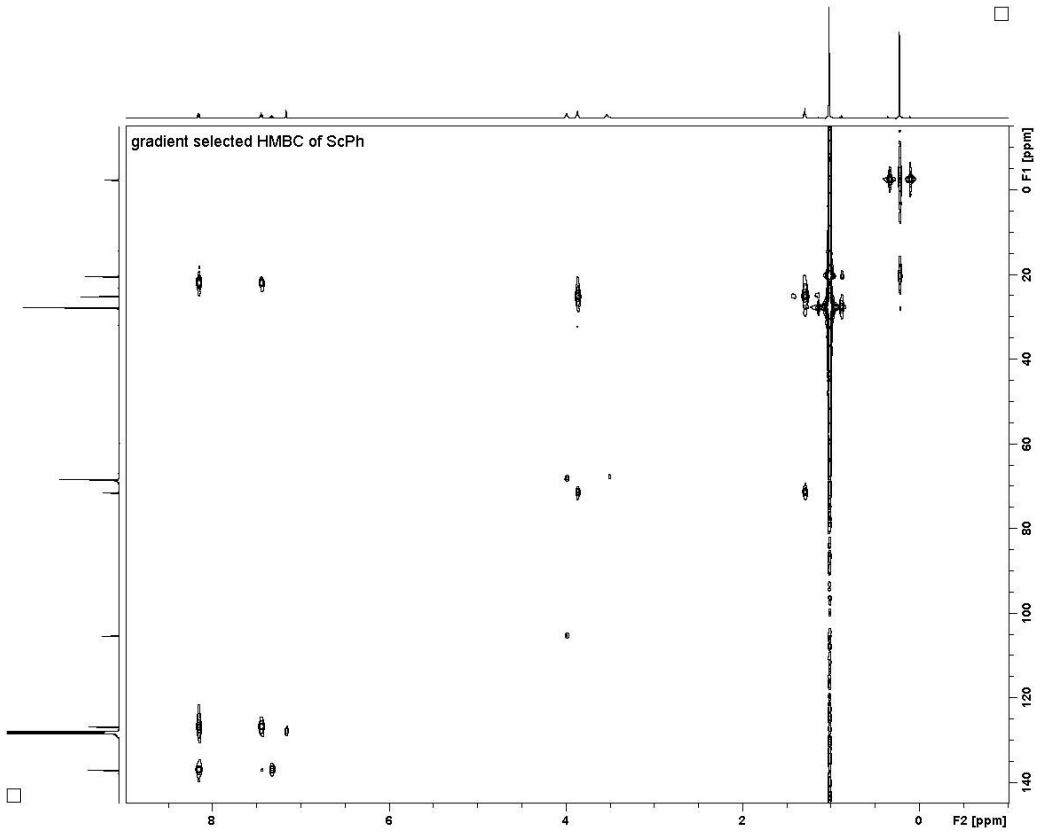


Figure S6. HMBC spectrum of **3a** (C_6D_6, 500 MHz, 228 K).

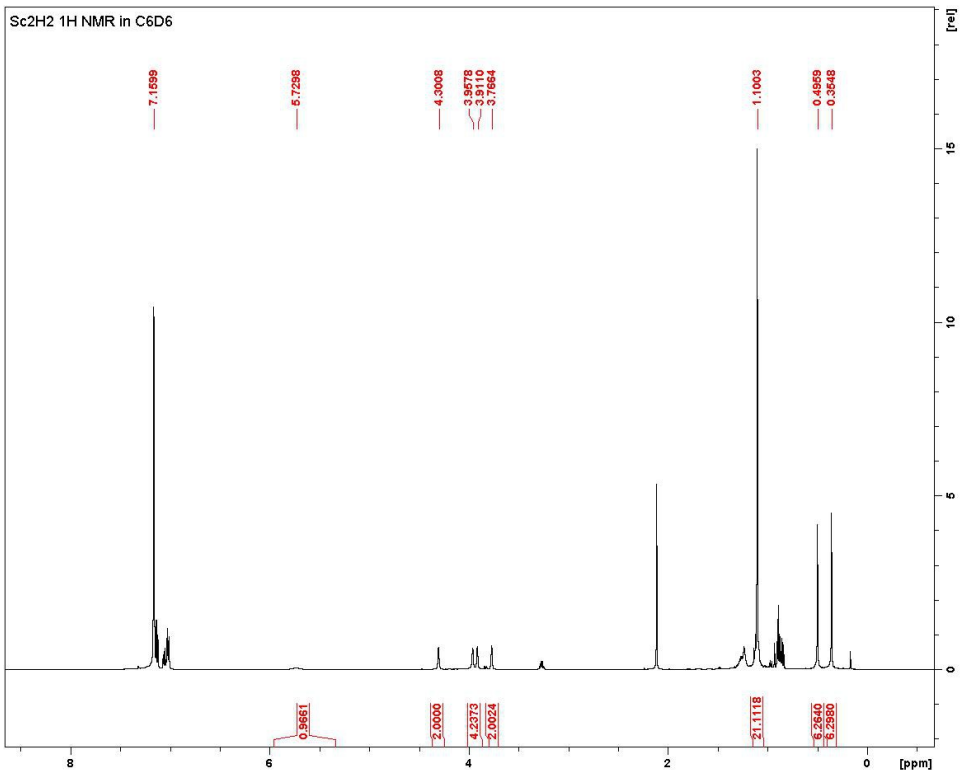


Figure S7. ^{1}H NMR spectrum of **2a** (C_6D_6, 500 MHz, 298 K).

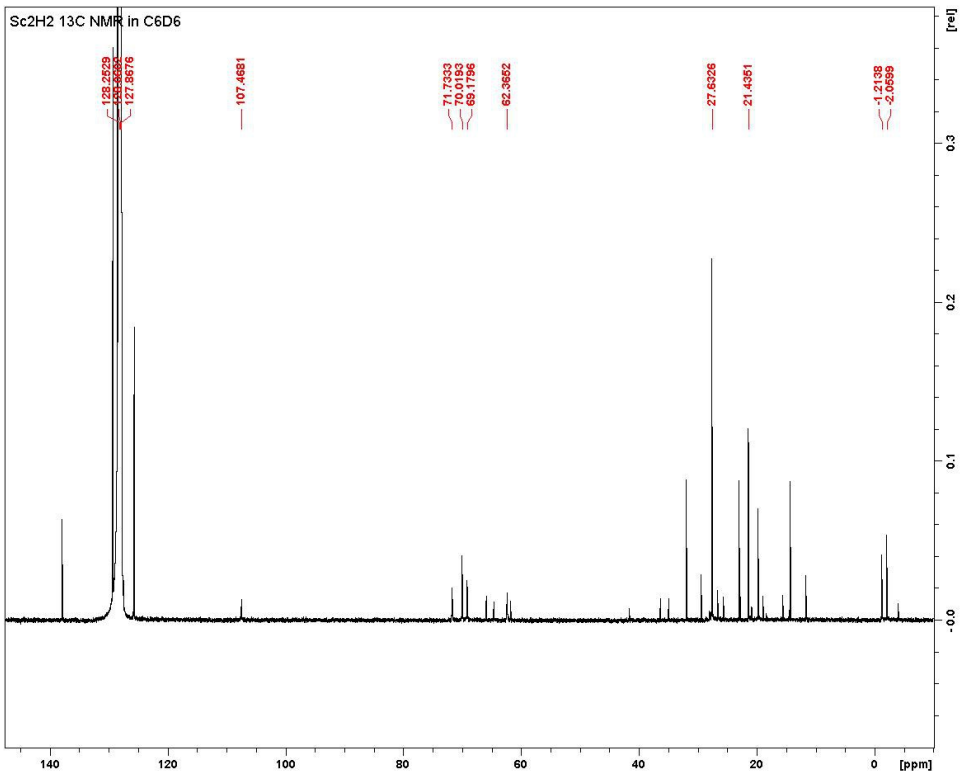


Figure S8. ^{13}C NMR spectrum of **2a** (C_6D_6, 126 MHz, 298 K).

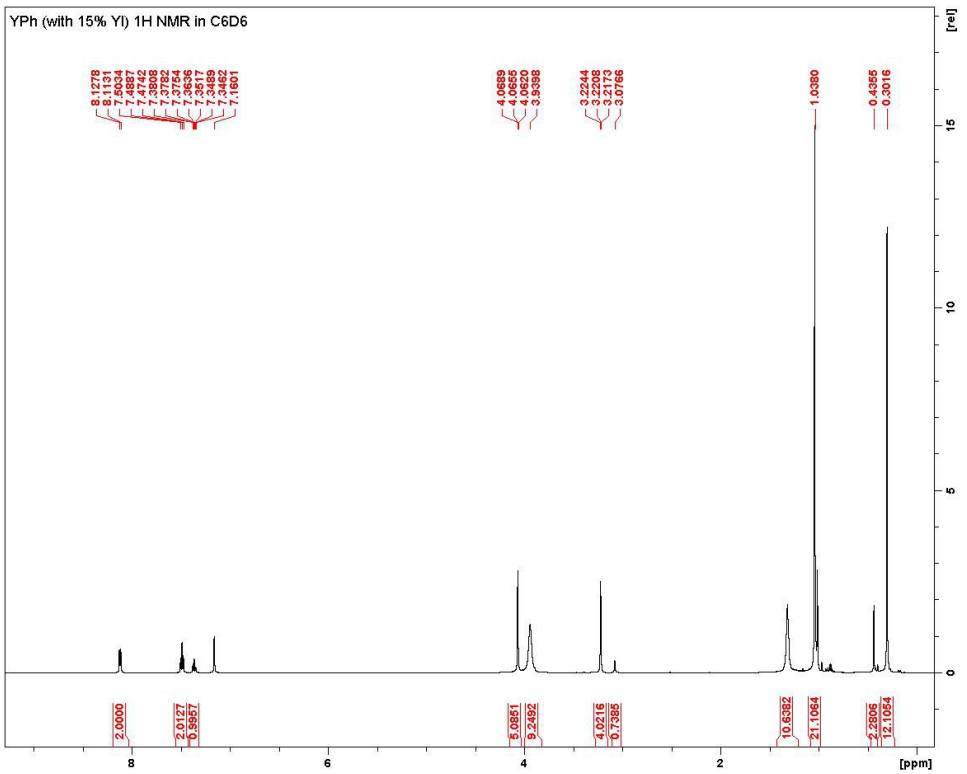


Figure S9. ^{1}H NMR spectrum of **3b** (C_6D_6, 500 MHz, 298 K).

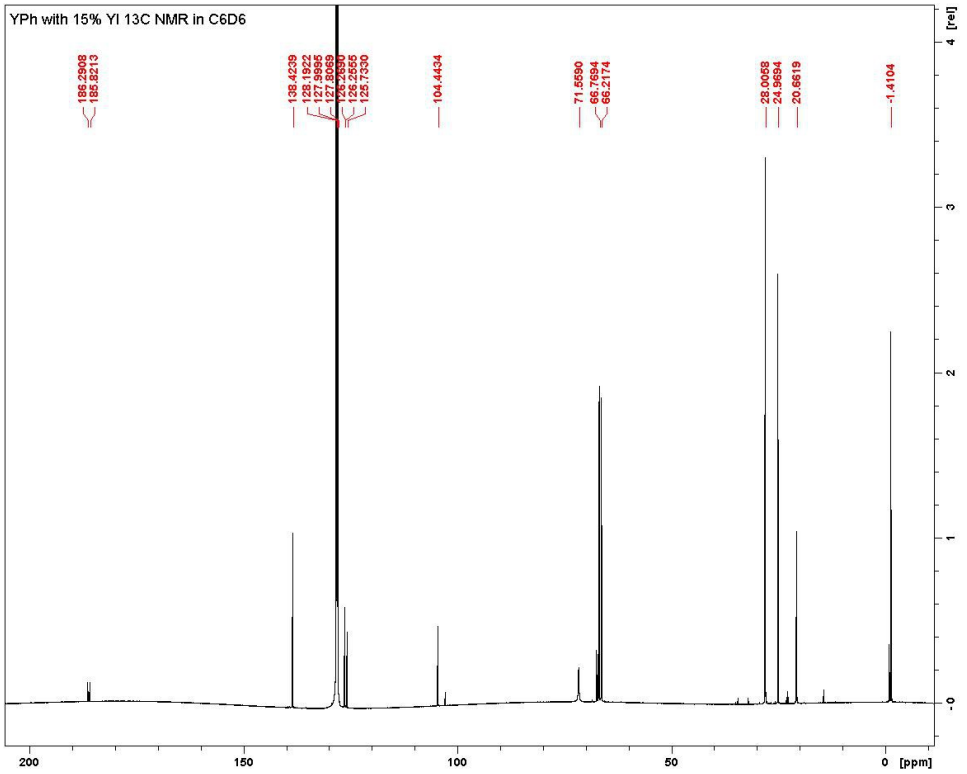


Figure S10. ^{13}C NMR spectrum of **3b** (C_6D_6, 126 MHz, 298 K).

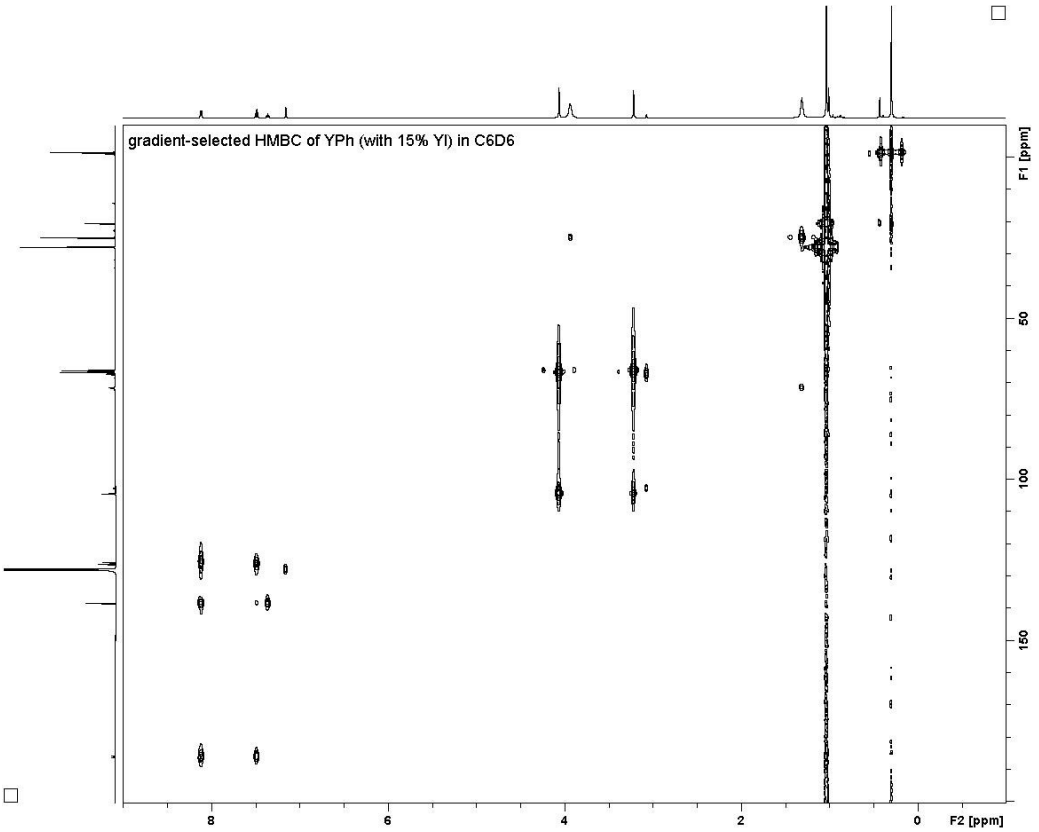


Figure S11. HMBC spectrum of **3b** (C_6D_6, 500 MHz, 228 K).

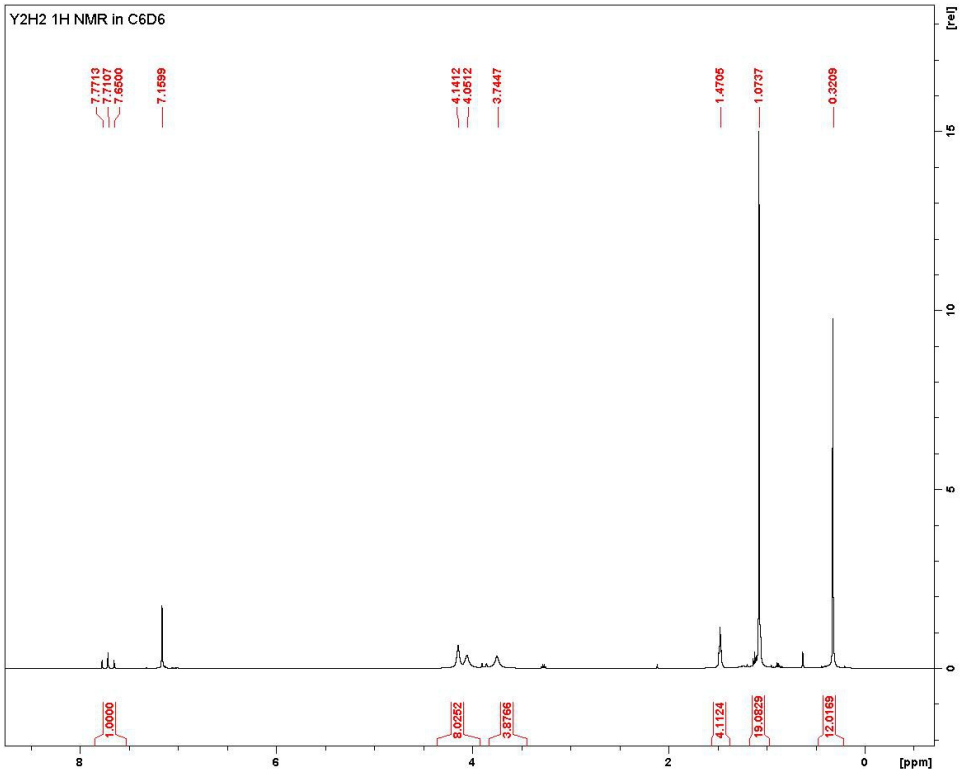


Figure S12. ^{1}H NMR spectrum of **2b** (C_6D_6, 500 MHz, 298 K).

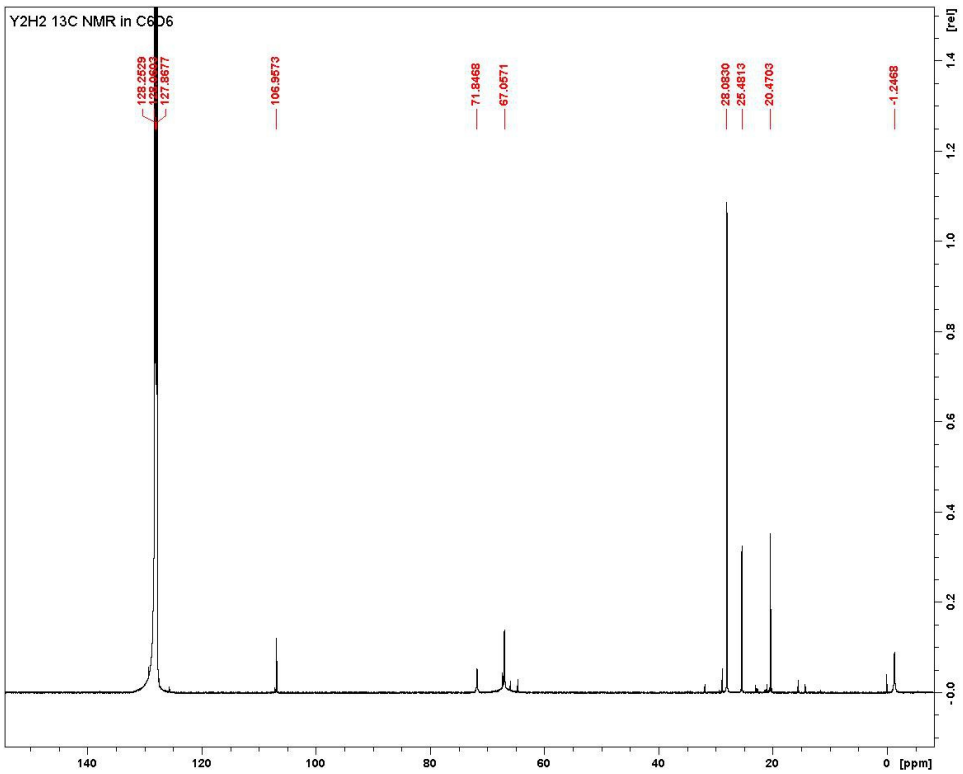


Figure S13. ^{13}C NMR spectrum of **2b** (C_6D_6, 126 MHz, 298 K).

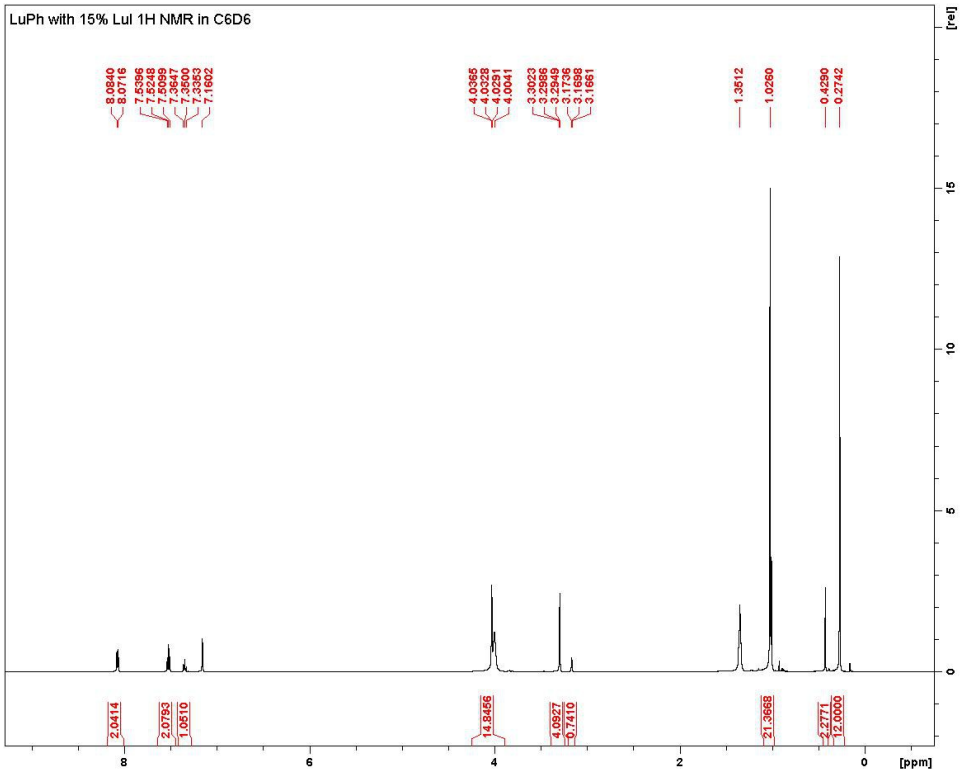


Figure S14. ^{1}H NMR spectrum of **3c** (C_6D_6, 500 MHz, 298 K).

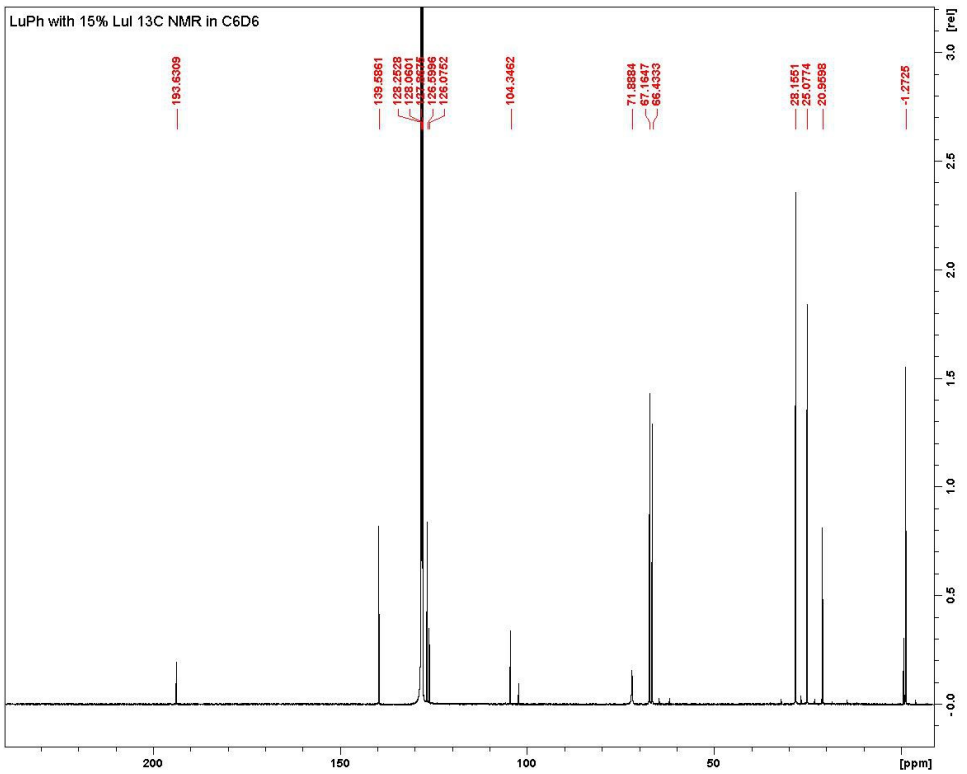


Figure S15. ^{13}C NMR spectrum of **3c** (C_6D_6, 126 MHz, 298 K).

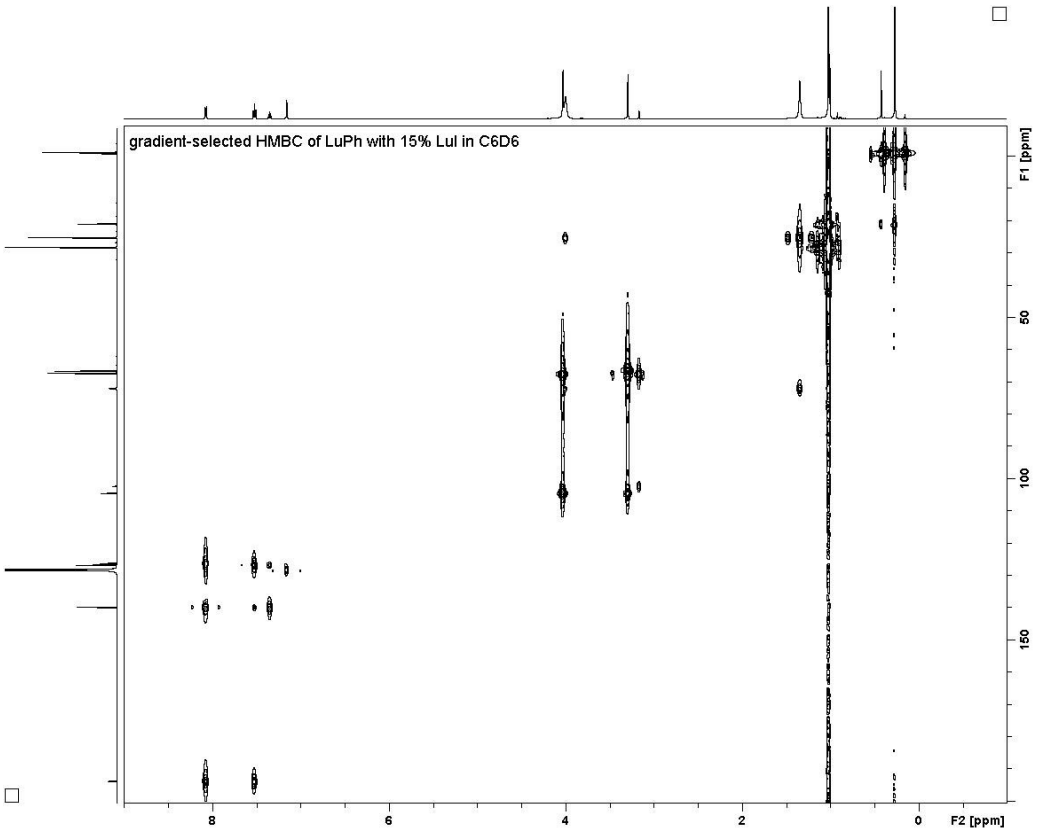


Figure S16. HMBC spectrum of **3c** (C_6D_6, 500 MHz, 228 K).

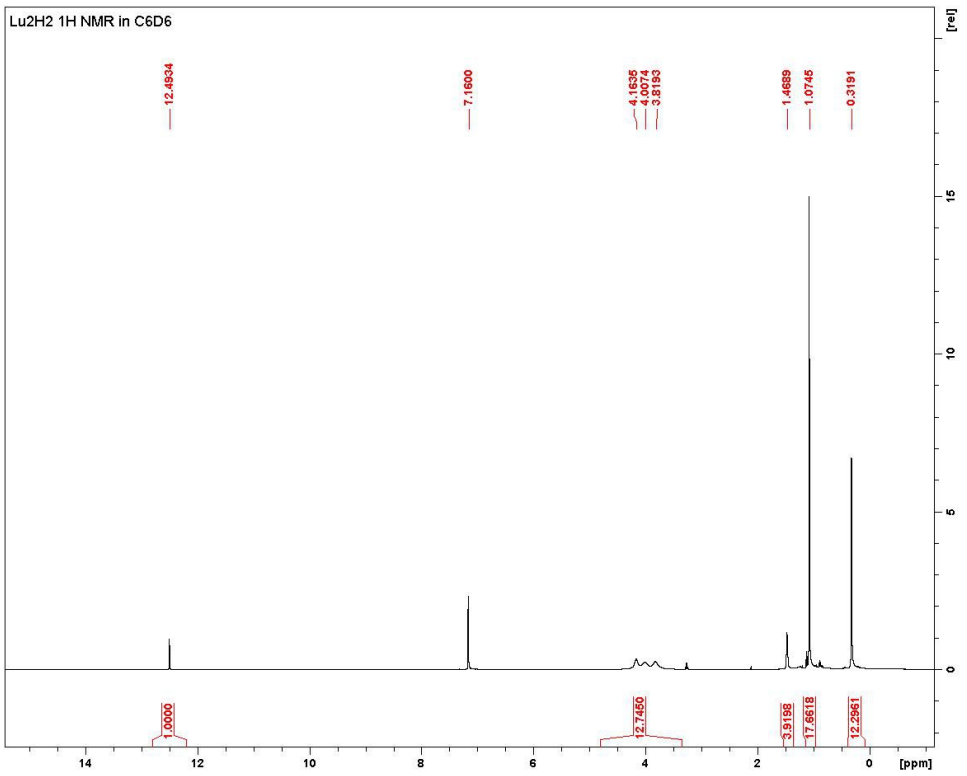


Figure S17. ^{1}H NMR spectrum of **2c** (C_6D_6, 500 MHz, 298 K).

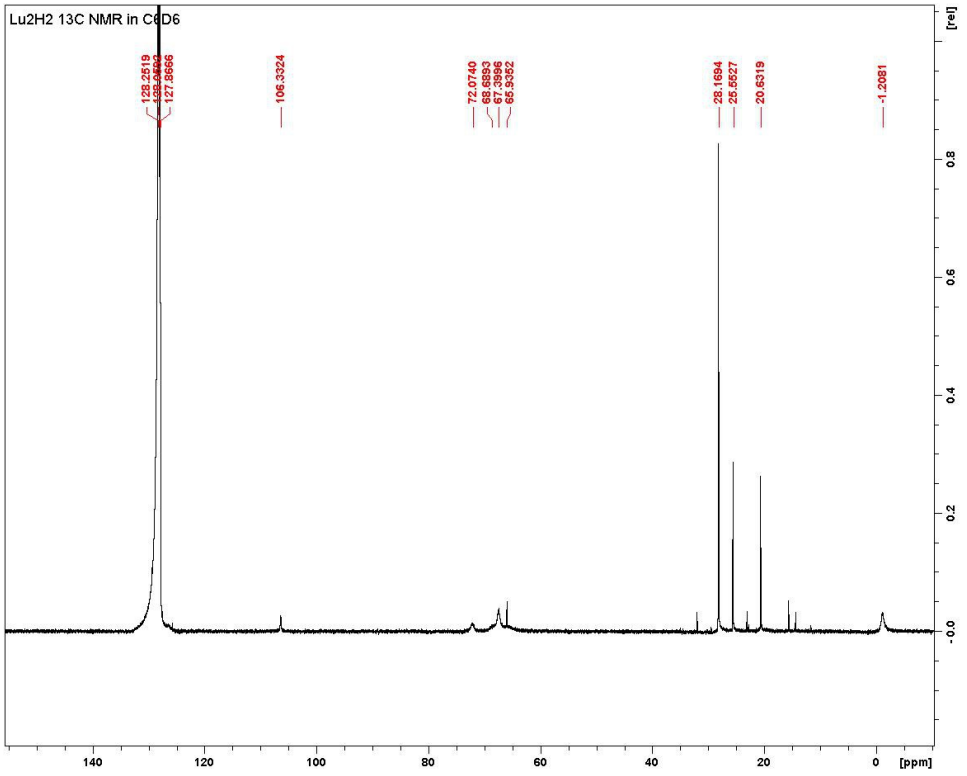


Figure S18. ^{13}C NMR spectrum of **2c** (C_6D_6, 126 MHz, 298 K).

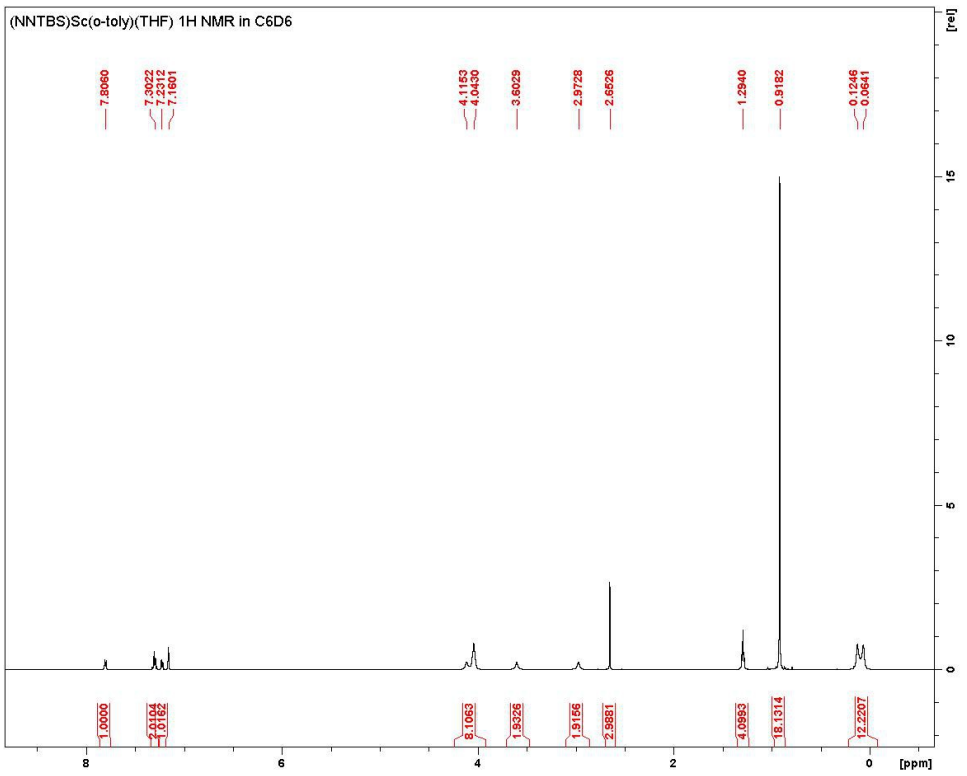


Figure S19. ^{1}H NMR spectrum of **4o** (C_6D_6, 500 MHz, 298 K).

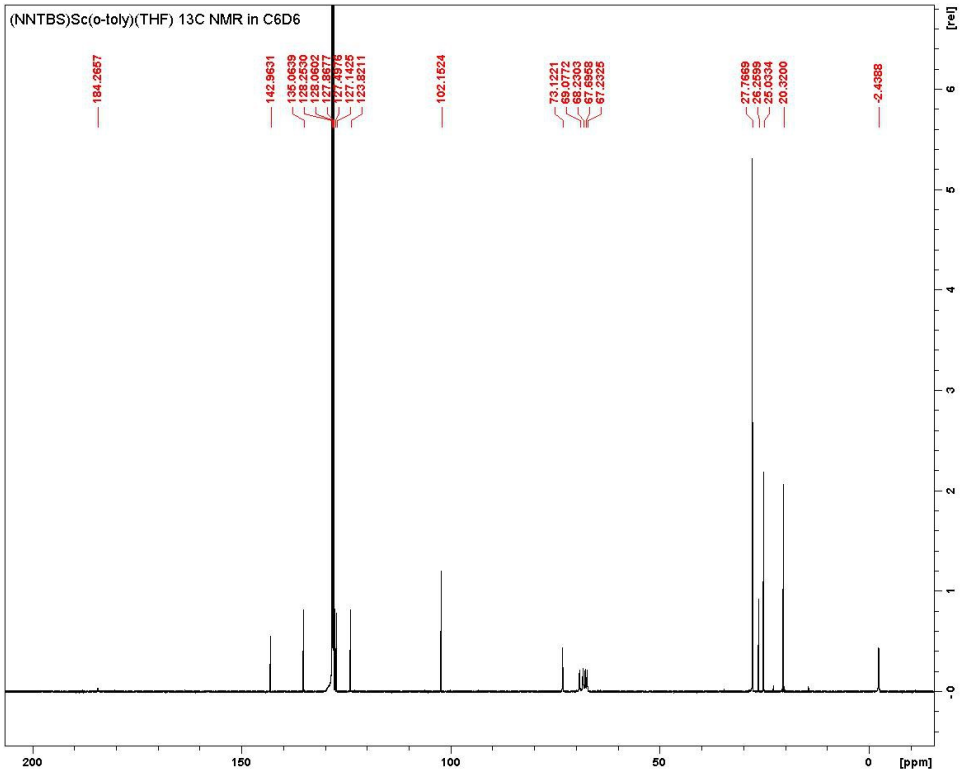


Figure S20. ^{13}C NMR spectrum of **4o** (C_6D_6, 126 MHz, 298 K).

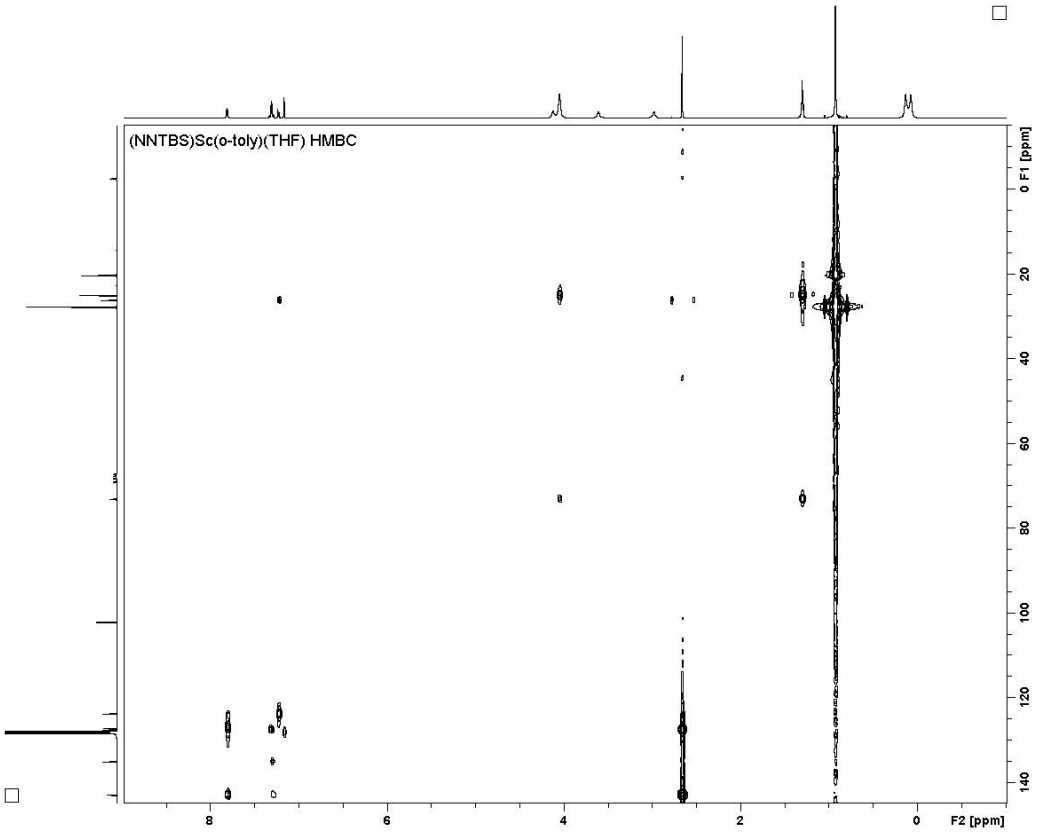


Figure S21. HMBC spectrum of **4o** (C_6D_6, 500 MHz, 228 K).

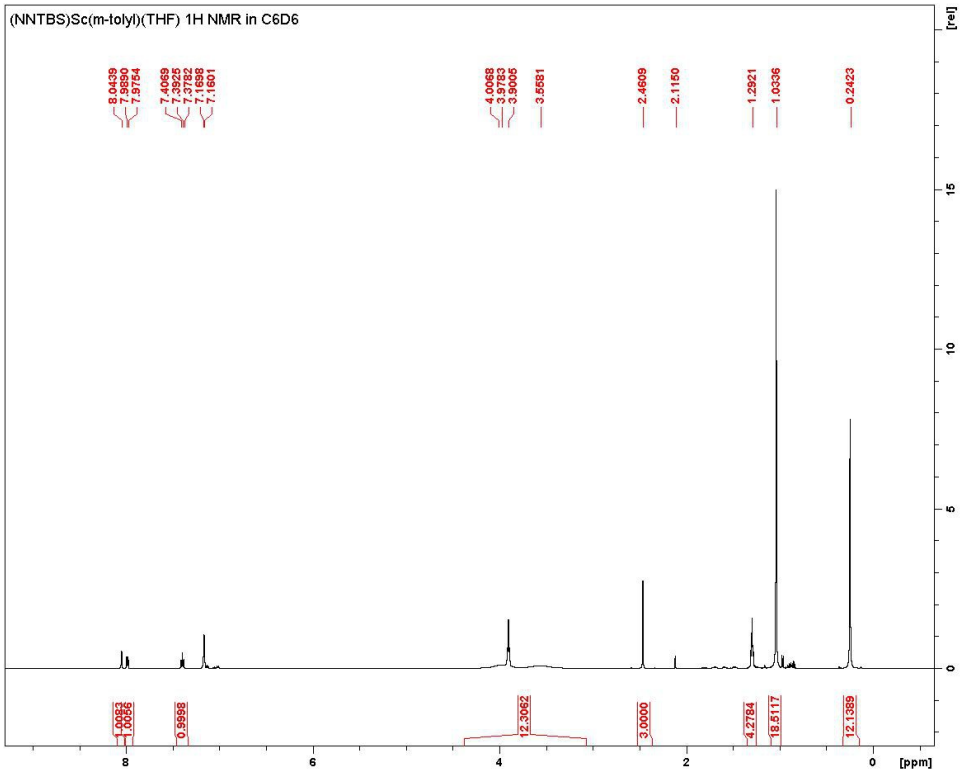


Figure S22. ^{1}H NMR spectrum of **4m** (C_6D_6, 500 MHz, 298 K).

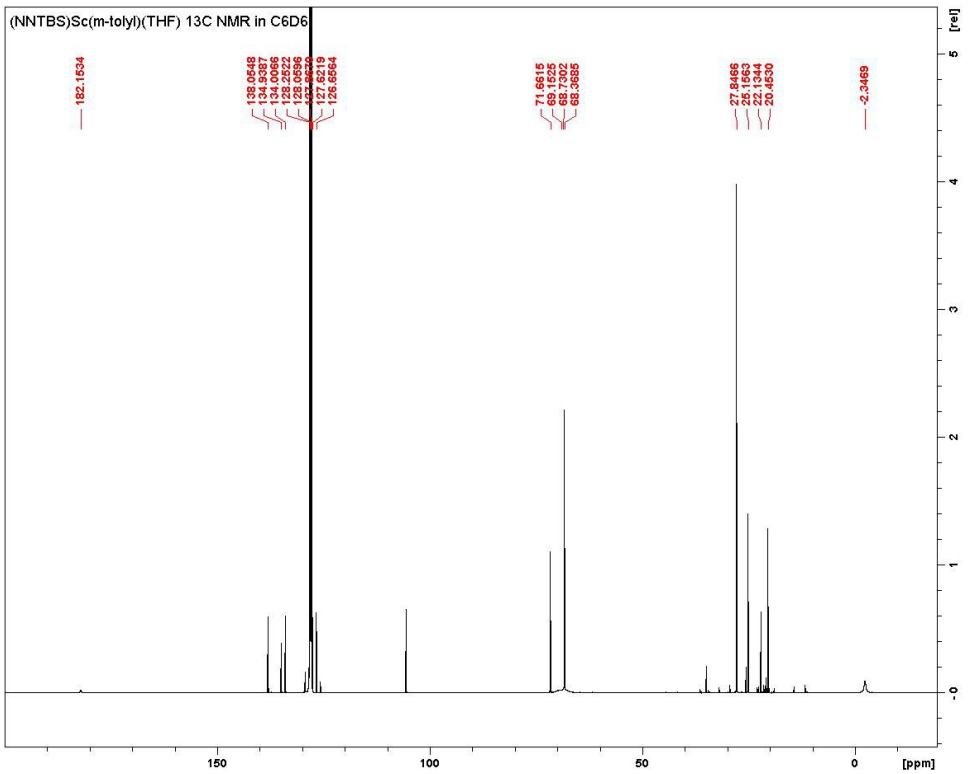


Figure S23. ^{13}C NMR spectrum of **4m** (C_6D_6, 126 MHz, 298 K).

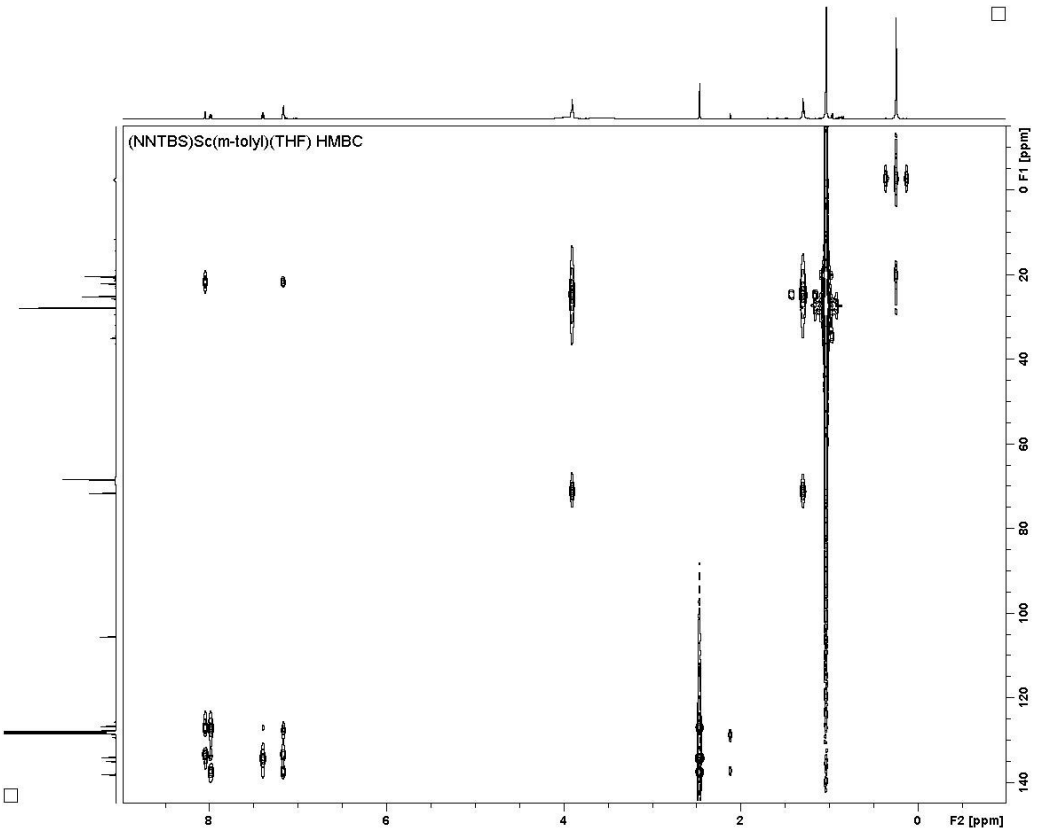


Figure S24. HMBC spectrum of **4m** (C_6D_6, 500 MHz, 228 K).

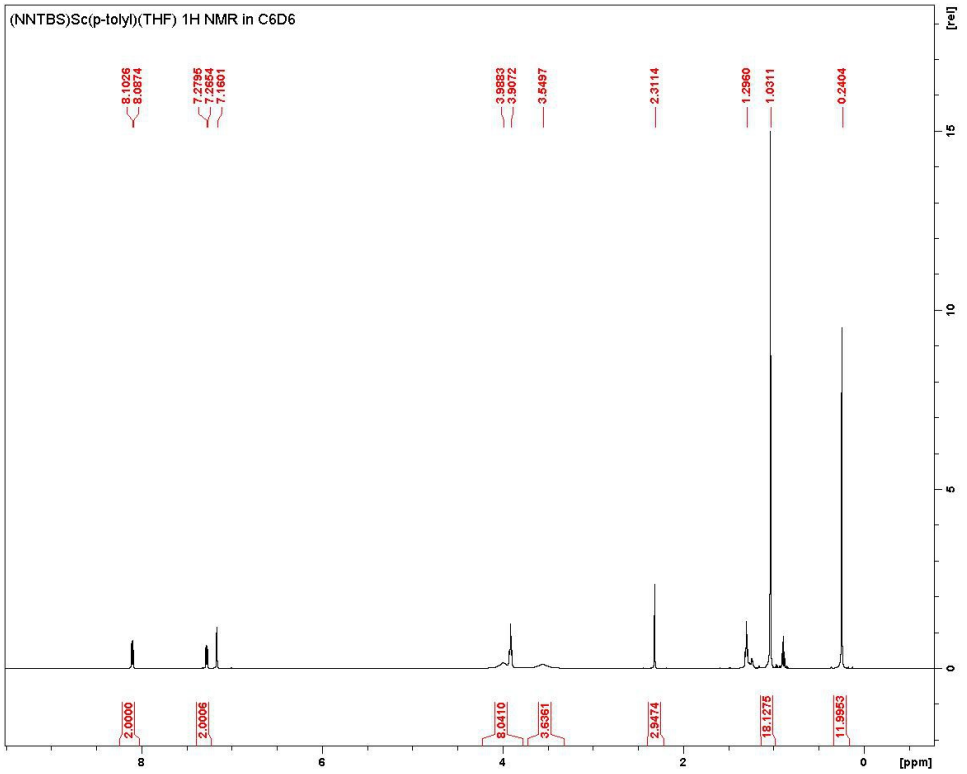


Figure S25. ^{1}H NMR spectrum of **4p** (C_6D_6, 500 MHz, 298 K).

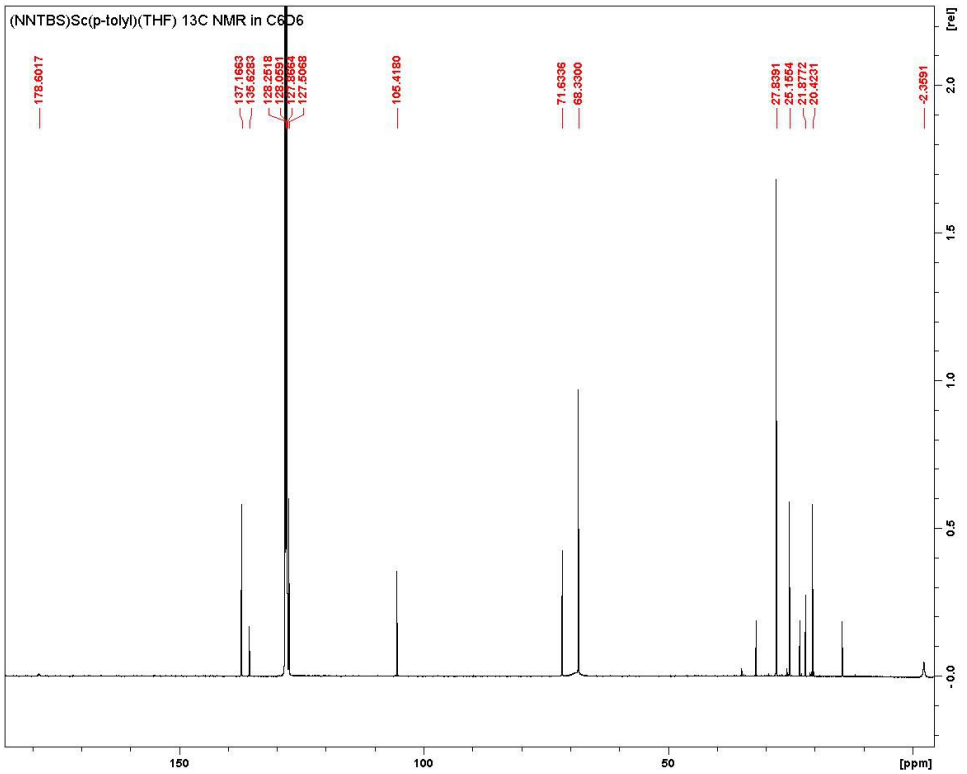


Figure S26. ^{13}C NMR spectrum of **4p** (C_6D_6, 126 MHz, 298 K).

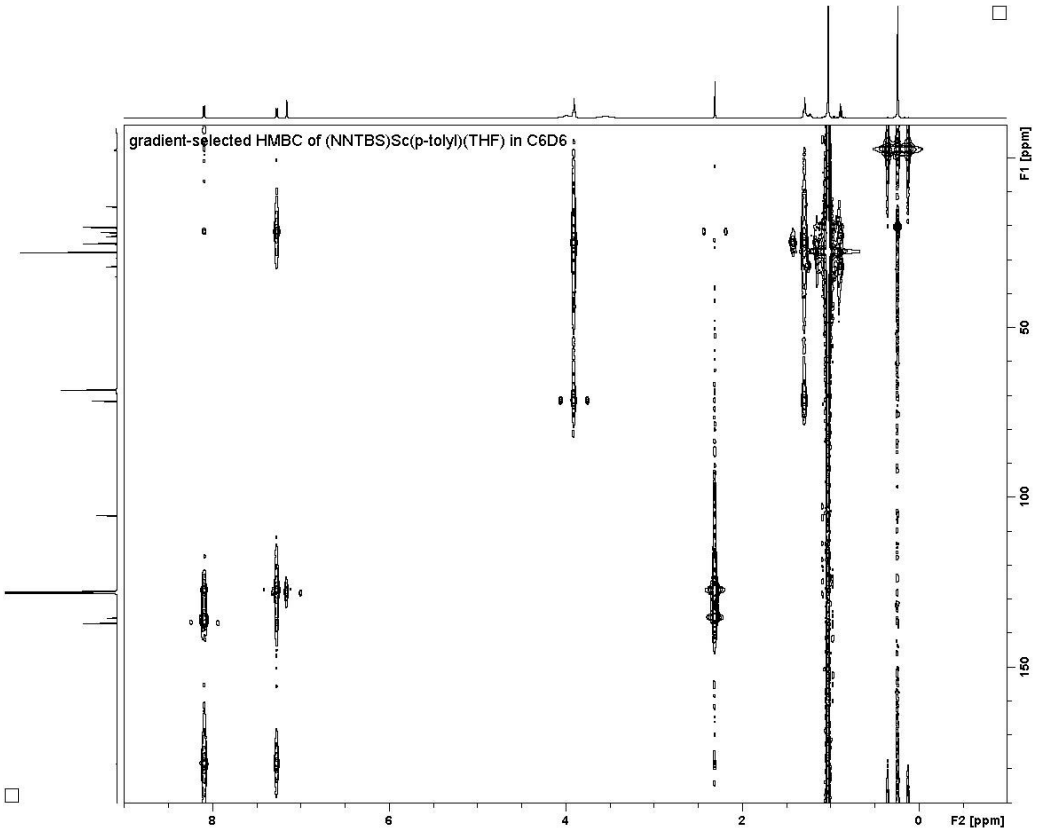


Figure S27. HMBC spectrum of **4p** (C_6D_6, 500 MHz, 228 K).

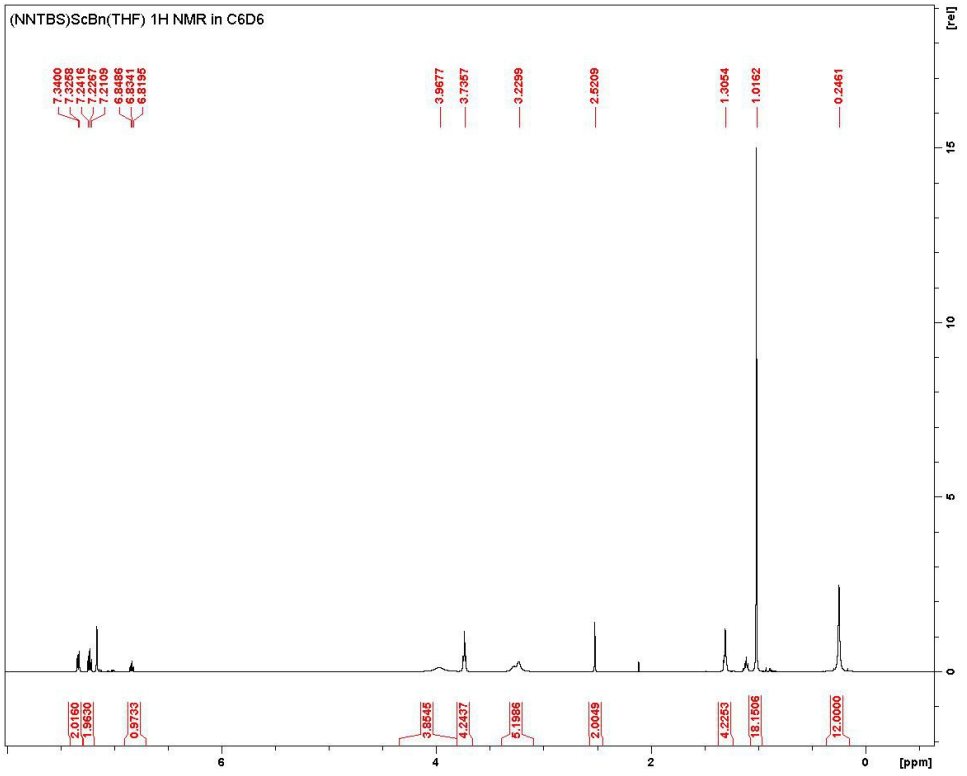


Figure S28. ^{1}H NMR spectrum of **7** (C_6D_6, 500 MHz, 298 K).

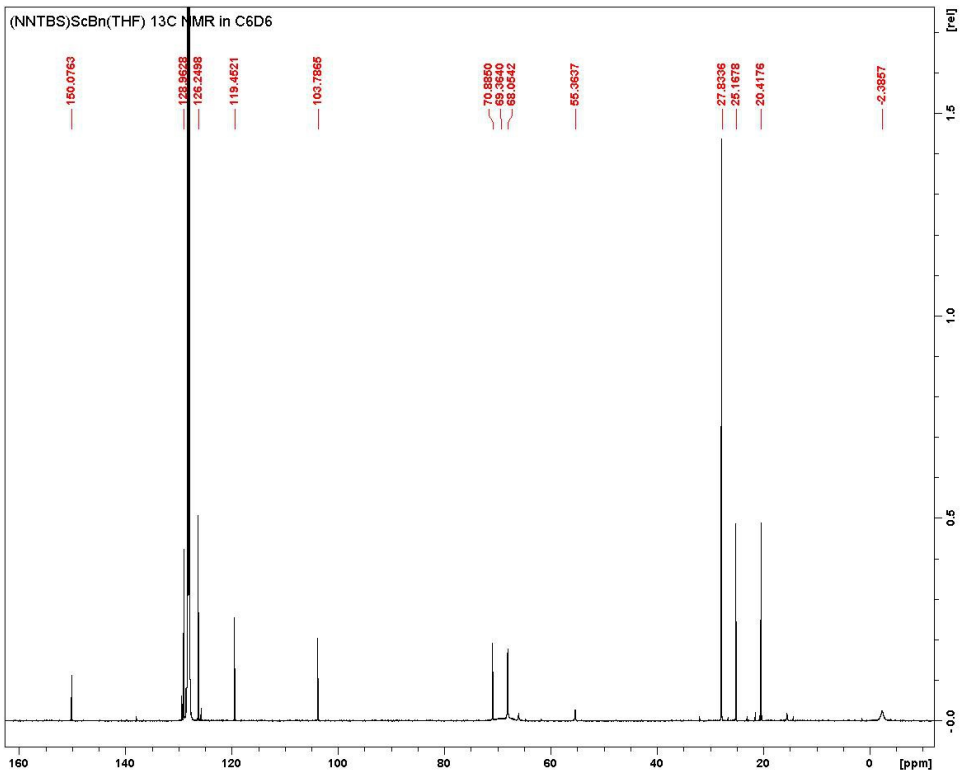


Figure S29. ^{13}C NMR spectrum of **7** (C_6D_6, 126 MHz, 298 K).

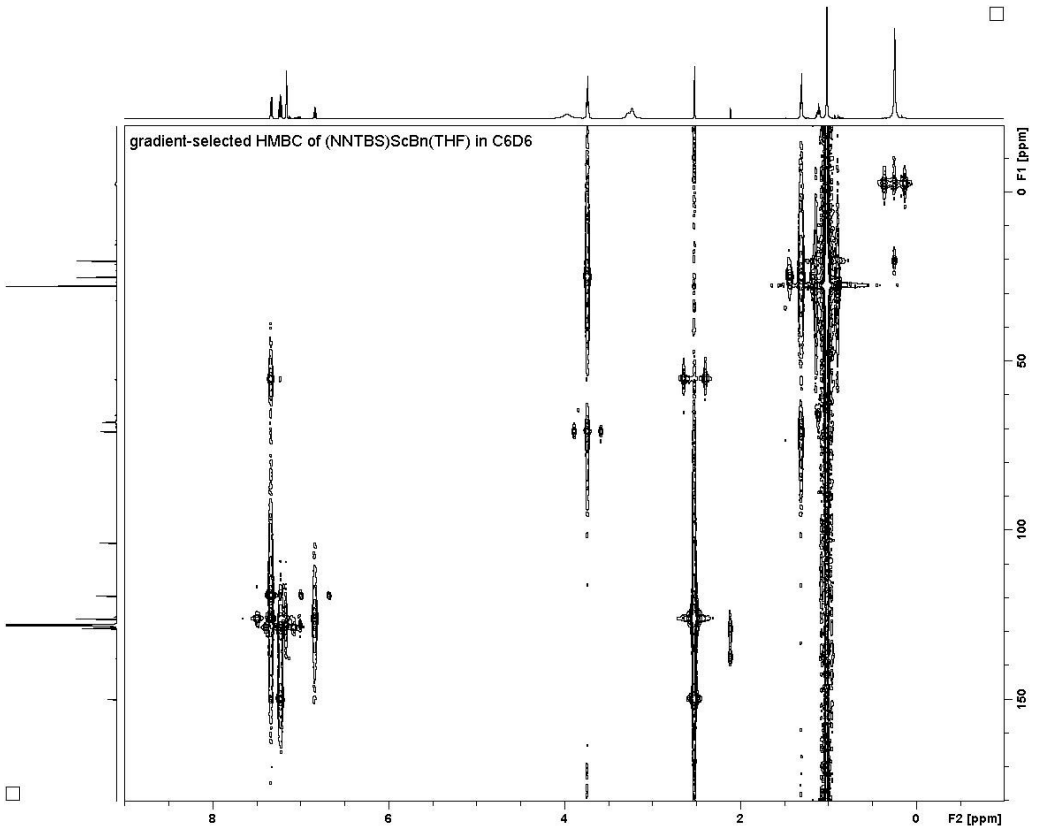


Figure S30. HMBC spectrum of **7** (C_6D_6, 500 MHz, 228 K).

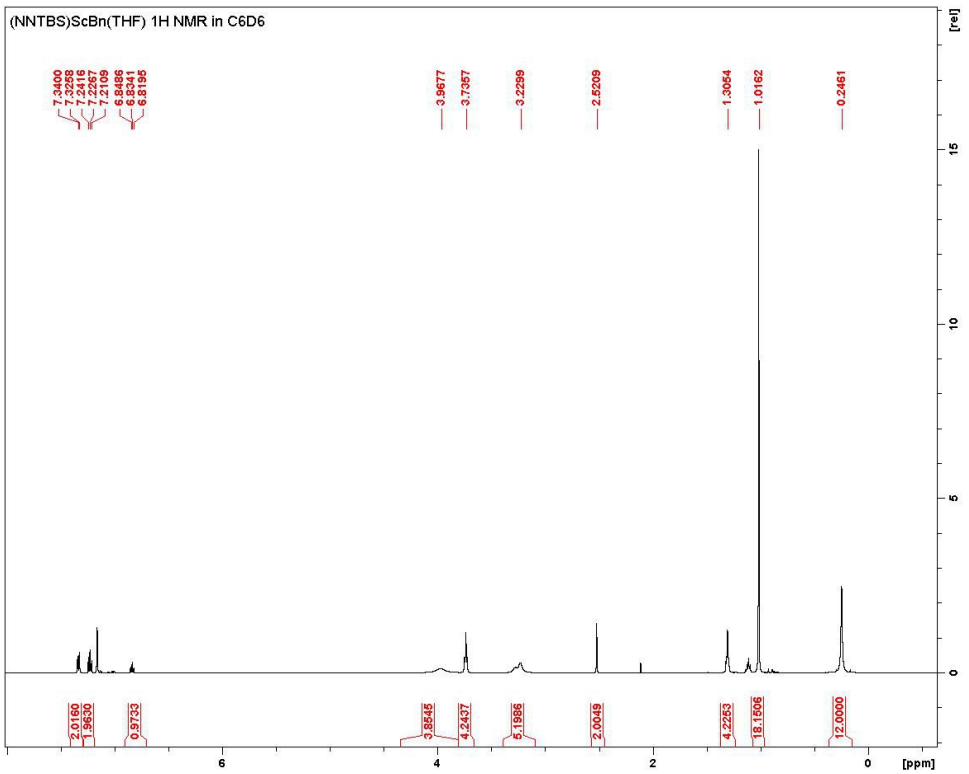


Figure S31. ^{1}H NMR spectrum of **7** (C_6D_6, 500 MHz, 298 K).

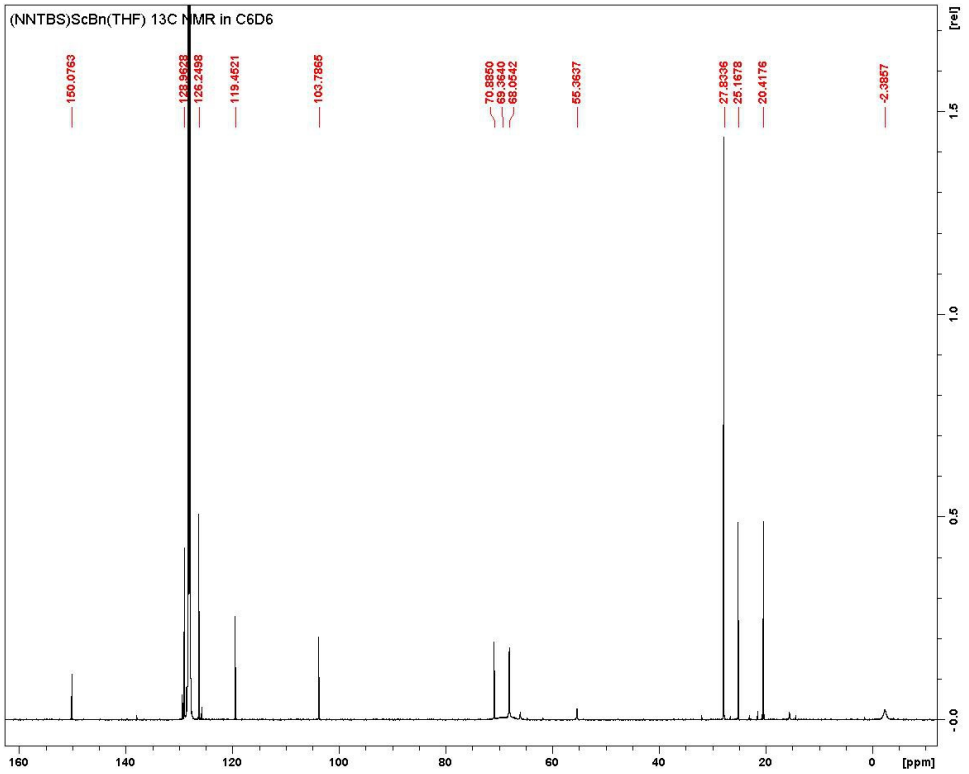


Figure S32. ^{13}C NMR spectrum of **7** (C_6D_6, 126 MHz, 298 K).

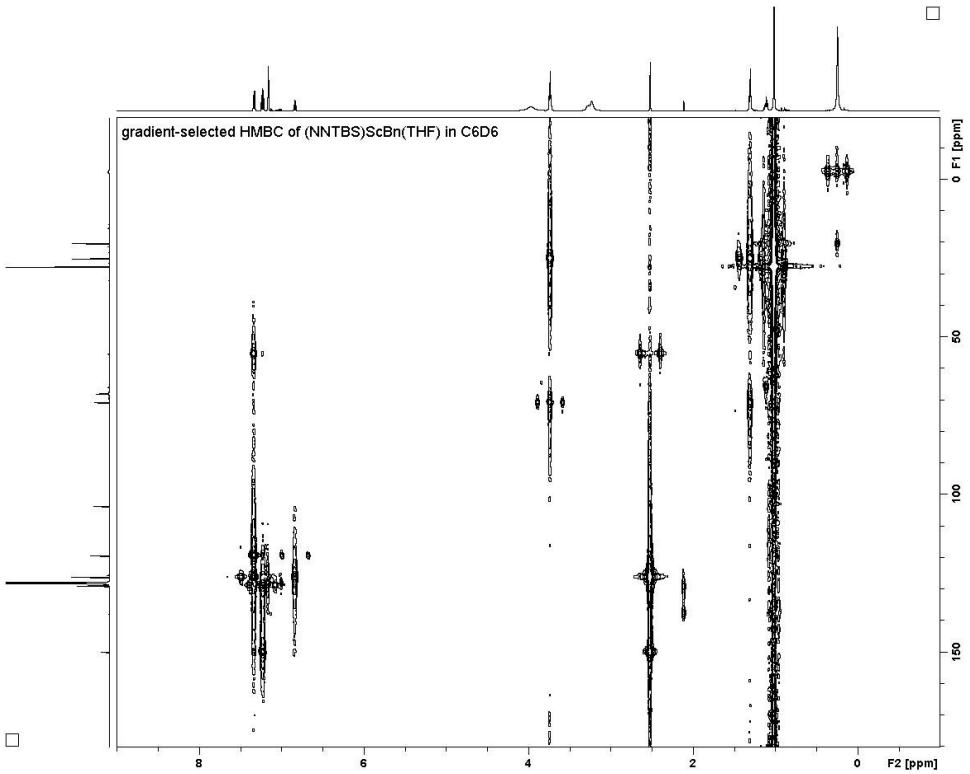


Figure S33. HMBC (C_6D_6, 500 MHz, 298 K) spectrum of **7**.

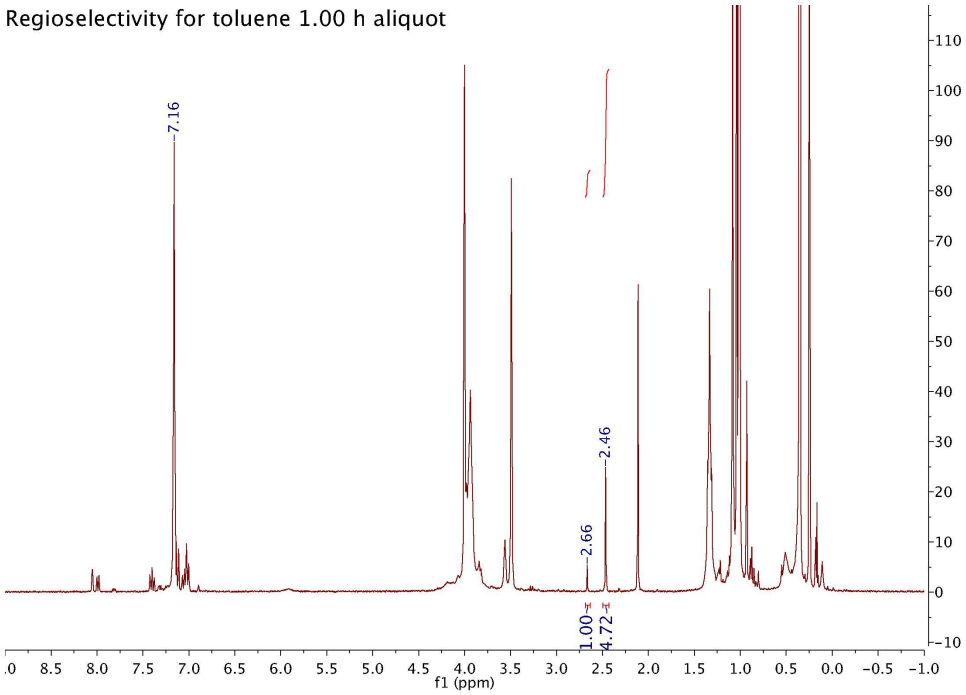


Figure S34. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of regioselectivity study on toluene activation at 25 °C after 1.00 h.

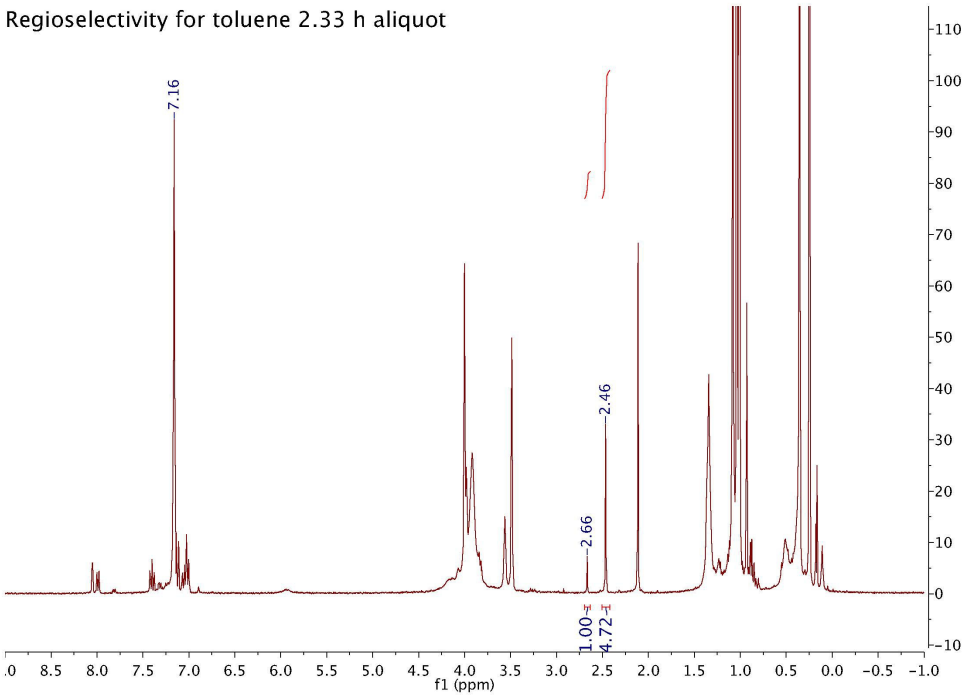


Figure S35. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of regioselectivity study on toluene activation at 25 °C after 2.33 h.

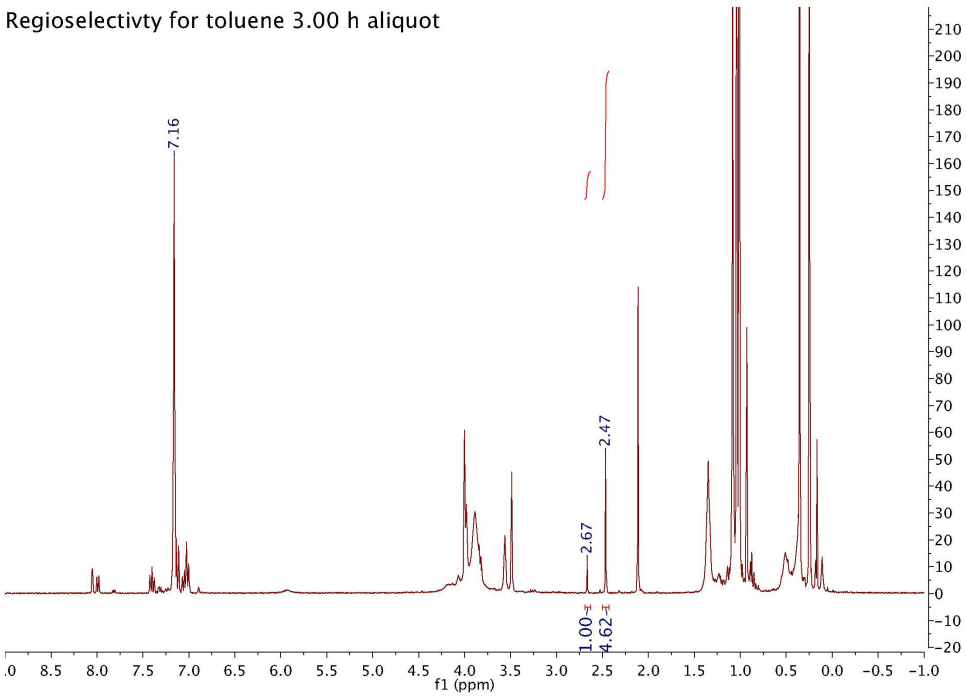


Figure S36. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of regioselectivity study on toluene activation at 25 °C after 3.00 h.

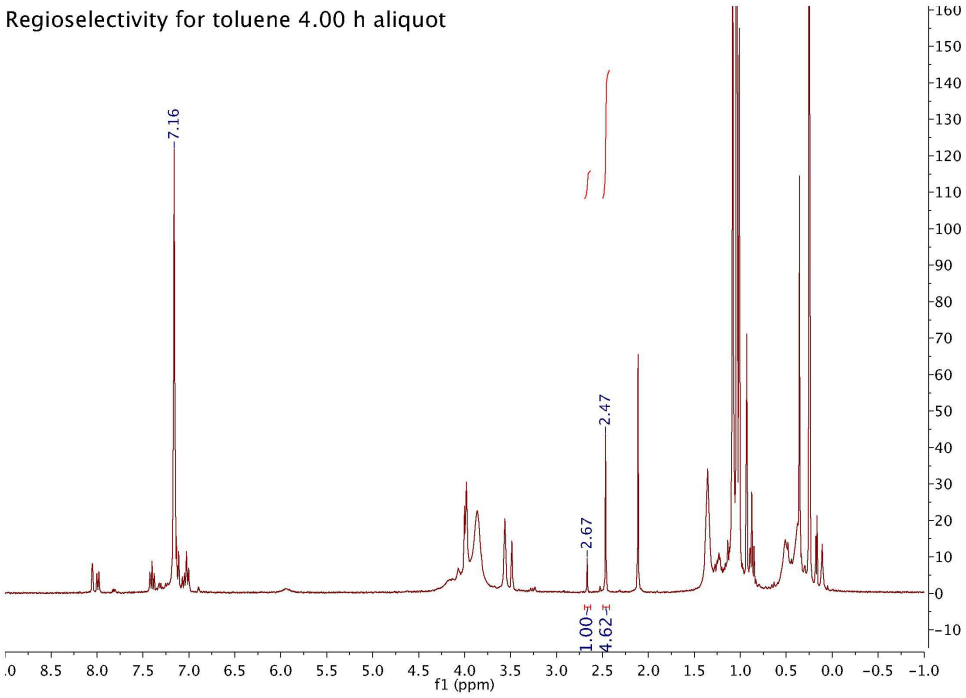


Figure S37. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of regioselectivity study on toluene activation at 25 °C after 4.00 h.

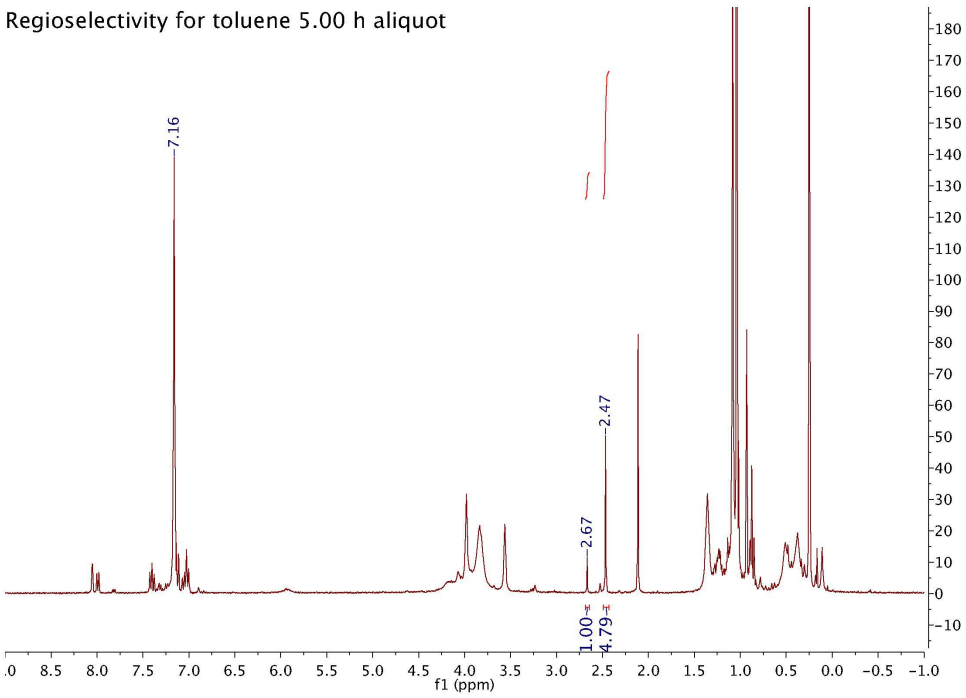


Figure S38. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of regioselectivity study on toluene activation at 25 °C after 5.00 h.

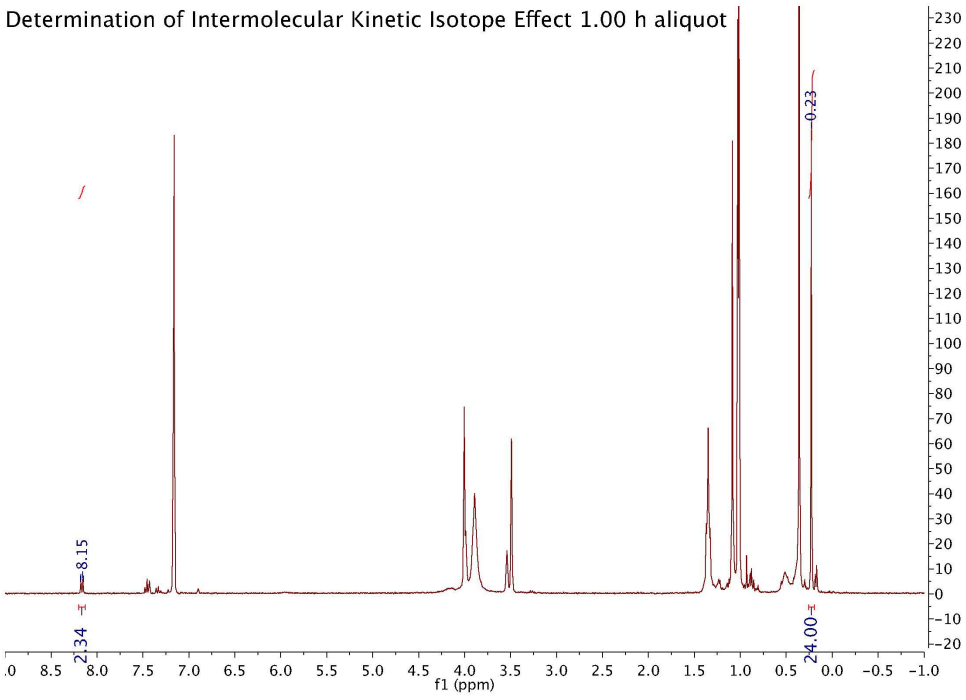


Figure S39. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of *inter*molecular KIE study at 25 °C after 1.00 h.

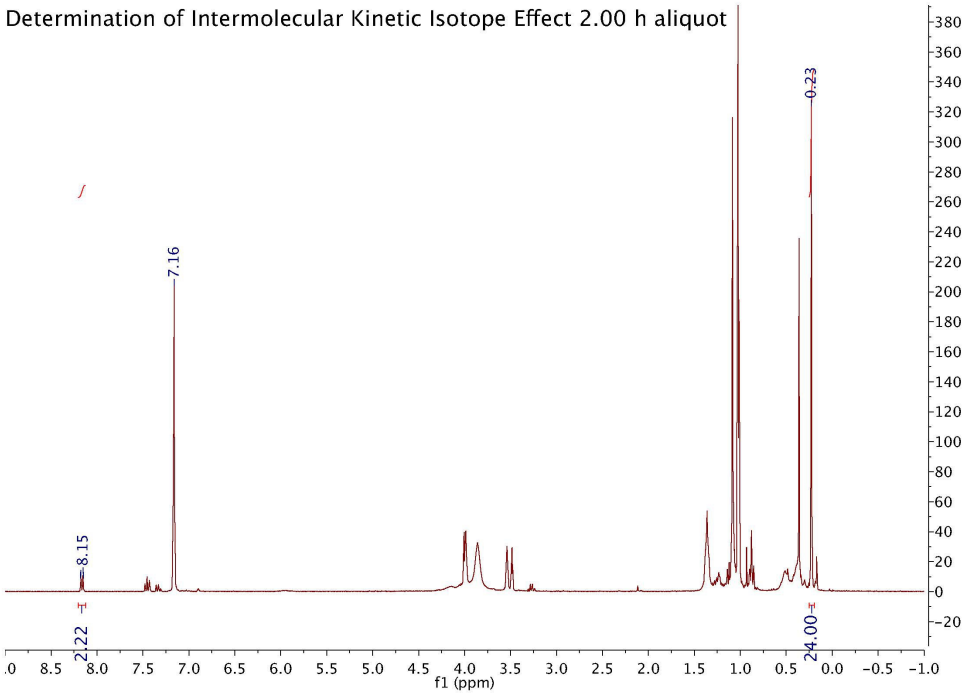


Figure S40. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of *inter*molecular KIE study at 25 °C after 2.00 h.

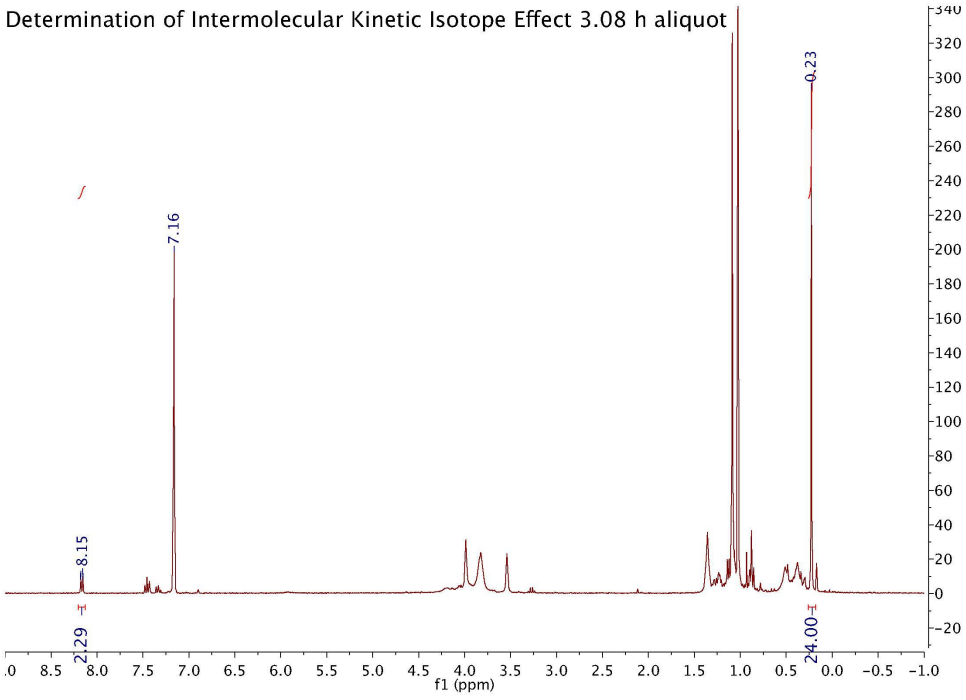


Figure S41. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of *inter*molecular KIE study at 25 °C after 3.08 h.

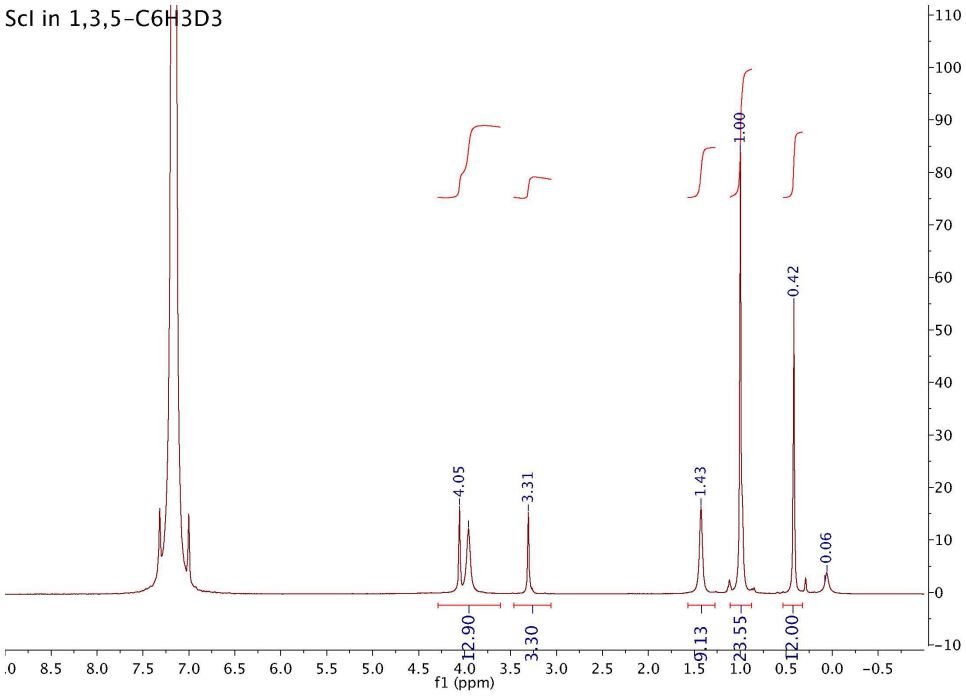


Figure S42. ^{1}H NMR spectrum ($C_6H_3D_3$, 300 MHz, 298 K) of **1a** in neat $C_6H_3D_3$.

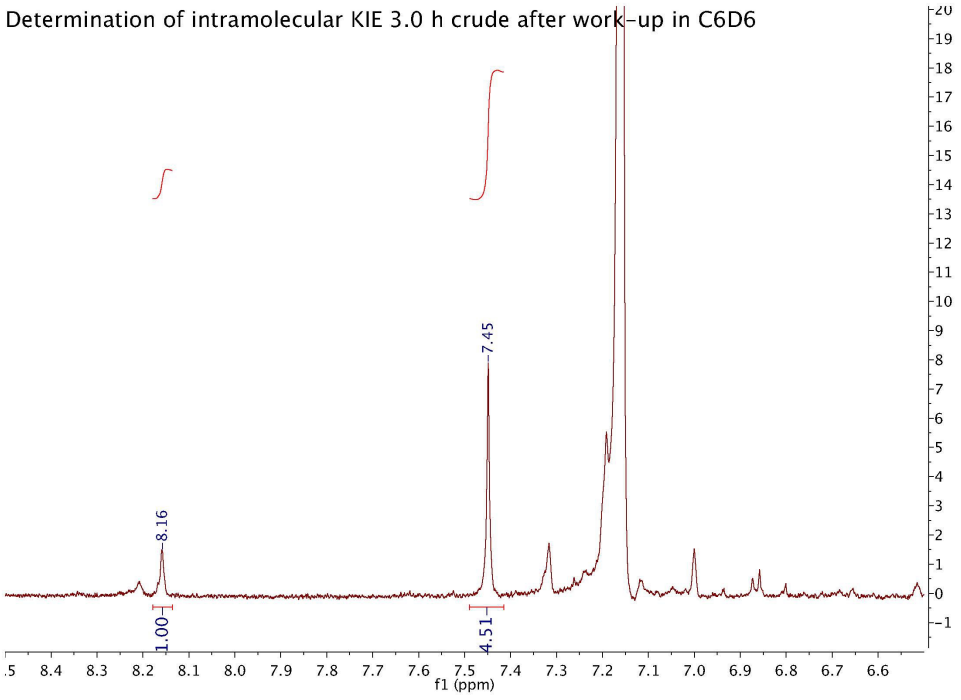


Figure S43. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) showing the aromatic region (8.5 to 6.5 ppm of *intra*molecular KIE study at 25 °C after 3 h (crude product).

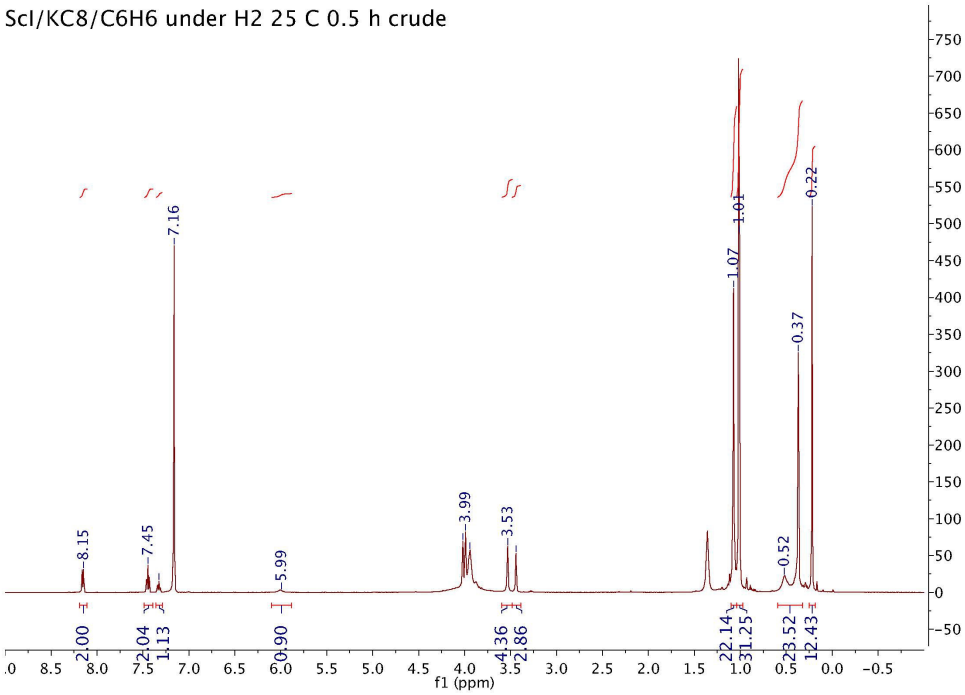


Figure S44. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation by **1a**/KC_8 under H_2 at 25 °C after 0.5 h (crude product).

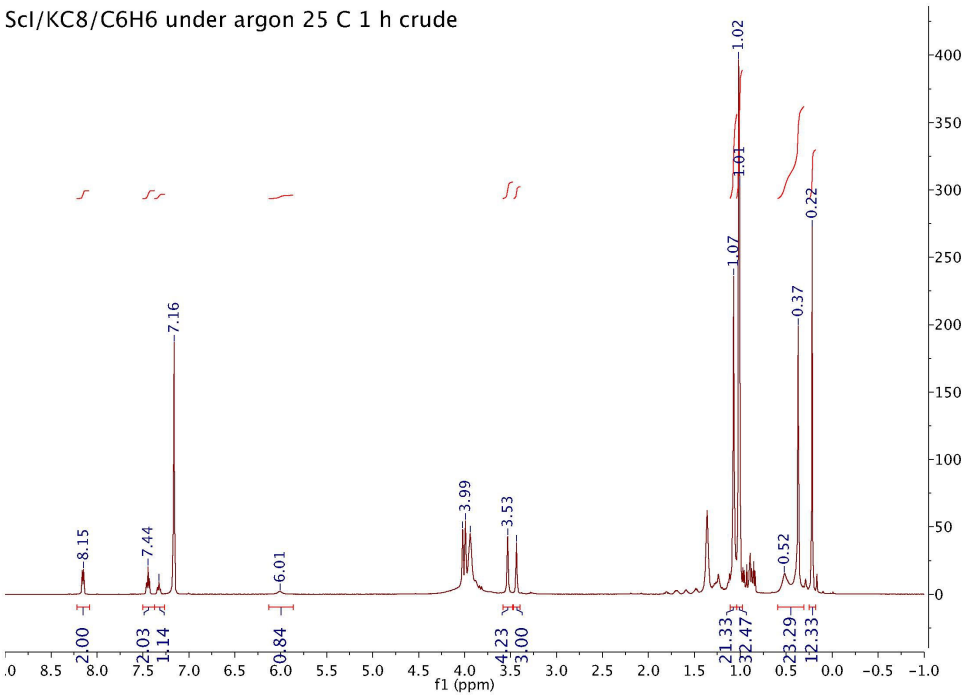


Figure S45. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation by **1a**/KC_8 under argon at 25 °C after 1.0 h (crude product).

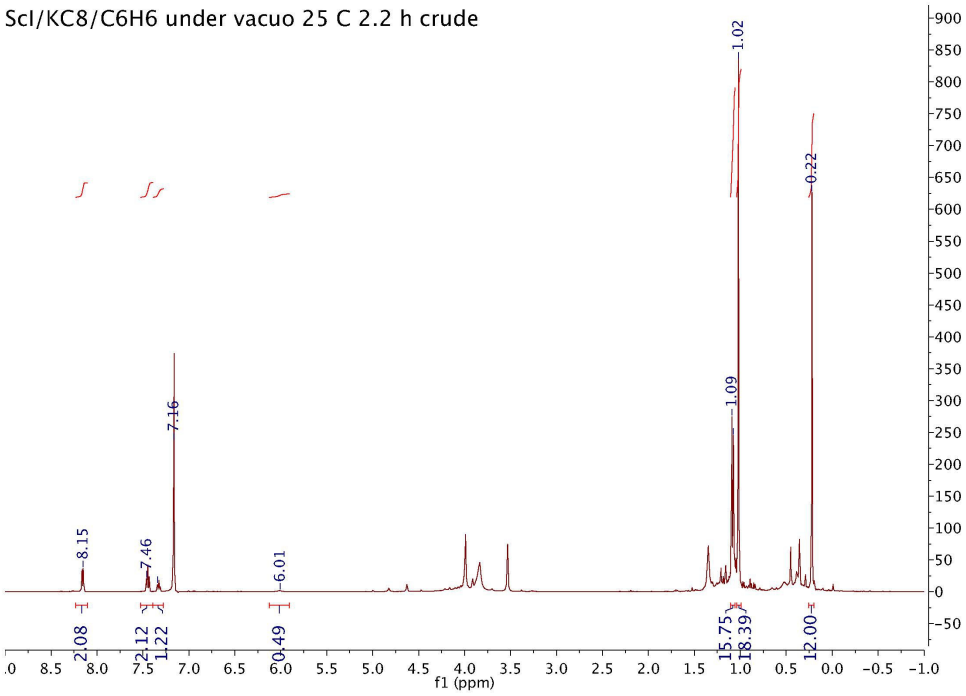


Figure S46. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation by **1a**/KC_8 under vacuum at 25 °C after 2.2 h (crude product).

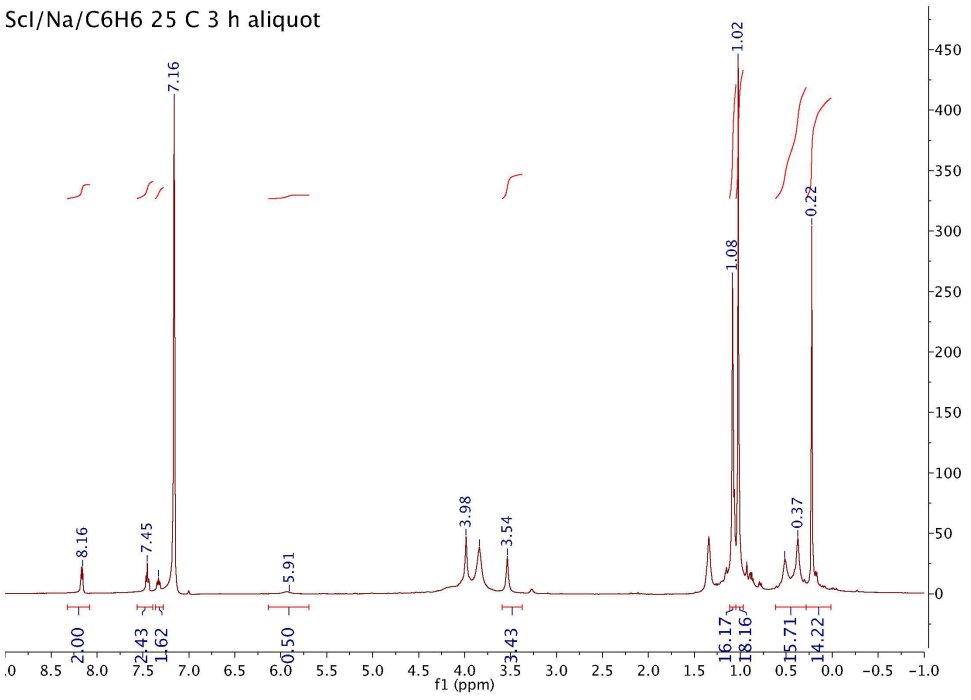


Figure S47. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation by **1a**/Na at 25 °C after 3 h (crude product).

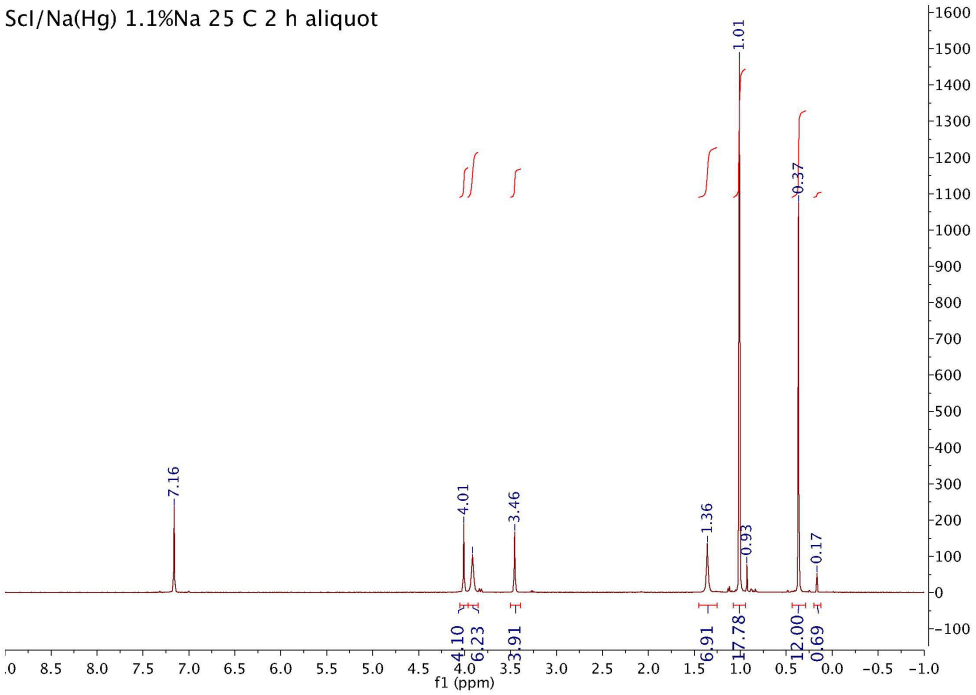


Figure S48. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation attempt by **1a**/Na(Hg) (1.1% sodium weight) at 25 °C after 2 h.

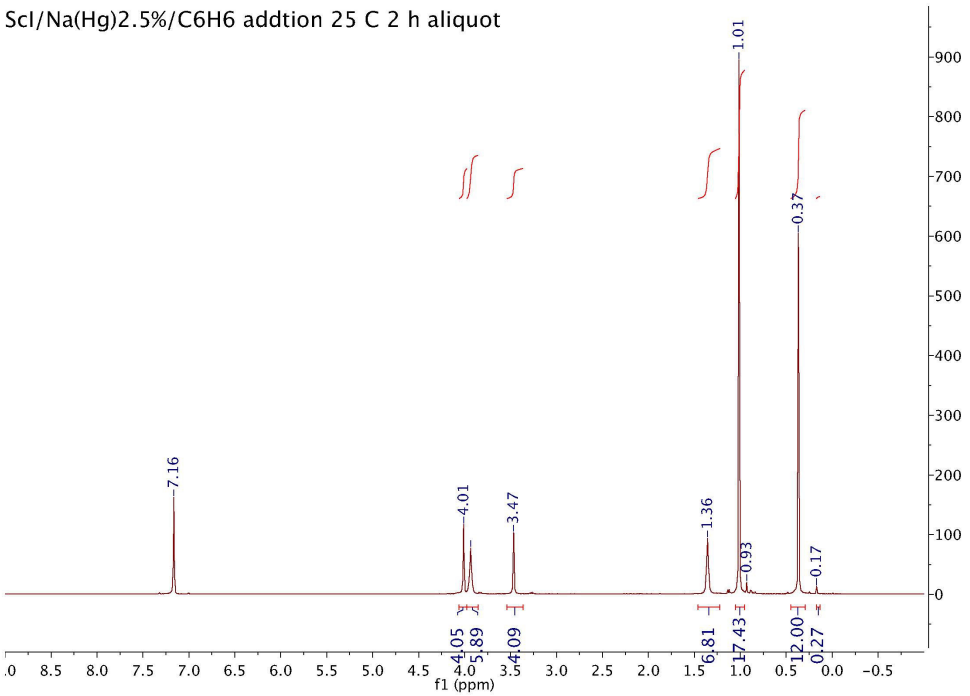


Figure S49. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of benzene activation attempt by **1a**/Na(Hg) (2.5% sodium weight) at 25 °C after 2 h.

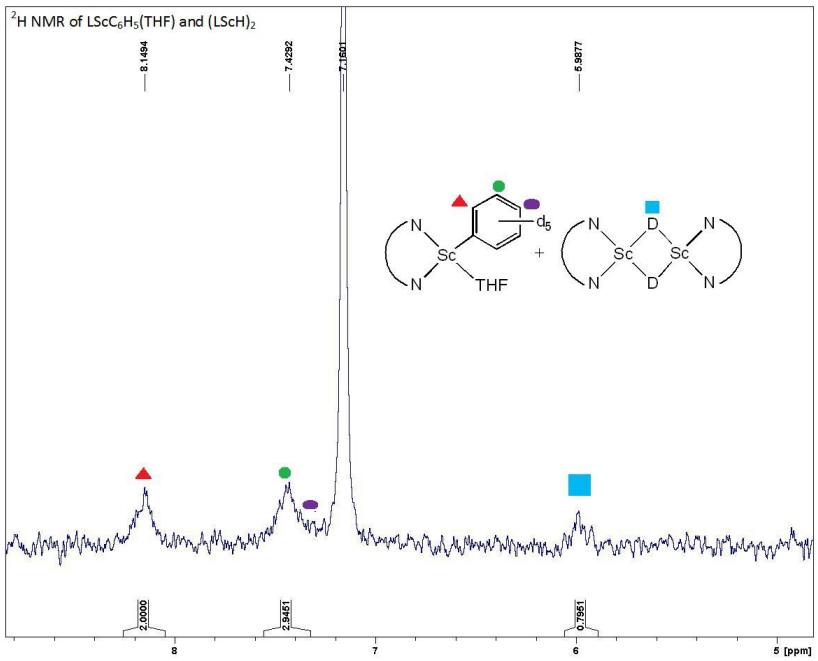


Figure S50. ^{2}H NMR spectrum (C_6H_6, 46 MHz, 298 K) showing only the aromatic region for clarity with assignment for C-D activation of C_6D_6 by **1a**/KC_8 system (crude product).

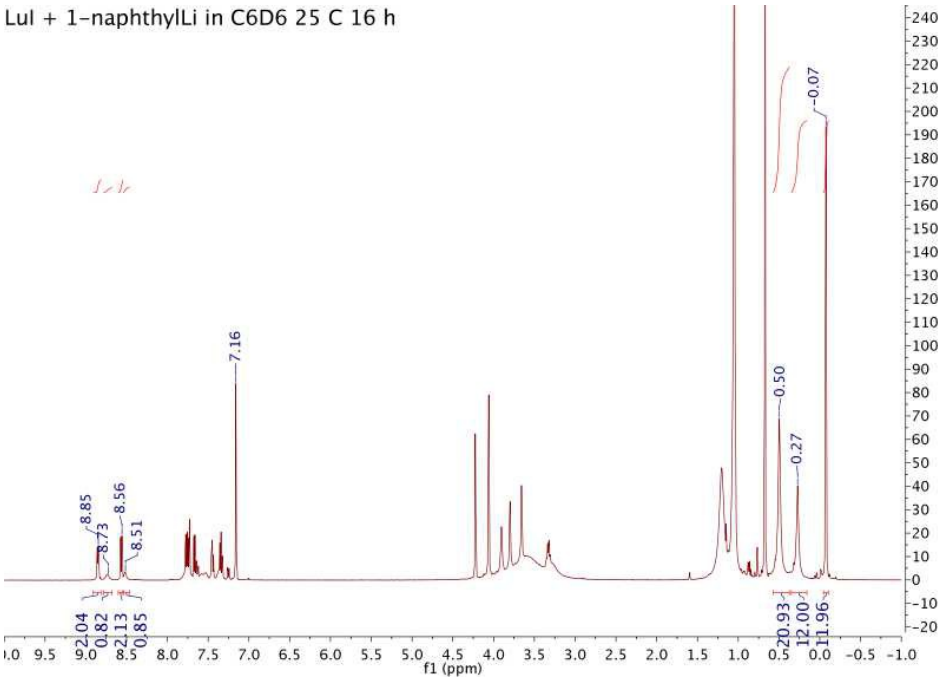


Figure S51. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of the reaction of **1c** and α-naphthylLi after 16 h at 25 °C. *Note*: the peaks at 8.73, 8.47, and 0.27 ppm were assigned to **6c-α**; the peaks at 8.85, 8.56, and -0.07 ppm were assigned to the ate complex, (NN^{fc})Lu(α-naphthyl)$_2$Li; the peak at 0.50 ppm was assigned to **1c**. The assignment of **6c-α** and (NN^{fc})Lu(α-naphthyl)$_2$Li was based on the relative integration of peaks in the aromatic region and the peak of SiCH_3 (close to 0 ppm). See also Figure S52 for the ^{1}H NMR spectrum of a pure sample of (NN^{fc})Lu(α-naphthyl)$_2$Li.

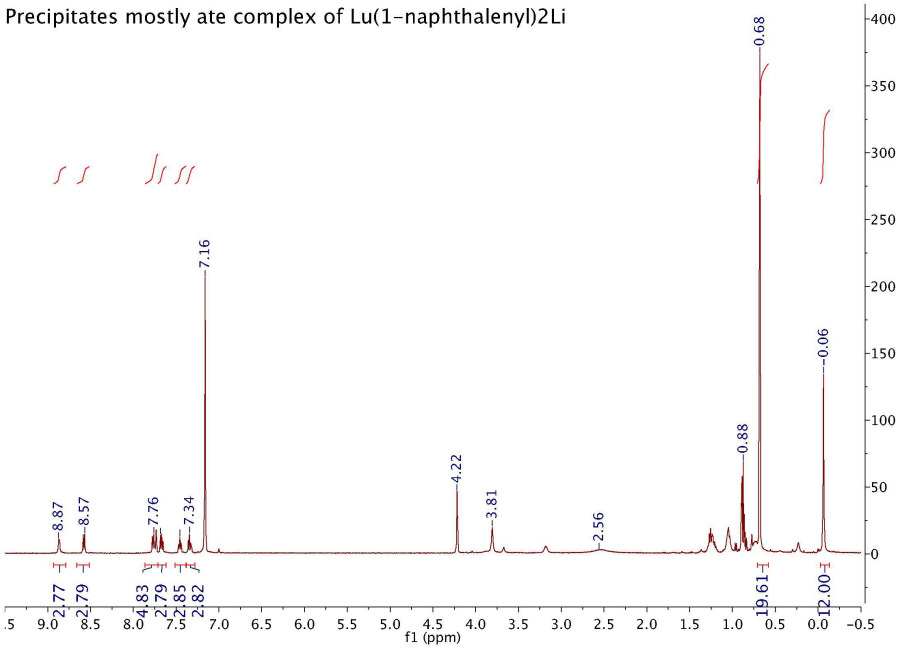


Figure S52. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of the ate complex, (NN^{fc})Lu(α-naphthyl)$_2$Li. The integration confirmed the 1 : 2 ratio for the NN^{fc} vs. α-naphthyl ligand.

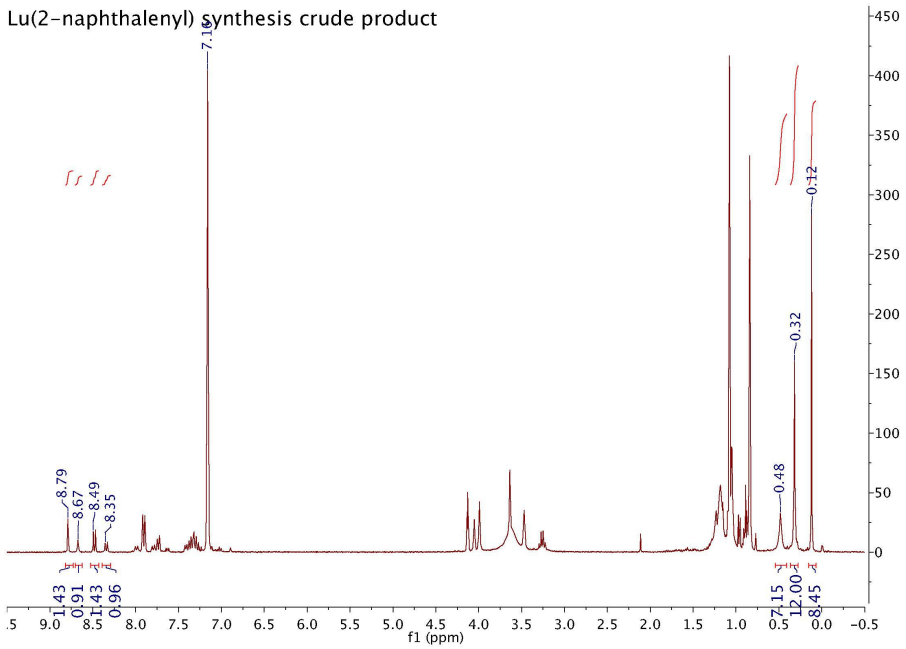


Figure S53. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of the crude product from **6c-β** synthesis. *Note*: the peaks at 8.67, 8.35, and 0.32 ppm were assigned to **6c-β**, while the peaks at 8.79, 8.49, and 0.12 ppm were assigned to the ate complex, (NN^{fc})Lu(β-naphthyl)$_2$Li. The peak at 0.48 ppm was assigned to **1c** present in the equilibrium. The assignment was based on the relative integration of peaks in the aromatic region and the peak of SiC*H*$_3$. The ratio of **1c** : **6c-β** : (NN^{fc})Lu(β-naphthyl)$_2$Li was 0.6 : 1 : 0.7.

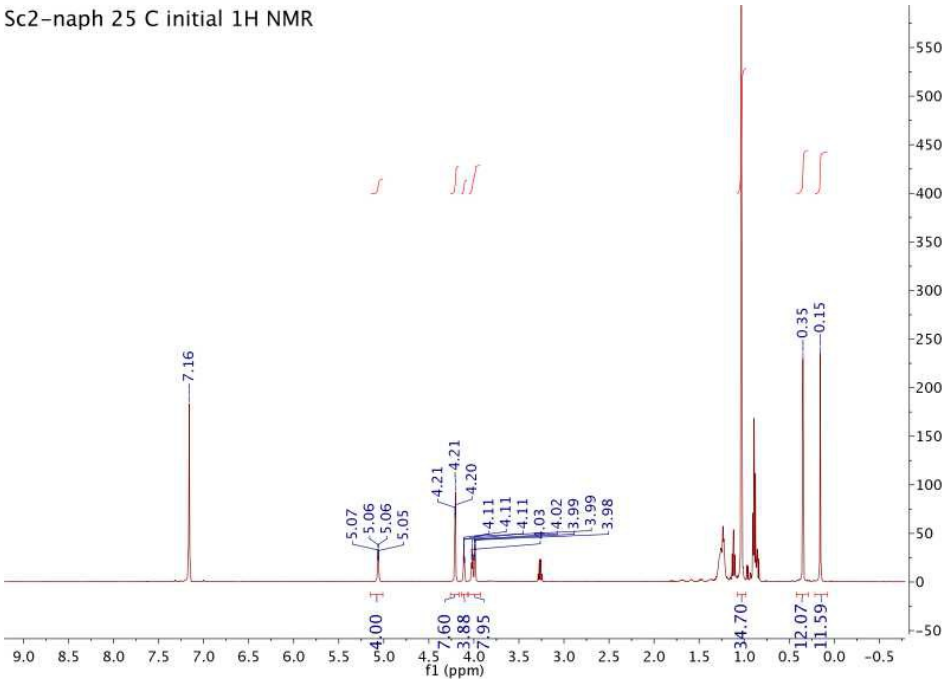


Figure S54. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of **5a** before heating. Labelled peaks are for **5a** and residue solvent peak (at 7.16 ppm), while unlabelled peaks are for residue hexanes and diethyl ether.

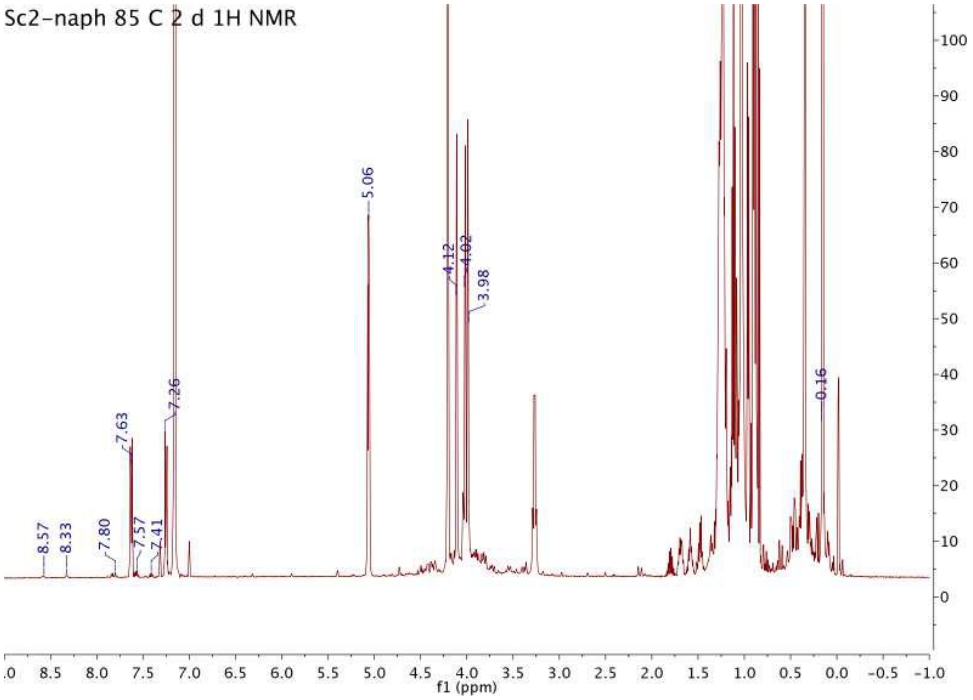


Figure S55. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of **5a** after heating at 85 °C for two days. Peaks at 8.57, 8.33, 7.80. 7.57, and 7.41 ppm were assigned to the scandium naphthyl species. Peaks at 7.63 and 7.26 ppm were from free naphthalene. Other labelled peaks were from **6a**.

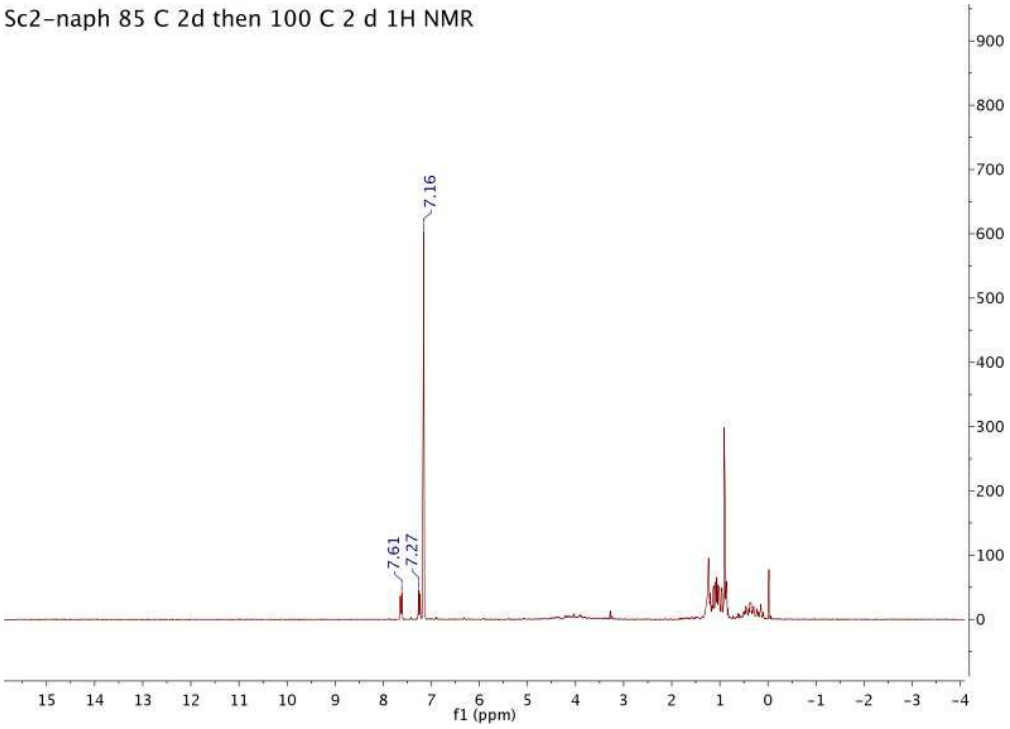


Figure S56. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of **5a** after heating at 85 °C for two days and then 100 °C for two days. Only free naphthalene could be identified with peaks at 7.61 and 7.27 ppm; other species could not be identified by ^{1}H NMR spectroscopy.

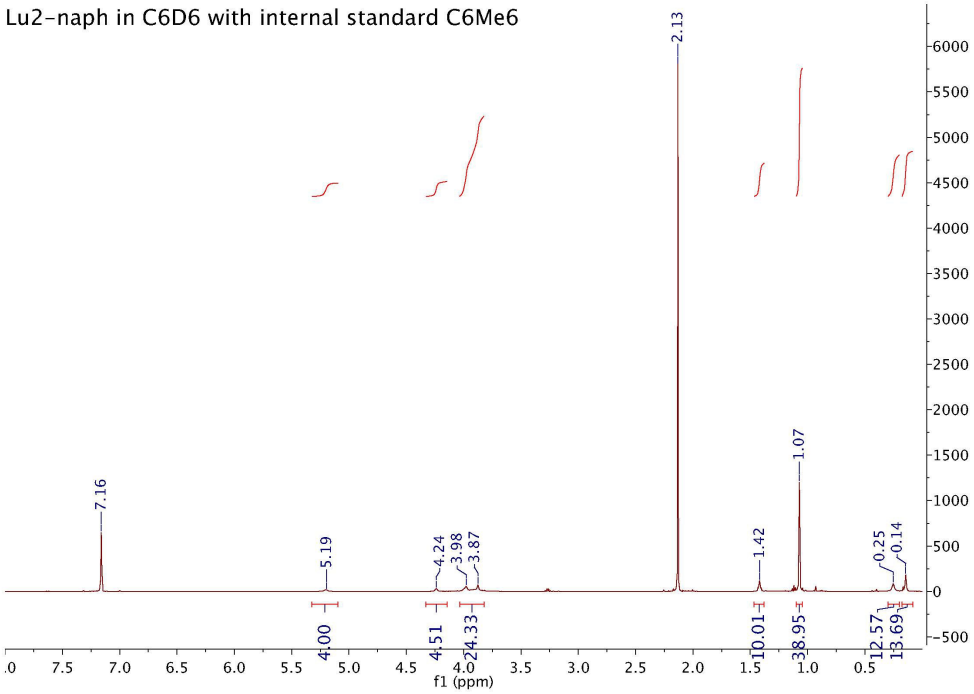


Figure S57. ^{1}H NMR spectrum of **5c** with internal standard C_6Me_6 for C-H activation study (C_6D_6, 300 MHz, 298 K).

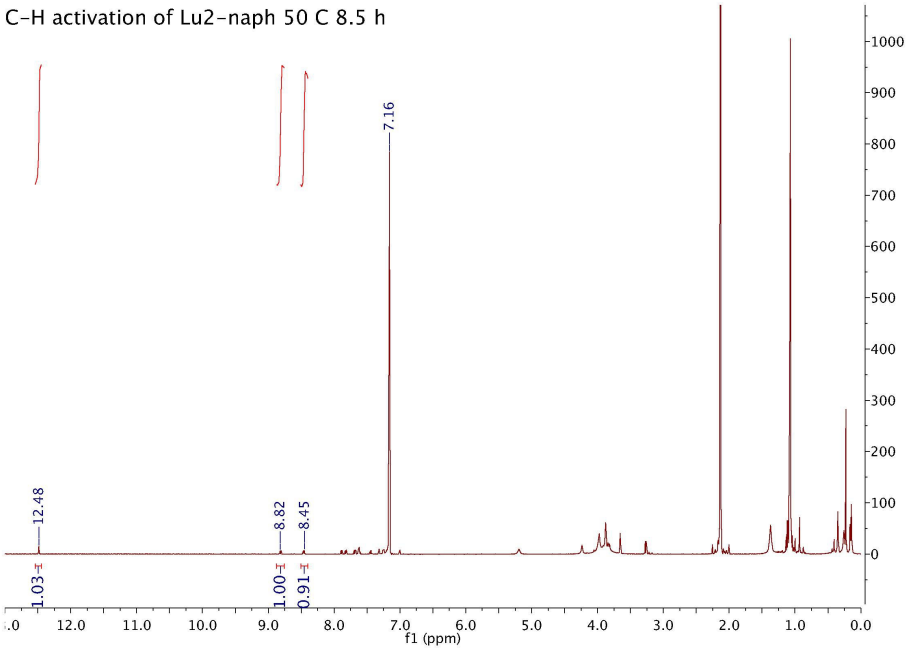


Figure S58. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of C-H activation of **5c** at 50 °C after 8.5 h. *Note*: The spectrum clearly shows that only one regioisomer of **6c** was formed in the

reaction, however, we were unable to determine which isomer (α-naphthyl or β-naphthyl). The relative integration between the hydride peak of **2c** (12.48 ppm) and the aromatic-CH peaks (8.82 and 8.45 ppm) of **6c** is close to 1.

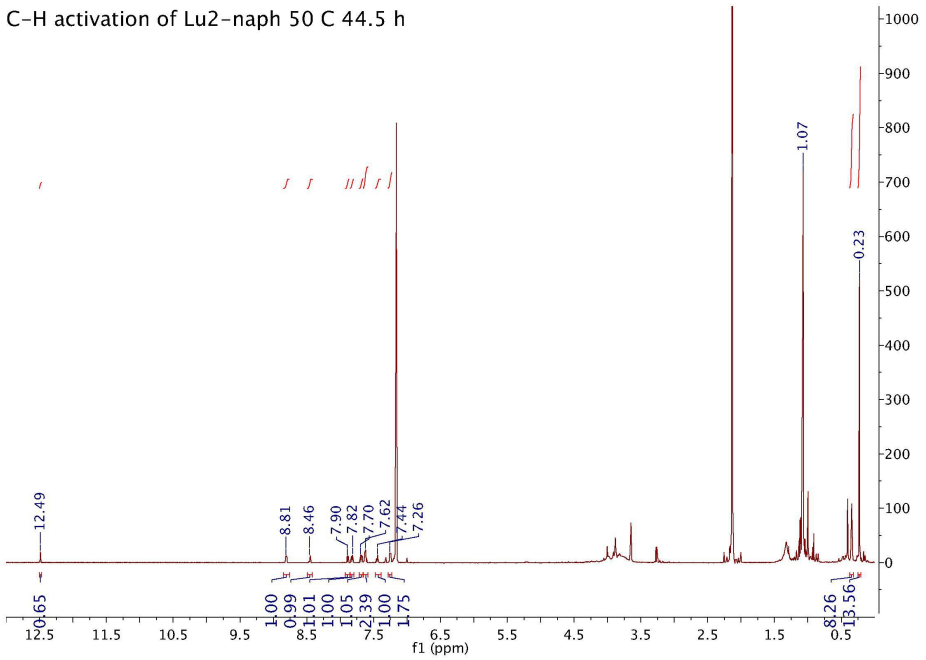


Figure S59. ^{1}H NMR spectrum (C_6D_6, 300 MHz, 298 K) of C-H activation of **5c** at 50 °C after 44.5 h. *Note*: The relative integration between the hydride peak of **2c** (12.48 ppm) and the aromatic peaks (8.82, 8.45, 7.90, 7.82, and 7.62 ppm) of **6c** is now smaller than 1 due to the thermal decomposition of **2c** after prolonged heating.

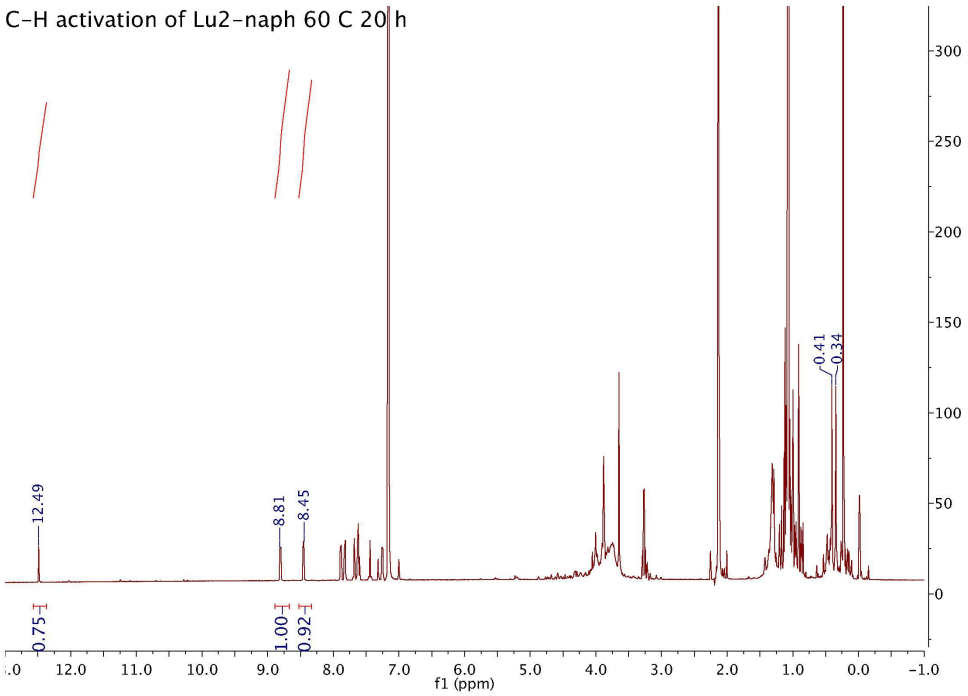


Figure S60. ^{1}H NMR (C_6D_6, 300 MHz, 298 K) spectrum of C-H activation of **5c** at 60 °C after 20.0 h. Labelled peaks indicate the formation of **2c** and **6c**. The reaction was completed after 20.0 h at 60 °C.

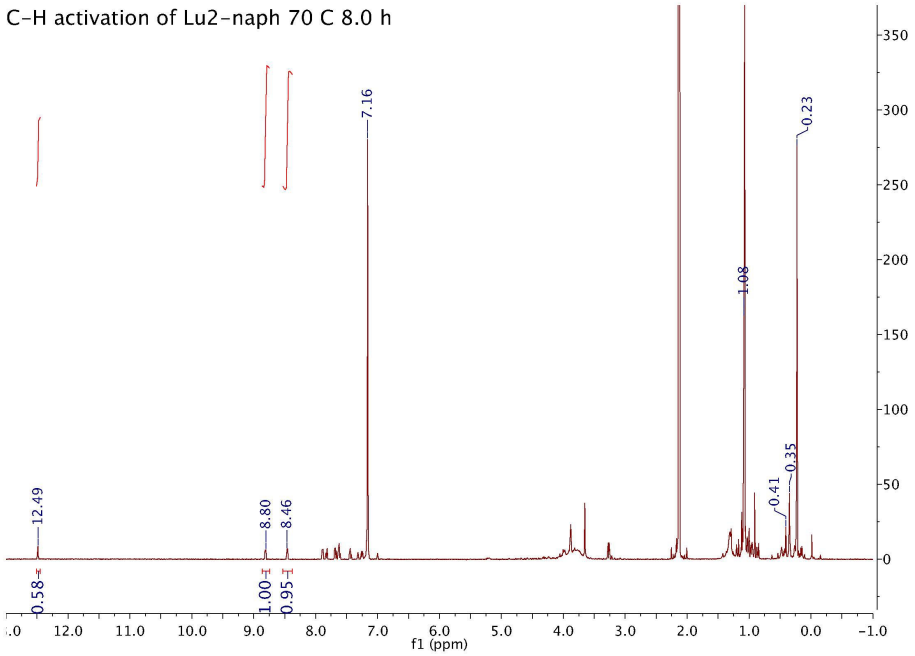


Figure S61. ^{1}H NMR (C_6D_6, 300 MHz, 298 K) spectrum of C-H activation of **5c** at 70 °C after 8.0 h. Labelled peaks indicate the formation of **2c** and **6c**. The reaction was completed after 8.0 h at 70 °C.

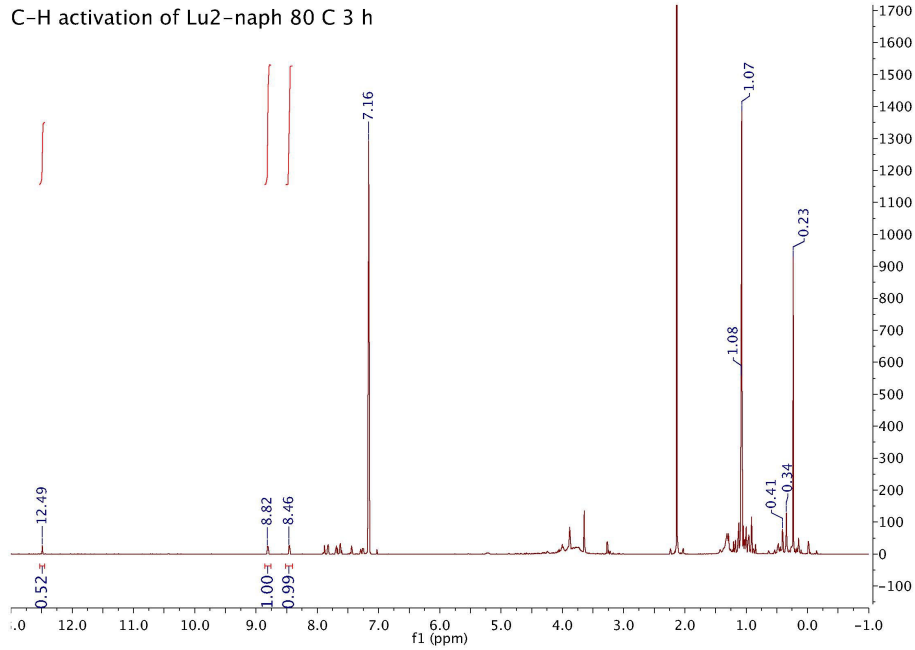


Figure S62. ^{1}H NMR (C_6D_6, 300 MHz, 298 K) spectrum of C-H activation of **5c** at 80 °C after 3.0 h. Labelled peaks indicate the formation of **2c** and **6c**. The reaction was completed after 3.0 h at 80 °C.

4. X-ray crystallography data

[(NN^{fc})Sc(THF)](μ-H)$_2$[Sc(NN^{fc})] (2a)

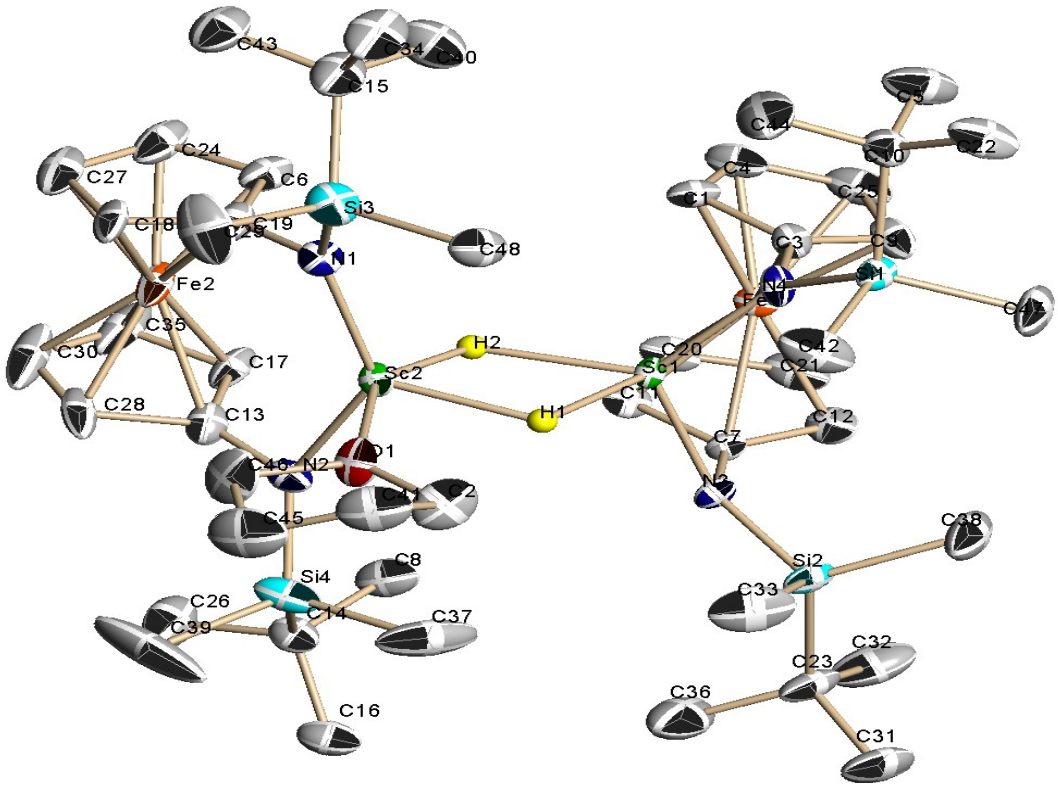


Figure S63. Thermal-ellipsoid (50% probability) representation of **2a** (code: pld1004). Hydrogen atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a diethyl ether solution layered with *n*-pentane. Crystal data for $C_{52}H_{96}Fe_2N_4O_2Sc_2Si_4$; M_r = 1123.31; Triclinic; space group P-1; *a* = 12.729(6) Å; *b* = 14.432(7) Å; *c* = 17.929(8) Å; α = 89.220(5)°; β = 72.659(6)°; γ = 76.126(6)°; V = 3046(2) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 0.797 mm^{-1}; d_{calc} = 1.225 g·cm^{-3}; 14943 reflections collected; 13856 unique (R_{int} = 0.1091); giving R_1 = 0.0943, wR_2 =

0.2420 for 9594 data with [I>2σ(I)] and R_1 = 0.1165, wR_2 = 0.2580 for all 13856 data. Residual electron density ($e^{-}\cdot Å^{-3}$) max/min: 1.266/-1.728.

(NN^{fc})Sc(*p*-Me-C$_6$H$_4$)(THF) (4p)

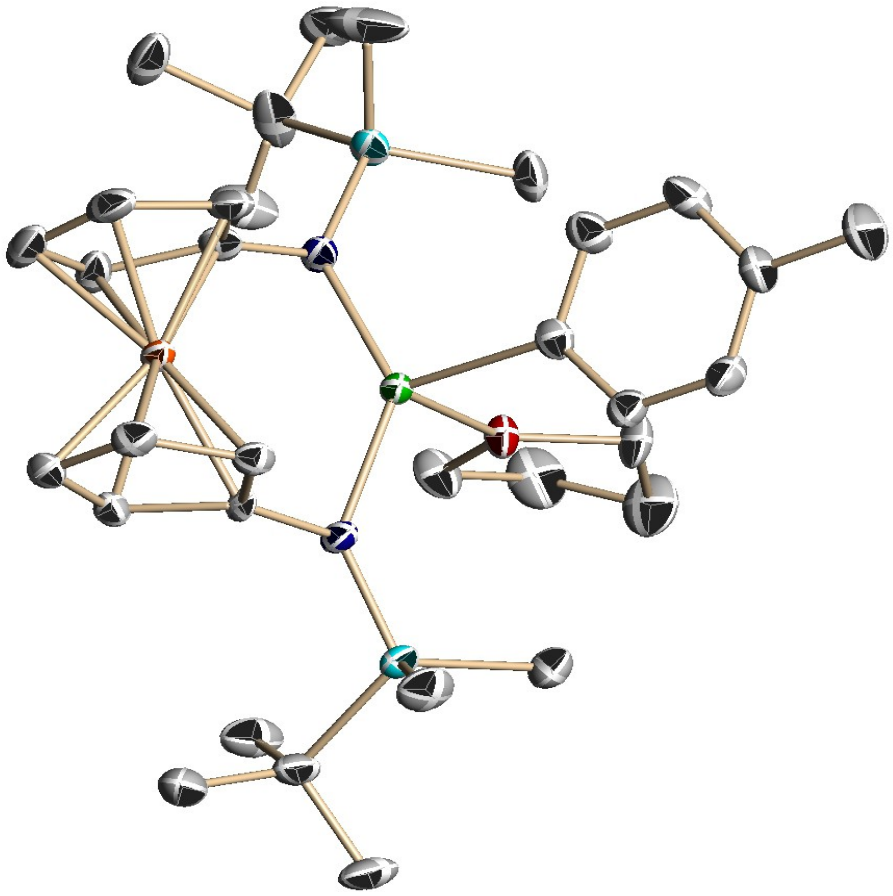


Figure S64. Thermal-ellipsoid (50% probability) representation of **4p** (code: pld1235sad). Hydrogen and solvent atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a concentrated toluene solution layered with hexanes. Crystal data for $C_{71}H_{117}Fe_2N_4O_2Sc_2Si_4$; M_r = 1372.67; Orthorhombic; space group Pbcn; *a* = 24.002(3) Å; *b* = 15.7124(16) Å; *c* = 20.586(2) Å; α = 90°; β = 90°; γ = 90°; V = 7763.5(14) Å^3; Z = 4; T = 100(2) K; λ = 0.71073 Å; μ = 0.637 mm^{-1}; d_{calc} = 1.174 g·cm^{-3}; 73849 reflections collected; 11376 unique (R_{int} = 0.0331); giving R_1 = 0.0632, wR_2 = 0.1593 for 9335 data with [I>2σ(I)] and R_1 = 0.0760, wR_2 = 0.1656 for all 11376 data. Residual electron density ($e^{-}\cdot Å^{-3}$) max/min: 1.337/-1.137.

(NN^{fc})Sc(*o*-Me-C$_6$H$_4$)(THF) (4o)

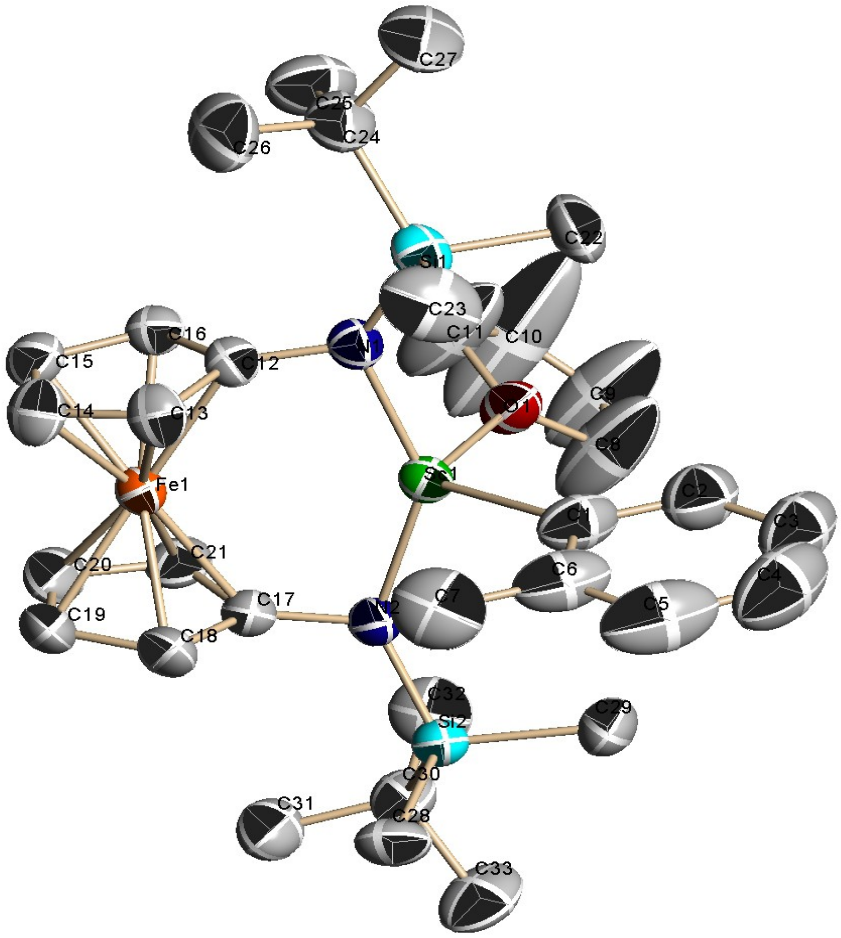


Figure S65. Thermal-ellipsoid (50% probability) representation of **4o** (code: pld1212sm). Hydrogen atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a concentrated THF solution layered with *n*-pentane. Crystal data for $C_{33}H_{53}FeN_2OScSi_2$; M_r = 650.76; Orthorhombic; space group P2(1)2(1)2(1)1; *a* = 14.381(2) Å; *b* = 14.514(2) Å; *c* = 17.253(3) Å; α = 90°; β = 90°; γ = 90°; V = 3601.3(10) Å^3; Z = 4; T = 100(2) K; λ = 0.71073 Å; μ = 0.684 mm^{-1}; d_{calc} = 1.200 g·cm^{-3}; 32710 reflections collected; 8902 unique (R_{int} = 0.0264); giving R_1 = 0.0584, wR_2 = 0.1634 for

7719 data with [I>2σ(I)] and R_1 = 0.0675, wR_2 = 0.1744 for all 8902 data. Residual electron density ($e^{-}\cdot Å^{-3}$) max/min: 2.088/-1.202.

[(NN^{fc})Y(THF)](μ-H)$_2$[Y(NN^{fc})] (2b)

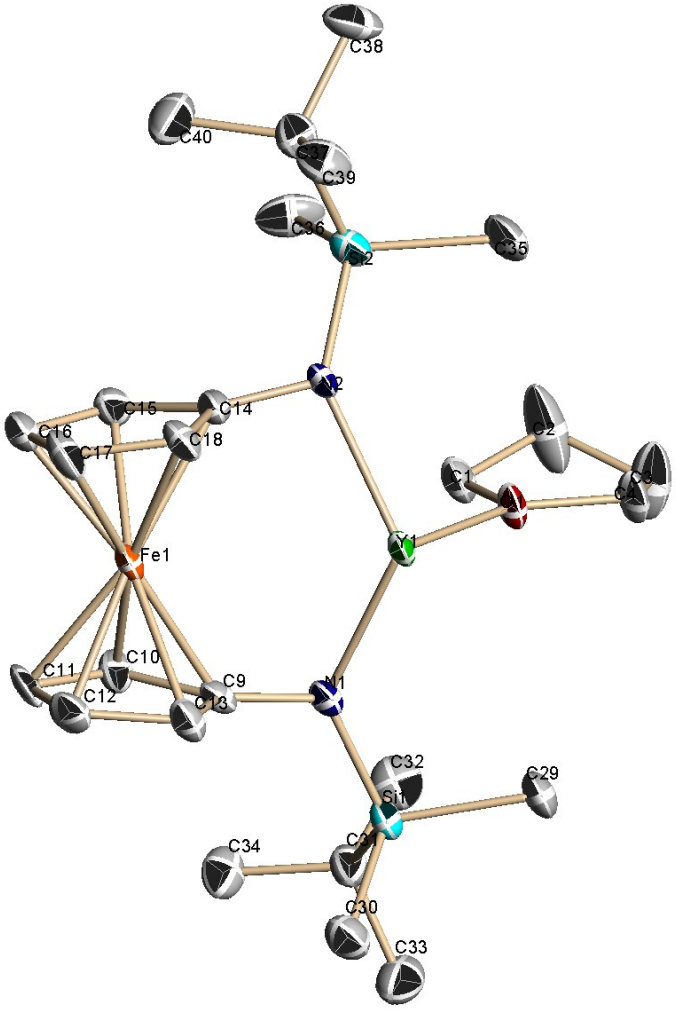


Figure S66. Thermal-ellipsoid (50% probability) representation of **2b** (code: pld1134sad). Hydrogen atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a THF solution layered with *n*-pentane. Crystal data for $C_{26}H_{46}FeN_2OSi_2Y$; M_r = 603.59; Triclinic; space group P-1; *a* = 11.618(6) Å; *b* = 15.479(6) Å; *c* = 16.953(7) Å; α = 77.348(5)°; β = 87.648(5)°; γ = 88.981(3)°;V = 2972(2) $Å^3$; Z = 4; T = 100(2) K; λ = 0.71073 Å; μ = 2.531 mm^{-1}; d_{calc} = 1.349 $g\cdot cm^{-3}$;20307 reflections collected; 10229 unique (R_{int} = 0.0405); giving R_1 = 0.0957, wR_2 = 0.2607 for 7885

data with [I>2σ(I)]and R_1 = 0.1156, wR_2 = 0.2659 for all 10229 data. Residual electron density ($e^-.Å^{-3}$) max/min: 5.332/-1.175.

$(NN^{fc})Y(C_6H_5)(THF)_2$ (3b)

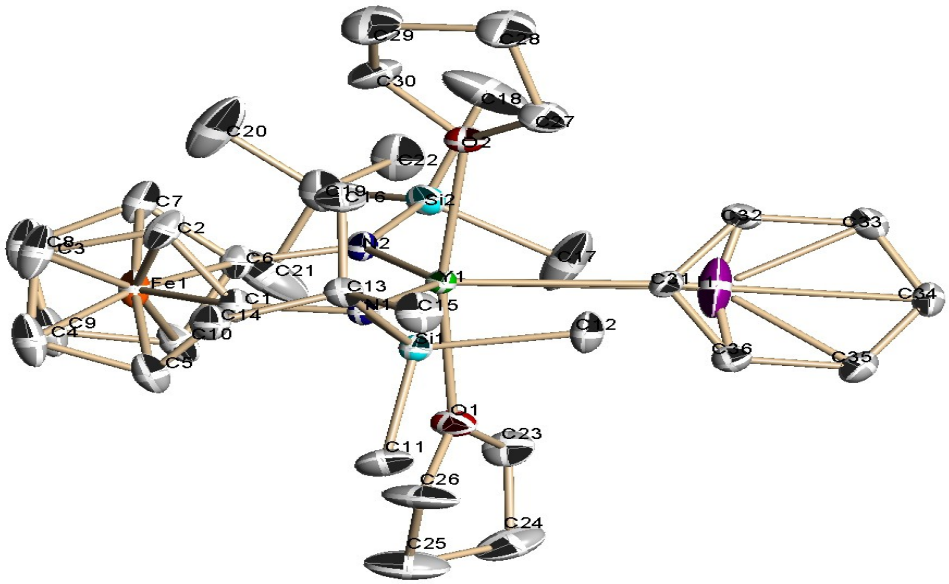


Figure S67. Thermal-ellipsoid (50% probability) representation of **3b** (code: pld1216sm). Hydrogen and solvent atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a diethyl ether solution. Crystal data for $C_{35.08}H_{58.22}FeI_{0.15}N_2O_2Si_2Y$; M_r = 760.28; Monoclinic; space group P(2)1/n; *a* = 9.7595(10) Å; *b* = 29.761(3) Å; *c* = 12.8474(13) Å; α = 90°; β = 94.5390(10)°; γ = 90°; V = 3719.8(6) $Å^3$; Z = 4; T = 100(2) K; λ = 0.71073 Å; μ = 2.165 mm^{-1}; d_{calc} = 1.358g·cm^{-3}; 25972 reflections collected; 6548 unique (R_{int} = 0.0237); giving R_1 = 0.0346, wR_2 = 0.0721 for 6104 data with [I>2σ(I)]and R_1 = 0.0380, wR_2 = 0.0731 for all 6548 data. Residual electron density (e^- ·$Å^{-3}$) max/min: 0.721/-0.323.

[(NN^{fc})Lu(THF)](μ-H)$_2$[Lu(NN^{fc})] (2c)

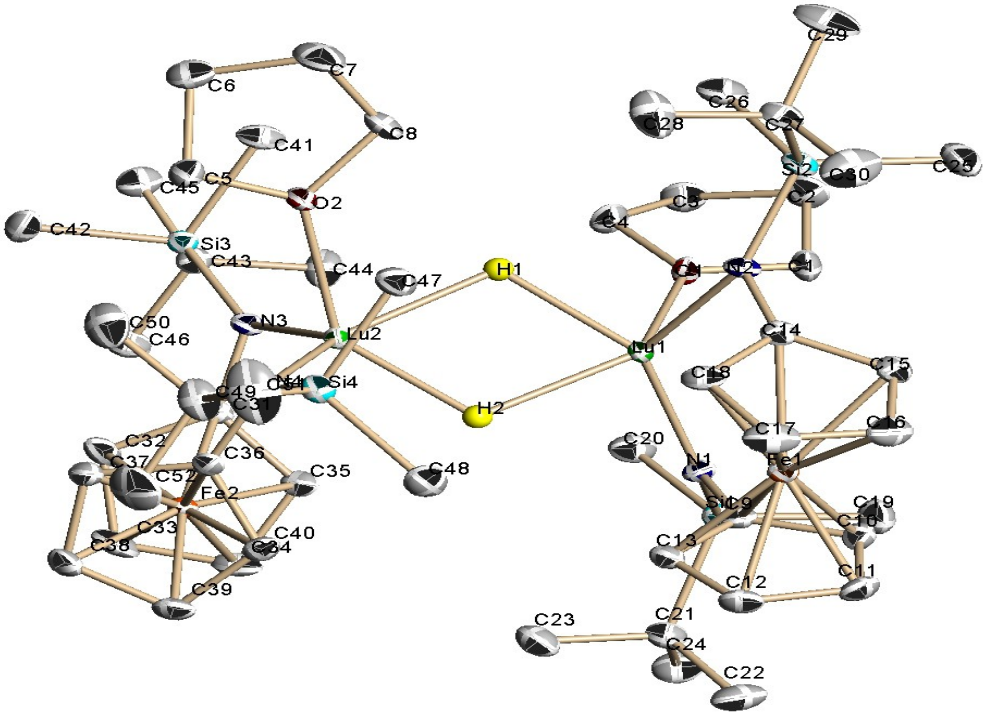


Figure S68. Thermal-ellipsoid (50% probability) representation of **2c** (code: pld1121s). Hydrogen atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a THF solution layered with *n*-pentane. Crystal data for $C_{52}H_{94}Fe_2Lu_2N_4O_2Si_4$; M_r = 1381.31; Triclinic; space group P-1; *a* = 10.8150(10) Å; *b* = 12.4852(11) Å; *c* = 23.535(2) Å; α = 95.9360(10)°; β = 100.1200(10)°; γ = 104.3810(10)°; V = 2994.2(5) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 3.862 mm^{-1}; d_{calc} = 1.532 g·cm^{-3}; 15326 reflections collected; 9671 unique (R_{int} = 0.0196); giving R_1 = 0.0232, wR_2 = 0.0555 for 8565 data with [I>2σ(I)] and R_1 = 0.0286, wR_2 = 0.0574 for all 9671 data. Residual electron density (e$^-$·Å^{-3}) max/min: 1.331/-0.904.

$(NN^{fc})Lu(C_6H_5)(THF)_2$ (3c)

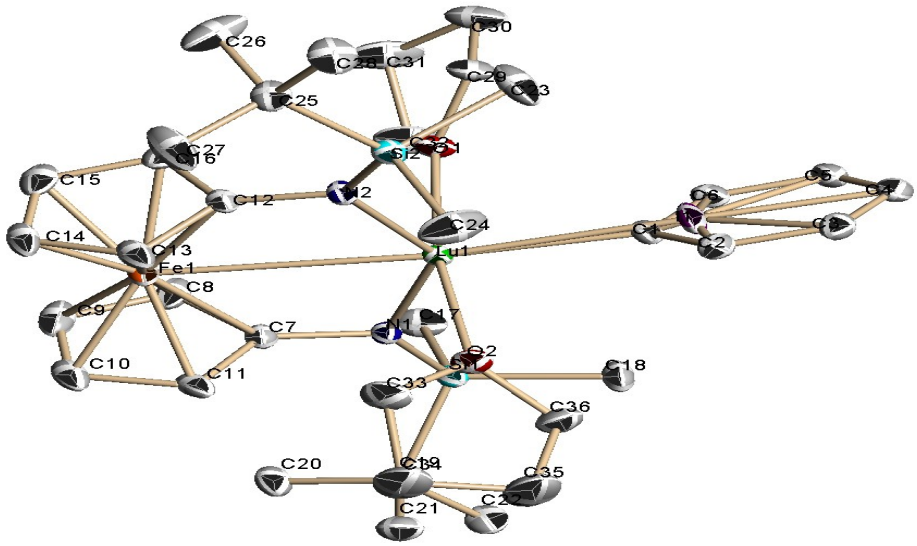


Figure S69. Thermal-ellipsoid (50% probability) representation of **3c** (code pld1219sm). Hydrogen and solvent atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a diethyl ether solution. Crystal data for $C_{35.70}H_{58.75}FeI_{0.05}LuN_2O_2Si_2$; M_r = 841.31; Monoclinic; space group P2(1)/n; *a* = 9.7679(12) Å; *b* = 29.678(4) Å; *c* = 12.8261(16) Å; α = 90°; β = 94.3910(10)°; γ = 90°; V = 3707.2(8) $Å^3$; Z = 4; T = 105(2) K; λ = 0.71073 Å; μ = 3.177 mm^{-1}; d_{calc} = 1.507 $g \cdot cm^{-3}$; 25908 reflections collected; 6525 unique (R_{int} = 0.0233); giving R_1 = 0.0193, wR_2 = 0.0404 for 6036 data with [I>2σ(I)]and R_1 = 0.0222, wR_2 = 0.0413 for all 6525 data. Residual electron density ($e^- \cdot Å^{-3}$) max/min: 0.956/-0.470.

(NN^{fc})Lu(α-$C_{10}H_7$)(THF)$_2$ (6c-α)

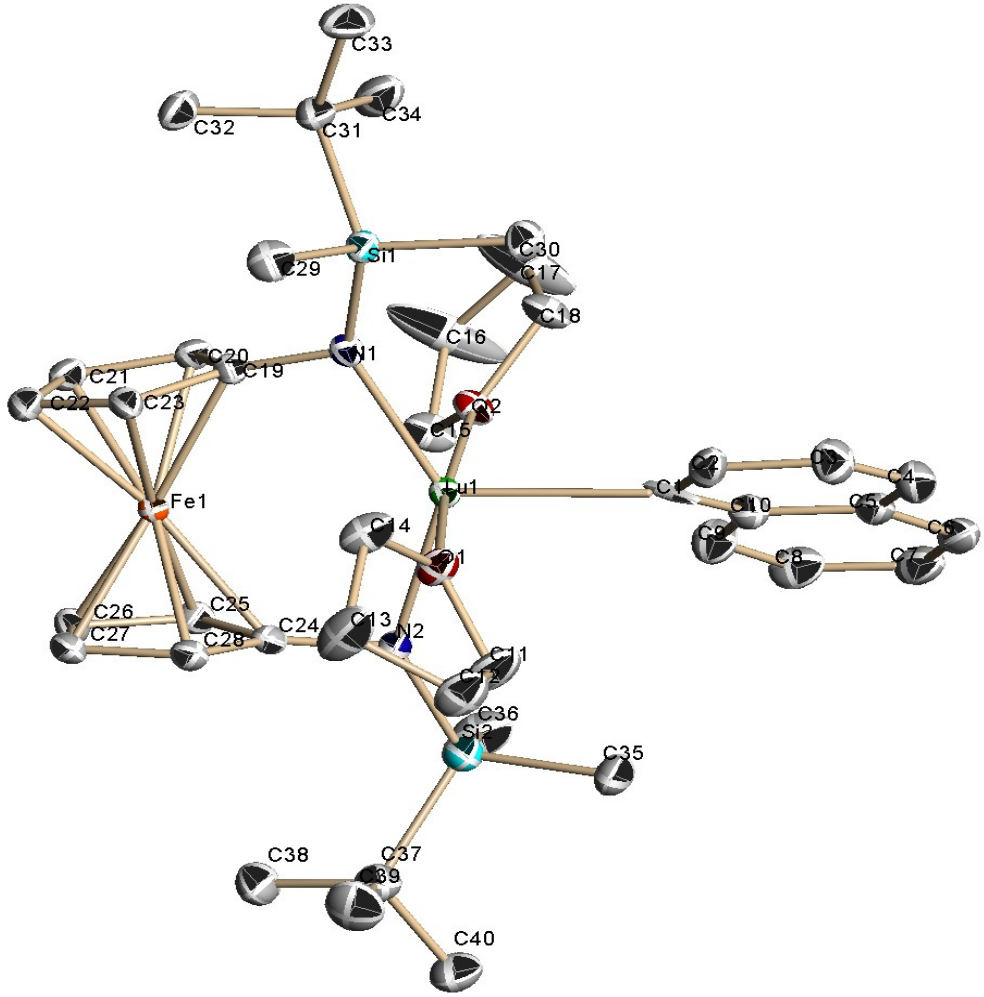


Figure S70. Thermal-ellipsoid (50% probability) representation of **6c-α** (code: pld1324sm). Hydrogen atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a THF solution layered with *n*-pentane. Crystal data for $C_{40}H_{61}FeLuN_2O_2Si_2$; M_r = 888.91; Monoclinic; space group P2(1)/c; *a* = 15.367(5) Å; *b* = 13.525(4) Å; *c* = 19.513(6) Å; α = 90°; β = 104.036(3)°; γ = 90°; V = 3934(2)

Å^3; Z = 4; T = 100(2) K; λ = 0.71073 Å; μ = 2.960 mm^{-1}; d_{calc} = 1.501 g·cm^{-3}; 54345 reflections collected; 11674 unique (R_{int} = 0.0321); giving R_1 = 0.0380, wR_2 = 0.0916 for 10055 data with [I>2σ(I)] and R_1 = 0.0461, wR_2 = 0.0961 for all 11674 data. Residual electron density (e$^-$·Å^{-3}) max/min: 5.284/-2.427.

(NN^{fc})Lu(β-C$_{10}$H$_7$)$_2$Li(THF) (6c-β)

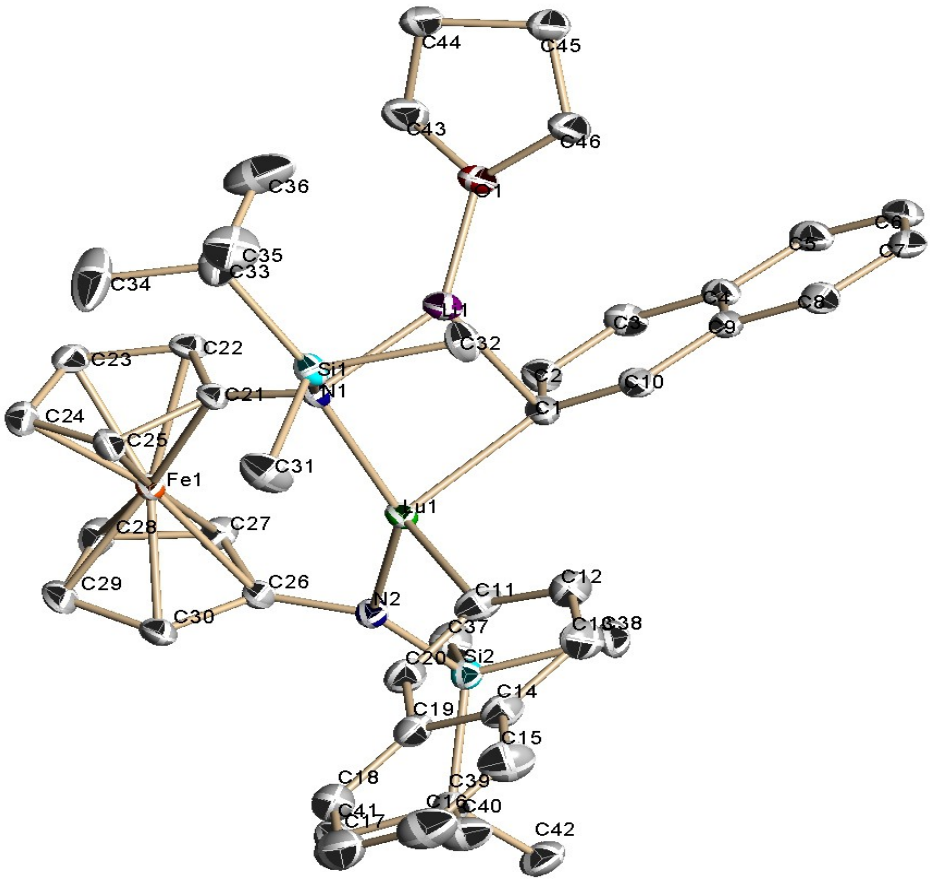


Figure S71. Thermal-ellipsoid (50% probability) representation of **6c-β** (code: pld1327sm). Hydrogen and solvent atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a concentrated hexanes solution. Crystal data for $C_{46}H_{60}FeLiLuN_2OSi_2$; M_r = 950.90; Triclinic; space group P-1; *a* = 11.682(4) Å; *b* = 11.922(4) Å; *c* = 17.793(5) Å; α = 80.603(3)°; β = 86.689(3)°; γ = 62.727(3)°;V = 2172.6(11) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 2.683 mm^{-1}; d_{calc} = 1.454 g.cm^{-3}; 28597 reflections collected; 12297 unique (R_{int} = 0.0274); giving R_1 = 0.0258, wR_2 = 0.0554 for 11015 data with

[I>2σ(I)] and R_1 = 0.0310, wR_2 = 0.0575 for all 12297 data. Residual electron density ($e^{-}.Å^{-3}$) max/min: 0.730/-0.839.

5. Optimized coordinates

*Optimized structure and free energy for **I***

21 10.989817000 8.029043000 0.871543000
26 8.555996000 9.844835000 0.921587000
14 9.954743000 6.302219000 3.829902000
14 13.278489000 10.742801000 1.376771000
7 9.757402000 7.276322000 2.340788000
7 11.739435000 9.931045000 0.945728000
6 12.030166000 5.201944000 0.225500000
6 8.569556000 7.931531000 1.965881000
6 7.830716000 8.951173000 2.681643000
1 8.069563000 9.308289000 3.670910000
6 6.739362000 9.392876000 1.860816000
1 6.007190000 10.139651000 2.128507000
6 6.815194000 8.704986000 0.603850000
1 6.142524000 8.830465000 -0.231146000
6 7.936419000 7.812684000 0.659150000
1 8.228195000 7.100837000 -0.100441000
6 10.552234000 10.646645000 0.656857000
6 9.755245000 11.454332000 1.556598000
1 9.996230000 11.646724000 2.590561000
6 8.607215000 11.939531000 0.846802000
1 7.830171000 12.569559000 1.252620000
6 8.648736000 11.411950000 -0.488201000
1 7.910950000 11.576514000 -1.258812000
6 9.831702000 10.615769000 -0.609176000
6 9.184239000 7.130197000 5.381550000
1 9.620918000 8.119625000 5.558929000
1 9.374067000 6.509448000 6.265958000
1 8.099915000 7.245240000 5.276056000
6 11.842948000 6.130582000 4.109438000
1 12.295732000 7.111113000 4.300453000
1 12.339008000 5.682551000 3.241031000
1 12.044296000 5.490797000 4.976950000
6 9.168597000 4.564043000 3.631824000
6 13.096387000 11.923674000 2.879954000
1 12.388738000 12.731764000 2.664299000
1 14.065046000 12.377507000 3.123211000
1 12.740257000 11.381874000 3.763670000
6 14.523467000 9.358374000 1.827661000
1 14.163139000 8.760088000 2.673171000
1 15.486572000 9.797599000 2.114169000
1 14.697967000 8.687755000 0.978737000
6 13.957228000 11.761519000 -0.100384000
6 12.375364000 6.564231000 -0.194601000
1 13.419587000 6.883423000 -0.157733000
6 11.398968000 7.179435000 -1.231899000

1	11.706855000	8.100080000	6	12.981494000	5.170232000
-1.723908000			-7.162987000		
6	10.529615000	6.310372000	1	13.412309000	4.175977000
-1.943465000			-6.999111000		
1	9.990683000	6.708511000	1	12.326276000	5.117161000
-2.799872000			-8.041274000		
6	10.387654000	4.959028000	1	13.795055000	5.867064000
-1.616960000			-7.390345000		
1	9.657789000	4.337357000	6	10.511355000	4.516464000
-2.118998000			-5.411498000		
6	11.062100000	4.456953000	1	10.882388000	3.506800000
-0.407717000			-5.201465000		
21	12.832589000	5.025700000	1	9.849066000	4.814867000
-2.205687000			-4.593226000		
26	15.807036000	5.642400000	1	9.917347000	4.474427000
-2.815014000			-6.332575000		
14	11.962812000	5.742786000	6	11.264617000	7.489173000
-5.639212000			-6.025563000		
14	13.568183000	1.532951000	6	14.372414000	0.818615000
-2.233093000			-3.826233000		
7	12.924663000	5.767731000	1	15.464467000	0.785925000
-4.121340000			-3.749120000		
7	13.897297000	3.286793000	1	14.016672000	-0.205632000
-2.009036000			-3.993881000		
6	14.202575000	6.368706000	1	14.105009000	1.421824000
-4.067313000			-4.701443000		
6	15.389947000	6.031714000	6	11.672542000	1.318488000
-4.827035000			-2.392970000		
1	15.440182000	5.275755000	1	11.265566000	1.934795000
-5.594243000			-3.202887000		
6	16.474815000	6.860022000	1	11.440008000	0.271181000
-4.383087000			-2.620289000		
1	17.483520000	6.841205000	1	11.156729000	1.583791000
-4.767209000			-1.464601000		
6	15.999729000	7.686996000	6	14.210581000	0.526229000
-3.311061000			-0.733740000		
1	16.582034000	8.407863000	1	14.157176000	11.114327000
-2.757569000			-0.961987000		
6	14.612619000	7.391502000	1	13.231349000	12.521922000
-3.112943000			-0.410709000		
1	13.947547000	7.897773000	1	14.889418000	12.270633000
-2.429464000			0.173042000		
6	15.210478000	3.790479000	1	15.073857000	5.052608000
-1.898944000			-0.035949000		
6	16.326284000	3.614734000	1	16.312899000	3.003167000
-2.806054000			-3.694040000		
6	17.431162000	4.402578000	1	15.288712000	0.672692000
-2.338739000			-0.601604000		
1	18.400533000	4.474532000	1	13.710332000	0.840775000
-2.808611000			0.188982000		
6	17.014254000	5.108876000	1	14.026890000	-0.545190000
-1.161528000			-0.879253000		
1	17.615670000	5.794735000	1	12.078091000	8.217193000
-0.584496000			-6.124037000		
6	15.658952000	4.738309000	1	10.696310000	7.482301000
-0.887468000			-6.963585000		

1 10.600153000 7.832636000 -5.224420000
1 9.299522000 3.967085000 4.542666000
1 8.094573000 4.648726000 3.429019000
1 9.628409000 4.027959000 2.794148000
1 10.172013000 10.108222000 -1.499042000
1 12.604090000 4.745038000 1.027567000
1 10.837606000 3.455348000 -0.061231000
Sum of electronic and thermal Free Energies= -3199.439504

Optimized structure and free energy for ***TS****$_{I\text{-}II}$*
21 2.199333000 0.382100000 0.376078000
26 3.525513000 -1.365321000 -1.513052000
14 4.581021000 3.057648000 0.039468000
14 3.012443000 -1.593594000 3.266360000
7 3.625685000 1.608470000 -0.422699000
7 2.703055000 -1.217125000 1.538908000
6 3.900258000 0.786862000 -1.534364000
6 5.088870000 0.012586000 -1.826344000
1 5.993720000 0.023722000 -1.239214000
6 4.857318000 -0.758866000 -3.013882000
1 5.564384000 -1.426608000 -3.482390000
6 3.508800000 -0.528331000 -3.446245000
1 3.028927000 -0.977500000 -4.302049000
6 2.914285000 0.411339000 -2.541340000
1 1.932411000 0.854367000 -2.635868000
6 2.965391000 -2.092323000 0.465896000
6 4.232534000 -2.629804000 0.016922000
1 5.178165000 -2.481917000 0.514739000
6 4.013723000 -3.378222000 -1.187406000
1 4.768819000 -3.903041000 -1.752979000
6 2.626515000 -3.271651000 -1.539265000
1 2.154412000 -3.715167000 -2.402380000
6 1.977991000 -2.480920000 -0.534363000
6 6.471846000 2.723045000 0.039032000
1 6.726959000 1.905651000 0.723267000
1 7.008107000 3.622239000 0.366401000
1 6.831913000 2.461699000 -0.962179000
6 4.026027000 3.528123000 1.807173000
1 4.310639000 2.752374000 2.527787000
1 2.940566000 3.667256000 1.862783000
1 4.503868000 4.465429000 2.116580000
6 4.229916000 4.506498000 -1.166129000
6 4.796054000 -2.238385000 3.566453000
1 4.972322000 -3.183078000 3.040143000
1 4.955529000 -2.413726000 4.637500000
1 5.539435000 -1.508641000 3.225455000
6 2.759122000 0.042935000 4.220613000
1 3.520178000 0.781460000 3.942561000
1 2.837553000 -0.129924000 5.300586000
1 1.771912000 0.472297000 4.015788000
6 1.781538000 -2.921144000 3.898452000
21 -1.946461000 0.276023000 0.147730000
26 -4.584093000 -0.871111000 0.978010000
14 -1.856311000 -2.249843000 -2.385671000
14 -3.403194000 3.021061000 -1.629116000
7 -2.014285000 -1.624500000 -0.701030000
7 -3.316426000 1.602864000 -0.526655000

6	-2.973003000	-2.132123000	1	-4.549345000	1.901522000
0.194947000			-3.585047000		
6	-4.292273000	-2.670587000	6	-1.694590000	3.173565000
-0.068028000			-2.476551000		
1	-4.708544000	-2.852244000	1	-1.487892000	2.305527000
-1.044887000			-3.113059000		
6	-4.952576000	-2.924863000	1	-1.666676000	4.069233000
1.182045000			-3.108783000		
1	-5.940029000	-3.344765000	1	-0.896678000	3.259408000
1.300188000			-1.730926000		
6	-4.095841000	-2.482472000	6	-3.794278000	4.624594000
2.239339000			-0.655177000		
1	-4.306813000	-2.531203000	1	0.749788000	-2.559400000
3.296559000			3.823650000		
6	-2.883486000	-1.990754000	1	1.861301000	-3.840148000
1.643480000			3.306432000		
1	-1.996166000	-1.695528000	1	1.983779000	-3.170809000
2.183802000			4.947103000		
6	-4.457065000	1.114121000	1	-4.012509000	1.670463000
0.160781000			2.295442000		
6	-5.576722000	0.378839000	1	-5.701970000	0.133065000
-0.388863000			-1.432195000		
6	-6.461695000	0.021472000	1	-4.754505000	4.537821000
0.681719000			-0.133780000		
1	-7.381548000	-0.535309000	1	-3.017680000	4.816534000
0.585042000			0.092659000		
6	-5.897313000	0.505571000	1	-3.848899000	5.486178000
1.911249000			-1.331731000		
1	-6.320355000	0.375491000	1	-2.107835000	-4.700395000
2.896025000			-1.846334000		
6	-4.671823000	1.171481000	1	-1.246006000	-4.482259000
1.602134000			-3.382809000		
6	-3.450814000	-2.082929000	1	-0.399009000	-4.237822000
-3.453100000			-1.836685000		
1	-3.886652000	-1.082238000	1	4.818669000	5.390601000
-3.355486000			-0.892792000		
1	-3.190566000	-2.239462000	1	4.488012000	4.228101000
-4.507800000			-2.194467000		
1	-4.215464000	-2.820476000	1	3.168753000	4.778998000
-3.187715000			-1.145291000		
6	-0.517353000	-1.197296000	1	0.915501000	-2.285881000
-3.252961000			-0.458800000		
1	-0.807937000	-0.140099000	1	0.006187000	0.886355000
-3.278250000			-0.222943000		
1	0.452960000	-1.276761000	6	0.314858000	1.363445000
-2.755070000			0.984677000		
1	-0.401370000	-1.536244000	6	0.212555000	2.837312000
-4.289970000			0.946566000		
6	-1.350271000	-4.098318000	6	-0.557370000	0.724207000
-2.360772000			2.007950000		
6	-4.755811000	2.784956000	6	-0.563659000	3.551114000
-2.969867000			1.824239000		
1	-5.744760000	2.662030000	1	0.830383000	3.374858000
-2.514344000			0.228626000		
1	-4.792398000	3.660731000	6	-1.324355000	1.528964000
-3.629417000			2.916599000		

1 -0.282000000 -0.278070000 2.349522000
6 -1.365062000 2.904115000 2.826517000
1 -0.541273000 4.638249000 1.792150000
1 -1.878176000 1.020779000 3.704662000
1 -1.959177000 3.495759000 3.514171000
Sum of electronic and thermal Free Energies= -3199.410131

Optimized structure and free energy for ***II***
21 11.200096000 7.700079000 0.369761000
26 8.192394000 8.407611000 0.059160000
14 10.619498000 6.597056000 3.733157000
14 11.827491000 11.283763000 0.605265000
7 10.228043000 6.960713000 2.005214000
7 11.087683000 9.726652000 0.037469000
6 8.884631000 7.025216000 1.551801000
6 7.818702000 7.875445000 2.043799000
1 7.905289000 8.564627000 2.867739000
6 6.645077000 7.649269000 1.250856000
1 5.690660000 8.137226000 1.379086000
6 6.971646000 6.695127000 0.229541000
1 6.306243000 6.336037000 -0.540873000
6 8.338932000 6.312159000 0.405653000
1 8.880060000 5.592334000 -0.185461000
6 9.759614000 9.789836000 -0.461698000
6 8.610452000 10.454151000 0.121028000
1 8.619273000 11.028214000 1.033886000
6 7.467113000 10.214664000 -0.712106000
1 6.467813000 10.583910000 -0.537728000
6 7.872280000 9.362853000 -1.793201000
1 7.235611000 8.983495000 -2.577781000
6 9.272369000 9.100833000 -1.645748000
6 9.207009000 7.078078000 4.939368000
1 9.053100000 8.162147000 4.971686000
1 9.479831000 6.746083000 5.948838000
1 8.258763000 6.602742000 4.669002000
6 12.171571000 7.600413000 4.233614000
1 11.970125000 8.674972000 4.150867000
1 13.041061000 7.362903000 3.613723000
1 12.430785000 7.383582000 5.277377000
6 10.942443000 4.720626000 3.975036000
6 11.287496000 11.733815000 2.396207000
1 10.209650000 11.914294000 2.468345000
1 11.805713000 12.644134000 2.722929000
1 11.543537000 10.926669000 3.092479000
6 13.735271000 11.168690000 0.613835000
1 14.104951000 10.374644000 1.269090000
1 14.139794000 12.122405000 0.975265000
1 14.123474000 10.995879000 -0.395286000
6 11.321468000 12.703355000 -0.577407000
21 12.883811000 5.692485000 -1.632256000
26 15.603182000 4.283697000 -3.078966000
14 12.588823000 7.793060000 -4.430341000
14 11.944701000 2.417892000 -0.581024000
7 13.444236000 6.602672000 -3.358366000
7 13.006716000 3.689949000 -1.313852000
6 14.705110000 6.094080000 -3.764414000
6 14.972785000 5.185902000 -4.858952000

1	14.222752000	4.771091000	1	9.768274000	3.615770000
-5.514790000			-0.986189000		
6	16.383711000	4.936527000	1	9.629405000	2.471960000
-4.913215000			0.360096000		
1	16.888189000	4.293200000	1	10.414315000	4.038299000
-5.618362000			0.616408000		
6	17.006249000	5.658751000	6	12.778690000	1.671885000
-3.839266000			0.977381000		
1	18.058645000	5.652444000	1	11.688390000	12.503917000
-3.598230000			-1.590334000		
6	15.982776000	6.368814000	1	10.234254000	12.819255000
-3.132425000			-0.627805000		
1	16.120333000	7.010481000	1	11.753408000	13.650956000
-2.275894000			-0.233819000		
6	14.284492000	3.250426000	1	15.671740000	4.071683000
-1.762806000			-0.193549000		
6	14.578460000	2.462281000	1	13.845694000	2.127248000
-2.940651000			-3.658079000		
6	15.991741000	2.224060000	1	13.781791000	1.300797000
-2.989413000			0.739283000		
1	16.516432000	1.674942000	1	12.872707000	2.421352000
-3.756715000			1.771382000		
6	16.594849000	2.877255000	1	12.186027000	0.835029000
-1.861240000			1.366044000		
1	17.650068000	2.902725000	1	13.604472000	9.919529000
-1.634065000			-3.573702000		
6	15.553900000	3.507670000	1	11.988480000	10.230317000
-1.106420000			-4.240675000		
6	13.465945000	7.952736000	1	12.161741000	9.534351000
-6.125854000			-2.617627000		
1	13.424873000	7.020402000	1	11.180991000	4.505623000
-6.697599000			5.023935000		
1	12.971599000	8.736383000	1	10.051855000	4.143603000
-6.713144000			3.700950000		
1	14.518649000	8.228906000	1	11.774677000	4.368508000
-6.003993000			3.356592000		
6	10.798669000	7.170053000	1	9.888252000	8.533559000
-4.729981000			-2.324560000		
1	10.822464000	6.278751000	1	11.116518000	6.481607000
-5.368421000			-1.235544000		
1	10.298727000	6.896601000	6	13.460547000	6.912300000
-3.794426000			0.353095000		
1	10.196088000	7.936160000	6	13.815168000	5.970207000
-5.232810000			1.363705000		
6	12.578544000	9.535232000	6	14.472292000	7.855693000
-3.630238000			0.011333000		
6	11.593823000	0.988295000	6	15.067109000	5.977096000
-1.811690000			1.994976000		
1	12.516895000	0.476618000	1	13.094322000	5.214077000
-2.103229000			1.663121000		
1	10.928718000	0.251946000	6	15.728079000	7.873311000
-1.343737000			0.637510000		
1	11.106071000	1.363296000	1	14.269815000	8.594739000
-2.718748000			-0.758678000		
6	10.282156000	3.222684000	6	16.024661000	6.933961000
-0.101631000			1.632619000		

1 15.294389000 5.244404000 2.764129000
1 16.467500000 8.617320000 0.354924000
1 16.994678000 6.945231000 2.120595000
Sum of electronic and thermal Free Energies= -3199.473859

*Optimized structure and free energy for **ScPh***
26 14.960985000 7.430884000 3.085346000
21 16.452624000 10.512133000 3.123927000
14 15.990024000 10.601952000 -0.401367000
14 15.670833000 10.654496000 6.602823000
7 15.860336000 9.902548000 1.254803000
7 15.697596000 9.940652000 4.947089000
8 15.964037000 12.621214000 3.065641000
6 18.686070000 10.623069000 3.204827000
6 19.485877000 10.549758000 2.032947000
6 20.885838000 10.635004000 2.067532000
6 21.546580000 10.797602000 3.291238000
6 20.799004000 10.865352000 4.473320000
6 19.399727000 10.776635000 4.423426000
6 14.552434000 13.107213000 2.963215000
6 14.645094000 14.608421000 3.247626000
6 16.049551000 14.987382000 2.722561000
6 16.914349000 13.782610000 3.100066000
6 15.380298000 8.567674000 1.326639000
6 16.194064000 7.367044000 1.370353000
6 15.327499000 6.227320000 1.400494000
6 13.970499000 6.700116000 1.385673000
6 13.999277000 8.133072000 1.350878000
6 15.263451000 8.590773000 4.855478000
6 16.115997000 7.416447000 4.857899000
6 15.288539000 6.249199000 4.793435000
6 13.917993000 6.678364000 4.743254000
6 13.899481000 8.111661000 4.767476000
6 16.807027000 12.334947000 -0.308468000
6 17.051224000 9.488165000 -1.547838000
6 14.259962000 10.808616000 -1.212487000
6 16.757480000 9.641833000 7.817041000
6 16.336138000 12.452284000 6.541554000
6 13.884564000 10.709595000 7.307248000
1 22.630614000 10.862964000 3.324154000
1 21.459729000 10.569116000 1.146036000
1 19.004171000 10.407136000 1.067247000
1 18.851852000 10.814467000 5.363753000
1 21.305166000 10.979823000 5.429122000
1 17.347687000 12.494783000 6.123657000
1 15.681674000 13.101421000 5.949941000
1 16.376058000 12.853249000 7.561645000
1 13.885016000 11.115735000 8.326229000
1 13.236365000 11.339317000 6.686256000
1 13.449466000 9.704832000 7.340340000
1 16.425974000 15.911482000 3.170239000
1 16.028767000 15.120616000 1.635255000
1 17.717422000 13.559106000 2.399565000
1 17.308697000 13.841925000 4.116005000
1 14.573736000 14.801552000 4.323758000
1 13.847668000 15.166384000 2.748768000
1 14.207909000 12.884978000 1.949814000

1 13.968695000 12.541119000 3.690771000
1 16.983802000 12.701185000 -1.327154000
1 16.160487000 13.058021000 0.199717000
1 17.771276000 12.296820000 0.208948000
1 18.087540000 9.436005000 -1.195600000
1 16.653117000 8.468093000 -1.576012000
1 17.054717000 9.884386000 -2.570557000
1 17.194562000 7.443024000 4.905375000
1 15.632993000 5.226399000 4.764461000
1 17.273757000 7.358029000 1.377318000
1 15.636969000 5.194196000 1.451345000
1 13.085630000 6.082239000 1.421171000
1 13.145227000 8.793469000 1.348400000
1 13.055851000 6.032256000 4.671092000
1 13.025224000 8.743577000 4.726706000
1 14.357417000 11.226896000 -2.221845000
1 13.748057000 9.843209000 -1.290145000
1 13.626452000 11.480749000 -0.621380000
1 16.680742000 10.047886000 8.833044000
1 16.437605000 8.594376000 7.841183000
1 17.810222000 9.665702000 7.514072000
Sum of electronic and thermal Free Energies= -1947.510711

Optimized structure and free energy for THF
8 10.393713000 9.435182000 6.698734000
6 11.036504000 9.304227000 8.017048000
1 11.858945000 10.023438000 8.065976000
1 11.447045000 8.290262000 8.110209000
6 9.931390000 9.565018000 9.054115000
1 9.851401000 10.637559000 9.268680000
1 10.109318000 9.043042000 9.999261000
6 8.661928000 9.071349000 8.323137000
1 8.580709000 7.980373000 8.400045000
1 7.742274000 9.508816000 8.723504000
6 8.932415000 9.489439000 6.868673000
1 8.590341000 10.514432000 6.673532000
1 8.481874000 8.820450000 6.130237000
Sum of electronic and thermal Free Energies= -232.292901

Optimized structure and free energy for ***Sc_2H_2***
21 14.453099000 9.384941000 4.616079000
21 11.204652000 9.661725000 4.725689000
26 16.228423000 9.529695000 2.215370000
26 9.260389000 9.921391000 1.772822000
14 16.336211000 11.906163000 6.331284000
14 15.966726000 6.339708000 5.716198000
14 10.887163000 13.157560000 4.941791000
14 10.385741000 6.245040000 4.670013000
7 10.596853000 11.540489000 4.189828000
7 10.284841000 7.952962000 4.081889000
7 15.376532000 7.562726000 4.542843000
7 15.618585000 11.031178000 4.938230000
8 10.394241000 9.678260000 6.772522000
6 15.213934000 11.401572000 2.455356000
1 14.148869000 11.573525000 2.510484000
6 11.069010000 9.578841000 8.103904000
1 11.903525000 10.277421000 8.092720000
1 11.442007000 8.557578000 8.202912000

6 16.075777000 11.187337000 3.609577000
6 16.017947000 11.404668000 1.270728000
1 15.661084000 11.545104000 0.261826000
6 10.634794000 11.517169000 1.624951000
1 11.698666000 11.398780000 1.488171000
6 15.816532000 7.638630000 3.202351000
6 17.418406000 11.023732000 3.087932000
1 18.294268000 10.811572000 3.680461000
6 16.054797000 13.794742000 6.169182000
6 14.940857000 7.826295000 2.053737000
1 13.861874000 7.809058000 2.097878000
6 17.172096000 7.715830000 2.694857000
1 18.065573000 7.654935000 3.295415000
6 9.632662000 8.111854000 2.827265000
6 11.498164000 5.184308000 3.524064000
6 11.973694000 14.264249000 3.814721000
6 10.254164000 8.077479000 1.518104000
1 11.313929000 7.970055000 1.345286000
6 8.554060000 11.695697000 2.643136000
1 7.784482000 11.741633000 3.398631000
6 9.971910000 11.571806000 2.912493000
6 15.744089000 7.973528000 0.877200000
1 15.377574000 8.121467000 -0.127238000
6 17.121626000 7.886592000 1.270833000
1 17.973319000 7.966307000 0.612242000
6 15.341787000 4.587371000 5.258766000
6 9.644832000 11.620821000 0.593851000
1 9.828365000 11.592510000 -0.469852000
6 17.381889000 11.189291000 1.662943000
1 18.229780000 11.132736000 0.997087000
6 8.358333000 11.736428000 1.222958000
1 7.409535000 11.812185000 0.713115000
6 8.214408000 8.301942000 2.606430000
1 7.473675000 8.384220000 3.387403000
6 9.237348000 14.085543000 5.273856000
1 8.673568000 14.222757000 4.344878000
1 9.436954000 15.075474000 5.702537000
1 8.605185000 13.529419000 5.976654000
6 7.973423000 8.365695000 1.194131000
1 7.015944000 8.515361000 0.718007000
6 15.276919000 6.856590000 7.425941000
1 15.702034000 7.815028000 7.746626000
1 15.538229000 6.104003000 8.179602000
1 14.186214000 6.952158000 7.404449000
6 9.235624000 8.229516000 0.521688000
1 9.389996000 8.262858000 -0.546465000
6 11.113557000 6.232410000 6.442344000
1 10.403831000 6.657798000 7.160405000
1 12.049381000 6.798132000 6.498542000
1 11.322609000 5.198814000 6.743366000
6 17.883245000 6.271040000 5.847876000
1 18.299574000 7.265030000 6.048357000
1 18.337658000 5.884174000 4.929309000
1 18.172304000 5.606707000 6.671873000
6 8.647116000 5.432850000 4.736595000
1 7.991661000 5.959636000 5.440298000

1 8.729349000 4.388133000 5.060845000
1 8.168902000 5.449242000 3.751412000
6 9.969238000 9.912032000 9.115257000
1 9.916338000 10.993839000 9.285181000
1 10.142655000 9.425952000 10.079691000
6 15.464492000 11.248780000 7.904539000
1 15.660508000 10.180161000 8.050626000
1 14.380941000 11.395591000 7.847707000
1 15.836404000 11.782800000 8.787339000
6 8.680043000 9.413487000 8.423127000
1 8.574561000 8.329456000 8.545981000
1 7.779169000 9.889053000 8.821568000
6 8.910854000 9.769407000 6.952592000
1 8.618401000 10.794595000 6.709812000
1 8.465502000 9.074326000 6.239435000
6 18.223393000 11.598489000 6.529554000
1 18.444242000 10.525278000 6.561752000
1 18.576338000 12.048928000 7.465717000
1 18.792893000 12.043937000 5.706663000
6 11.782175000 12.915519000 6.617546000
1 12.686737000 12.309029000 6.501792000
1 11.127616000 12.437256000 7.353645000
1 12.079216000 13.894156000 7.013488000
1 12.915112000 9.406687000 5.858799000
1 12.527580000 5.559636000 3.528010000
1 11.508690000 4.138365000 3.854477000
1 11.129031000 5.212757000 2.492847000
1 15.717404000 3.844568000 5.973098000
1 14.247380000 4.551983000 5.262457000
1 15.685619000 4.302932000 4.257668000
1 16.500539000 14.175010000 5.242909000
1 14.984693000 14.026481000 6.149558000
1 16.511171000 14.327789000 7.012171000
1 12.971166000 13.828693000 3.687433000
1 11.521904000 14.376722000 2.823037000
1 12.087734000 15.262586000 4.254676000
1 12.825164000 9.601748000 3.571098000

Sum of electronic and thermal Free Energies= -3200.864710

*Optimized structure and free energy for **IV***

21 2.337533000 -0.390867000 1.281218000
26 3.708479000 0.939901000 3.460403000
14 0.568321000 -2.606196000 3.500415000
14 5.133363000 -2.589630000 0.653947000
7 1.383698000 -1.111011000 2.927492000
7 4.250781000 -1.109503000 1.155187000
6 0.004556000 3.190700000 0.116326000
1 0.278690000 4.197297000 -0.186221000
6 -1.022574000 2.999159000 1.053393000
1 -1.528412000 3.859345000 1.480743000
6 -1.401772000 1.704607000 1.420708000
1 -2.206774000 1.546349000 2.130455000
6 -0.721700000 0.602819000 0.879177000
1 -0.993467000 -0.400267000 1.190551000
6 0.307031000 0.768181000 -0.071119000
6 1.826131000 -0.085838000 3.790580000
6 2.711102000 -0.177988000 4.933972000

1	3.105839000	-1.096536000	6	3.872040000	-3.695542000
5.339525000			-0.268231000		
6	2.980838000	1.145902000	1	3.029693000	-3.965963000
5.417418000			0.378733000		
1	3.601590000	1.395739000	1	4.357336000	-4.624748000
6.264507000			-0.589656000		
6	2.317853000	2.082896000	1	3.478022000	-3.199718000
4.557354000			-1.162426000		
1	2.337987000	3.157872000	6	6.583791000	-2.141956000
4.651236000			-0.515189000		
6	1.612053000	1.339906000	6	1.052619000	-0.394896000
3.555645000			-0.656848000		
1	0.941653000	1.754244000	1	0.551685000	-1.350430000
2.816086000			-0.798115000		
6	4.827902000	-0.058884000	6	2.315918000	-0.083655000
1.892637000			-1.376723000		
6	5.512543000	-0.098262000	1	3.010639000	-0.883799000
3.168091000			-1.605547000		
1	5.765232000	-0.996043000	6	2.622293000	1.217391000
3.709844000			-1.729132000		
6	5.780589000	1.247284000	1	3.560898000	1.427953000
3.591255000			-2.234014000		
1	6.289111000	1.534965000	6	1.607604000	2.254506000
4.498971000			-1.616525000		
6	5.220396000	2.145581000	1	1.893682000	3.271127000
2.624678000			-1.869369000		
1	5.247449000	3.223704000	6	0.652647000	2.100199000
2.665189000			-0.493322000		
6	4.630771000	1.355299000	21	0.549377000	0.681973000
1.582475000			-3.058482000		
6	1.733281000	-3.752764000	26	-0.892255000	-1.781416000
4.509574000			-4.501404000		
1	2.642138000	-3.982967000	14	2.624655000	1.116771000
3.942132000			-5.900524000		
1	1.224137000	-4.696699000	14	-2.431495000	2.614927000
4.740522000			-3.480167000		
1	2.029298000	-3.290840000	7	1.527827000	0.222290000
5.458082000			-4.796136000		
6	-0.006917000	-3.548157000	7	-1.435951000	1.120033000
1.936973000			-3.358078000		
1	0.839304000	-3.819543000	6	1.067510000	-1.083095000
1.295204000			-5.074986000		
1	-0.705039000	-2.944892000	6	0.294121000	-1.541052000
1.346415000			-6.210518000		
1	-0.518337000	-4.474636000	1	-0.000546000	-0.926816000
2.224040000			-7.046349000		
6	-0.943359000	-2.164566000	6	-0.022192000	-2.929113000
4.591144000			-6.025926000		
6	5.842290000	-3.579899000	1	-0.586376000	-3.546439000
2.139454000			-6.708668000		
1	6.639409000	-3.023966000	6	0.503569000	-3.344825000
2.645350000			-4.757543000		
1	6.266406000	-4.528440000	1	0.418320000	-4.330327000
1.787430000			-4.325315000		
1	5.060116000	-3.805984000	6	1.169896000	-2.219495000
2.873003000			-4.170721000		

1 1.719896000 -2.221101000 -3.241295000
6 -1.999055000 -0.145294000 -3.644814000
6 -2.578218000 -0.606389000 -4.889868000
6 -2.962979000 -1.981384000 -4.740590000
1 -3.422713000 -2.597422000 -5.498691000
6 -2.596868000 -2.407677000 -3.419579000
1 -2.741087000 -3.395286000 -3.007979000
6 -2.006219000 -1.290297000 -2.747268000
6 2.041832000 1.083333000 -7.729735000
1 1.027315000 1.486471000 -7.826097000
1 2.713760000 1.697443000 -8.342091000
1 2.050127000 0.066035000 -8.135176000
6 2.660312000 2.940514000 -5.316650000
1 1.658684000 3.383866000 -5.354602000
1 3.036414000 3.035001000 -4.292367000
1 3.315435000 3.526403000 -5.972821000
6 4.403289000 0.397163000 -5.832697000
6 -3.405560000 2.726542000 -5.134370000
1 -4.159333000 1.936404000 -5.216624000
1 -3.921808000 3.693489000 -5.185814000
1 -2.731582000 2.654031000 -5.995821000
6 -1.249560000 4.118195000 -3.410440000
1 -0.577357000 4.127443000 -4.276235000
1 -1.833010000 5.047116000 -3.423873000
1 -0.642801000 4.108130000 -2.500817000
6 -3.704212000 2.714259000 -2.049451000
1 6.214435000 -1.669227000 -1.431958000
1 7.273429000 -1.443214000 -0.027818000
1 7.147755000 -3.040436000 -0.793121000
1 -1.665597000 -1.264557000 -1.723267000
1 -2.682385000 -0.008158000 -5.780743000
1 -4.365478000 1.839946000 -2.062281000
1 -3.192446000 2.739378000 -1.081853000
1 -4.324444000 3.614315000 -2.142843000
1 4.401863000 -0.666258000 -6.098414000
1 5.063281000 0.924495000 -6.532289000
1 4.822695000 0.493930000 -4.824615000
1 -1.423132000 -3.074660000 4.970611000
1 -0.640093000 -1.555191000 5.449998000
1 -1.685130000 -1.596629000 4.019035000
1 4.214930000 1.734998000 0.658335000

Sum of electronic and thermal Free Energies= -3353.011006

*Optimized structure and free energy for **III***

21 -0.766314000 -0.067277000 2.783273000
26 1.072782000 0.729557000 5.073697000
14 -3.674875000 0.208955000 4.833034000
14 0.358407000 -3.495495000 3.022881000
7 -1.971970000 0.483064000 4.341378000
7 0.408648000 -1.704527000 3.165148000
6 -0.144532000 1.604138000 0.978133000
1 0.472909000 2.465261000 1.214002000
6 -1.575082000 1.701502000 1.148367000
1 -2.014126000 2.615102000 1.533870000
6 -2.354554000 0.584968000 0.901585000
1 -3.425560000 0.601406000 1.069116000
6 -1.714120000 -0.630958000 0.450424000

1 -2.319913000 -1.517685000 0.294888000
6 -0.410339000 -0.584715000 -0.131914000
6 -1.033651000 1.182346000 5.127415000
6 -0.517797000 0.835018000 6.435309000
1 -0.845799000 -0.006529000 7.024770000
6 0.499290000 1.780425000 6.796240000
1 1.065855000 1.780875000 7.715242000
6 0.664083000 2.702964000 5.708889000
1 1.366811000 3.521457000 5.671072000
6 -0.269029000 2.342906000 4.684608000
1 -0.434331000 2.872445000 3.757837000
6 1.423242000 -1.052100000 3.897394000
6 1.793775000 -1.224145000 5.288131000
1 1.353741000 -1.941273000 5.962562000
6 2.826513000 -0.281280000 5.611027000
1 3.307821000 -0.173262000 6.571293000
6 3.079293000 0.523703000 4.450162000
1 3.790554000 1.332619000 4.380356000
6 2.225842000 0.058201000 3.398778000
6 -3.843739000 -0.246110000 6.689279000
1 -3.301704000 -1.169596000 6.921764000
1 -4.901136000 -0.398928000 6.937958000
1 -3.456738000 0.551709000 7.332372000
6 -4.335068000 -1.248969000 3.780397000
1 -3.767412000 -2.163418000 3.987943000
1 -4.271001000 -1.039011000 2.706778000
1 -5.387691000 -1.441076000 4.020589000
6 -4.745430000 1.767707000 4.503536000
6 0.180206000 -4.371612000 4.725747000
1 1.074897000 -4.241453000 5.344240000
1 0.031229000 -5.447967000 4.573285000
1 -0.682243000 -3.981569000 5.278627000
6 -1.170016000 -3.964986000 1.972006000
1 -2.094346000 -3.572093000 2.410748000
1 -1.258006000 -5.057235000 1.923087000
1 -1.078684000 -3.582586000 0.951157000
6 1.951425000 -4.150753000 2.181222000
6 0.144532000 -1.604138000 -0.978133000
1 -0.472909000 -2.465261000 -1.214002000
6 1.575082000 -1.701502000 -1.148367000
1 2.014126000 -2.615102000 -1.533870000
6 2.354554000 -0.584968000 -0.901585000
1 3.425560000 -0.601406000 -1.069116000
6 1.714120000 0.630958000 -0.450424000
1 2.319913000 1.517685000 -0.294888000
6 0.410339000 0.584715000 0.131914000
21 0.766314000 0.067277000 -2.783273000
26 -1.072782000 -0.729557000 -5.073697000
14 3.674875000 -0.208955000 -4.833034000
14 -0.358407000 3.495495000 -3.022881000
7 1.971970000 -0.483064000 -4.341378000
7 -0.408648000 1.704527000 -3.165148000
6 1.033651000 -1.182346000 -5.127415000
6 0.517797000 -0.835018000 -6.435309000
1 0.845799000 0.006529000 -7.024770000
6 -0.499290000 -1.780425000 -6.796240000

1 -1.065855000 -1.780875000 -7.715242000
6 -0.664083000 -2.702964000 -5.708889000
1 -1.366811000 -3.521457000 -5.671072000
6 0.269029000 -2.342906000 -4.684608000
1 0.434331000 -2.872445000 -3.757837000
6 -1.423242000 1.052100000 -3.897394000
6 -1.793775000 1.224145000 -5.288131000
6 -2.826513000 0.281280000 -5.611027000
1 -3.307821000 0.173262000 -6.571293000
6 -3.079293000 -0.523703000 -4.450162000
1 -3.790554000 -1.332619000 -4.380356000
6 -2.225842000 -0.058201000 -3.398778000
6 3.843739000 0.246110000 -6.689279000
1 3.301704000 1.169596000 -6.921764000
1 4.901136000 0.398928000 -6.937958000
1 3.456738000 -0.551709000 -7.332372000
6 4.335068000 1.248969000 -3.780397000
1 3.767412000 2.163418000 -3.987943000
1 4.271001000 1.039011000 -2.706778000
1 5.387691000 1.441076000 -4.020589000
6 4.745430000 -1.767707000 -4.503536000
6 -0.180206000 4.371612000 -4.725747000
1 -1.074897000 4.241453000 -5.344240000
1 -0.031229000 5.447967000 -4.573285000
1 0.682243000 3.981569000 -5.278627000
6 1.170016000 3.964986000 -1.972006000
1 2.094346000 3.572093000 -2.410748000
1 1.258006000 5.057235000 -1.923087000
1 1.078684000 3.582586000 -0.951157000
6 -1.951425000 4.150753000 -2.181222000
1 2.061325000 -3.715098000 1.182318000
1 2.838447000 -3.883015000 2.766838000
1 1.921192000 -5.243081000 2.086857000
1 -2.225064000 -0.404571000 -2.375510000
1 -1.353741000 1.941273000 -5.962562000
1 -2.838447000 3.883015000 -2.766838000
1 -2.061325000 3.715098000 -1.182318000
1 -1.921192000 5.243081000 -2.086857000
1 4.363604000 -2.624924000 -5.070138000
1 5.786846000 -1.596534000 -4.802189000
1 4.731567000 -2.032659000 -3.440110000
1 -5.786846000 1.596534000 4.802189000
1 -4.363604000 2.624924000 5.070138000
1 -4.731567000 2.032659000 3.440110000
1 2.225064000 0.404571000 2.375510000

Sum of electronic and thermal Free Energies= -3353.020418

Optimized structure and free energy for ***TS****$_{IV\text{-}V}$*

21 1.910609000 0.242373000 0.157722000
26 2.761882000 -2.371035000 -1.120488000
14 4.705675000 1.941219000 -1.373266000
14 3.246238000 -0.821871000 3.325556000
7 3.400608000 0.713274000 -1.170926000
7 2.443157000 -0.974077000 1.714511000
6 3.333696000 -0.455377000 -1.956603000
6 4.344020000 -1.475392000 -2.155020000
1 5.348224000 -1.437120000 -1.765935000

6	3.783407000	-2.536802000	1	2.757717000	1.633398000
-2.941354000			3.675561000		
1	4.299818000	-3.430834000	1	2.896090000	0.780358000
-3.257079000			5.221760000		
6	2.406134000	-2.229045000	1	1.411894000	0.627319000
-3.196280000			4.257225000		
1	1.709220000	-2.839883000	6	2.944740000	-2.396741000
-3.749267000			4.372196000		
6	2.124202000	-0.957116000	21	-2.155290000	-0.053479000
-2.597340000			-0.096936000		
1	1.198193000	-0.405556000	26	-4.720282000	1.191147000
-2.676534000			0.140932000		
6	2.484687000	-2.202608000	14	-2.601073000	-2.123096000
1.014198000			2.863253000		
6	3.634987000	-3.015674000	14	-2.813215000	-1.696102000
0.675983000			-3.250057000		
1	4.655479000	-2.792469000	7	-2.747940000	-0.700609000
0.946190000			1.771998000		
6	3.192600000	-4.144995000	7	-2.999210000	-0.536762000
-0.091499000			-1.895124000		
1	3.822563000	-4.927719000	6	-3.739044000	0.290857000
-0.486579000			1.883726000		
6	1.773381000	-4.035799000	6	-5.180893000	0.138230000
-0.276388000			1.903319000		
1	1.148226000	-4.720167000	1	-5.702360000	-0.805756000
-0.829076000			1.915211000		
6	1.337515000	-2.850185000	6	-5.784118000	1.439279000
0.393998000			1.929451000		
6	6.418961000	1.159494000	1	-6.843277000	1.645640000
-1.755413000			1.964951000		
1	6.734577000	0.476922000	6	-4.740456000	2.420399000
-0.958126000			1.845833000		
1	7.164386000	1.961381000	1	-4.873470000	3.491227000
-1.827981000			1.820494000		
1	6.418810000	0.612374000	6	-3.486098000	1.726709000
-2.703778000			1.808120000		
6	4.868870000	2.911483000	1	-2.504424000	2.179777000
0.263846000			1.814128000		
1	5.180298000	2.246313000	6	-4.091893000	0.349926000
1.077831000			-1.759142000		
1	3.935856000	3.403019000	6	-5.469677000	0.025448000
0.553002000			-1.445229000		
1	5.634971000	3.688823000	6	-6.214348000	1.244497000
0.153414000			-1.332278000		
6	4.284978000	3.135054000	1	-7.267092000	1.325999000
-2.812670000			-1.107453000		
6	5.144245000	-0.557873000	6	-5.310403000	2.344159000
3.174270000			-1.525493000		
1	5.636078000	-1.429418000	1	-5.566092000	3.391557000
2.728008000			-1.472269000		
1	5.582604000	-0.393038000	6	-4.010345000	1.807206000
4.166534000			-1.779146000		
1	5.369244000	0.315133000	6	-4.124716000	-2.331387000
2.551466000			4.009594000		
6	2.502671000	0.706270000	1	-5.020517000	-2.624911000
4.200779000			3.452064000		

1 -3.913197000 -3.116765000 4.745482000
1 -4.346645000 -1.406954000 4.553445000
6 -2.420187000 -3.708324000 1.799386000
1 -3.313386000 -3.859739000 1.182096000
1 -1.548525000 -3.661460000 1.137313000
1 -2.295586000 -4.585867000 2.445627000
6 -1.046016000 -1.910983000 3.958144000
6 -4.460705000 -2.578256000 -3.683571000
1 -5.233858000 -1.859212000 -3.976348000
1 -4.305160000 -3.268489000 -4.521752000
1 -4.834236000 -3.156505000 -2.830867000
6 -1.533195000 -2.996425000 -2.675566000
1 -1.931848000 -3.585437000 -1.840832000
1 -1.298477000 -3.687360000 -3.494484000
1 -0.596800000 -2.528039000 -2.350670000
6 -2.177798000 -0.808802000 -4.828561000
1 1.876578000 -2.542350000 4.560990000
1 3.325426000 -3.286863000 3.859291000
1 3.458740000 -2.312458000 5.337224000
1 -3.114305000 2.370349000 -1.993812000
1 -5.853750000 -0.975473000 -1.322832000
1 -2.873729000 -0.018959000 -5.134568000
1 -1.199346000 -0.347526000 -4.651948000
1 -2.078309000 -1.516919000 -5.660337000
1 -1.169848000 -1.053608000 4.630023000
1 -0.871992000 -2.805787000 4.568238000
1 -0.158758000 -1.732384000 3.341057000
1 5.086108000 3.871871000 -2.948307000
1 4.164489000 2.580865000 -3.750730000
1 3.352415000 3.669839000 -2.607348000
1 0.320537000 -2.505102000 0.493242000
1 -0.038364000 -0.005210000 -0.487174000
6 -0.455400000 1.360683000 -0.234224000
6 -0.281128000 2.078361000 -1.511867000
6 0.338095000 3.290795000 -1.596129000
1 -0.728067000 1.648653000 -2.406071000
6 0.950534000 3.927244000 -0.448407000
6 0.348644000 1.887816000 0.865410000
1 0.117319000 1.531788000 1.874434000
6 0.951057000 3.212537000 0.792812000
6 1.511495000 5.218118000 -0.515712000
1 1.501781000 5.744716000 -1.466691000
6 1.502486000 3.855385000 1.929110000
1 1.479487000 3.342416000 2.886102000
6 2.053959000 5.825823000 0.615079000
1 2.475616000 6.823358000 0.552131000
6 2.037248000 5.139223000 1.842258000
1 2.439101000 5.613738000 2.732543000
1 0.356085000 3.824668000 -2.543993000

Sum of electronic and thermal Free Energies= -3352.983933

Optimized structure and free energy for ***$TS_{IV\text{-}VI}$***

21 1.969280000 0.040387000 -0.529001000
26 3.010819000 0.296260000 2.274479000
14 4.826168000 -1.996592000 -1.423558000
14 3.363575000 3.197500000 -1.415207000
7 3.527986000 -1.291602000 -0.392007000

7 2.534886000 1.997705000 -0.352686000
6 3.540863000 -1.391120000 1.013010000
6 4.590847000 -1.037371000 1.947873000
1 5.581302000 -0.711026000 1.675930000
6 4.089503000 -1.186230000 3.284985000
1 4.645139000 -1.005090000 4.192715000
6 2.710708000 -1.571734000 3.208443000
1 2.051654000 -1.749993000 4.044147000
6 2.367821000 -1.699230000 1.821336000
1 1.432560000 -2.072643000 1.427816000
6 2.655344000 2.046474000 1.054322000
6 3.850597000 2.176448000 1.862417000
1 4.851521000 2.300167000 1.479093000
6 3.484063000 2.091442000 3.247785000
1 4.160922000 2.157524000 4.086172000
6 2.068681000 1.868126000 3.326127000
1 1.491718000 1.741429000 4.229061000
6 1.559059000 1.835876000 1.989900000
6 6.597223000 -1.657769000 -0.754675000
1 6.776763000 -0.585216000 -0.617992000
1 7.329218000 -2.033755000 -1.480607000
1 6.778119000 -2.166904000 0.197704000
6 4.718774000 -1.197714000 -3.158933000
1 4.861888000 -0.112243000 -3.102796000
1 3.755069000 -1.398098000 -3.633961000
1 5.510547000 -1.608573000 -3.797267000
6 4.611774000 -3.895864000 -1.554514000
6 5.254930000 2.878991000 -1.554805000
1 5.770281000 3.110523000 -0.615787000
1 5.685478000 3.513396000 -2.339750000
1 5.460703000 1.832732000 -1.806240000
6 2.592848000 3.018375000 -3.157085000
1 2.749112000 2.013861000 -3.567571000
1 3.053304000 3.735618000 -3.846964000
1 1.516277000 3.215669000 -3.124391000
6 3.117756000 4.977221000 -0.752723000
21 -2.101166000 0.053184000 -0.041728000
26 -4.745711000 -0.318773000 -1.050545000
14 -2.362196000 3.685214000 -0.074789000
14 -2.788733000 -1.298388000 3.251344000
7 -2.605098000 1.980198000 -0.594136000
7 -2.966424000 -0.990712000 1.491567000
6 -3.644096000 1.538604000 -1.430923000
6 -5.073589000 1.743853000 -1.302178000
1 -5.544998000 2.368689000 -0.560537000
6 -5.743342000 1.005282000 -2.333832000
1 -6.809482000 0.978105000 -2.501777000
6 -4.759455000 0.265463000 -3.068868000
1 -4.949959000 -0.402812000 -3.894669000
6 -3.472092000 0.577083000 -2.518134000
1 -2.517517000 0.241834000 -2.900285000
6 -4.124441000 -1.342368000 0.756011000
6 -5.459853000 -0.789164000 0.873750000
6 -6.295169000 -1.388611000 -0.124526000
1 -7.341364000 -1.176757000 -0.285840000
6 -5.490679000 -2.287638000 -0.904193000

1 -5.827655000 -2.869868000 -1.748463000
6 -4.161552000 -2.260260000 -0.378956000
6 -3.859163000 4.805574000 -0.502211000
1 -4.730397000 4.579438000 0.121912000
1 -3.582771000 5.852569000 -0.327586000
1 -4.152033000 4.701985000 -1.552395000
6 -2.092916000 3.731501000 1.822759000
1 -2.969818000 3.333597000 2.346343000
1 -1.215492000 3.150125000 2.126457000
1 -1.933127000 4.764780000 2.154669000
6 -0.810102000 4.386306000 -0.945378000
6 -4.338899000 -0.762521000 4.248316000
1 -5.228330000 -1.321135000 3.936515000
1 -4.177712000 -0.951931000 5.316701000
1 -4.540493000 0.306958000 4.118703000
6 -1.286036000 -0.272906000 3.840325000
1 -1.494674000 0.800572000 3.759482000
1 -1.068331000 -0.494720000 4.892285000
1 -0.386409000 -0.494178000 3.255086000
6 -2.483158000 -3.161433000 3.594243000
1 2.061555000 5.262159000 -0.772442000
1 3.475065000 5.058911000 0.279906000
1 3.681691000 5.690066000 -1.366343000
1 -3.325200000 -2.850667000 -0.722853000
1 -5.759054000 -0.048724000 1.599163000
1 -3.305883000 -3.767209000 3.196795000
1 -1.553190000 -3.501932000 3.125056000
1 -2.411750000 -3.349095000 4.672542000
1 -0.970253000 4.443078000 -2.028430000
1 -0.579772000 5.393710000 -0.577503000
1 0.056468000 3.741975000 -0.760881000
1 5.357729000 -4.326376000 -2.233836000
1 4.734595000 -4.363298000 -0.570513000
1 3.611741000 -4.146040000 -1.922465000
1 0.525183000 1.732200000 1.700916000
1 0.041238000 -0.406468000 0.107147000
6 -0.432478000 -0.887346000 -1.172233000
6 -0.188837000 -2.360865000 -1.236875000
6 0.518892000 -2.946679000 -2.338840000
6 1.066629000 -2.107123000 -3.377279000
6 0.277449000 -0.106258000 -2.188831000
1 0.010584000 0.946432000 -2.306960000
6 0.944073000 -0.742951000 -3.290052000
6 0.663130000 -4.355682000 -2.391315000
6 0.154634000 -5.174776000 -1.391299000
6 -0.696205000 -3.222545000 -0.235862000
1 -1.230374000 -2.787839000 0.605525000
6 -0.524037000 -4.603761000 -0.298943000
1 1.571236000 -2.574663000 -4.216639000
1 1.346888000 -0.110558000 -4.078309000
1 -0.914387000 -5.236051000 0.492383000
1 0.285509000 -6.250829000 -1.449603000
1 1.196286000 -4.790677000 -3.232595000
Sum of electronic and thermal Free Energies= -3352.979979

*Optimized structure and free energy for **V***
21 11.140280000 7.755538000 0.388636000

26	8.119407000	8.402446000	0.033462000		
14	10.546581000	6.689285000	3.758812000		
14	11.678246000	11.356840000	0.581733000		
7	10.162122000	7.032058000	2.025928000		
7	10.990297000	9.775055000	0.015998000		
6	8.820303000	7.070104000	1.564112000		
6	7.742679000	7.919884000	2.030656000		
1	7.818056000	8.630500000	2.837497000		
6	6.575034000	7.659774000	1.239361000		
1	5.614643000	8.140036000	1.350861000		
6	6.916195000	6.681767000	0.245477000		
1	6.257790000	6.294756000	-0.517460000		
6	8.286830000	6.319320000	0.436541000		
1	8.839580000	5.591739000	-0.133918000		
6	9.670465000	9.798426000	-0.506306000		
6	8.498906000	10.457450000	0.036116000		
1	8.481648000	11.062609000	0.928542000		
6	7.374621000	10.169766000	-0.807706000		
1	6.365938000	10.525868000	-0.662226000		
6	7.813725000	9.291158000	-1.853233000		
1	7.198027000	8.875395000	-2.636111000		
6	9.216227000	9.061357000	-1.674350000		
6	9.134035000	7.196593000	4.954048000		
1	8.984049000	8.281683000	4.965593000		
1	9.403502000	6.882294000	5.970099000		
1	8.184643000	6.719769000	4.690349000		
6	12.104247000	7.687958000	4.249650000		
1	11.913850000	8.762450000	4.142627000		
1	12.977033000	7.429842000	3.643015000		
1	12.353504000	7.491249000	5.299680000		
6	10.854101000	4.813170000	4.023502000		
6	11.102151000	11.805355000	2.362164000		
1	10.018719000	11.955009000	2.420122000		
1	11.589982000	12.732874000	2.687303000		
1	11.372743000	11.011725000	3.068462000		
6	13.588266000	11.300269000	0.617292000		
1	13.973570000	10.522795000	1.283134000		
1	13.957090000	12.268999000	0.977077000		
1	13.996403000	11.132895000	-0.384936000		
6	11.150456000	12.753717000	-0.618774000		
21	12.888009000	5.735671000	-1.553092000		
26	15.646200000	4.347636000	-2.935857000		
14	12.619326000	7.809498000	-4.374583000		
14	11.942627000	2.452456000	-0.530962000		
7	13.468234000	6.640285000	-3.275287000		
7	13.017474000	3.733131000	-1.228128000		
6	14.747036000	6.149618000	-3.644397000		
6	15.060365000	5.247007000	-4.731523000		
1	14.336815000	4.823378000	-5.411005000		
6	16.475524000	5.016412000	-4.742262000		
1	17.010024000	4.381292000	-5.432587000		
6	17.054653000	5.743510000	-3.647493000		
1	18.098947000	5.750137000	-3.373501000		
6	16.000541000	6.439312000	-2.972132000		
1	16.101907000	7.083072000	-2.111889000		
6	14.305972000	3.300512000	-1.653812000		

6 14.625739000 2.521667000 -2.831284000
6 16.040651000 2.288986000 -2.854063000
1 16.582369000 1.748071000 -3.615362000
6 16.618746000 2.934924000 -1.708810000
1 17.668929000 2.962584000 -1.459882000
6 15.561246000 3.555984000 -0.969993000
6 13.528032000 7.967706000 -6.053603000
1 13.511806000 7.030177000 -6.618006000
1 13.034338000 8.739200000 -6.657291000
1 14.573909000 8.260353000 -5.912801000
6 10.845150000 7.156538000 -4.704481000
1 10.894438000 6.266478000 -5.343239000
1 10.334928000 6.872808000 -3.777471000
1 10.237380000 7.912734000 -5.215948000
6 12.567147000 9.559339000 -3.593004000
6 11.613248000 1.038568000 -1.785258000
1 12.541721000 0.530603000 -2.065906000
1 10.939408000 0.296478000 -1.339390000
1 11.142809000 1.425295000 -2.696526000
6 10.273437000 3.252585000 -0.067893000
1 9.773811000 3.656511000 -0.955626000
1 9.613030000 2.498011000 0.376276000
1 10.396672000 4.060776000 0.660103000
6 12.748196000 1.685183000 1.032319000
1 11.533288000 12.554279000 -1.625828000
1 10.061660000 12.844616000 -0.682443000
1 11.557025000 13.713753000 -0.278695000
1 15.661494000 4.108768000 -0.048460000
1 13.908338000 2.189825000 -3.565638000
1 13.751742000 1.308163000 0.805955000
1 12.836184000 2.427054000 1.834215000
1 12.142917000 0.849980000 1.404905000
1 13.586604000 9.957177000 -3.515968000
1 11.983758000 10.239836000 -4.225961000
1 12.125747000 9.565330000 -2.590807000
1 11.102802000 4.608721000 5.072096000
1 9.955317000 4.241111000 3.766099000
1 11.675477000 4.447045000 3.398651000
1 9.853911000 8.485222000 -2.325188000
1 11.099654000 6.491575000 -1.186133000
6 13.410098000 7.013198000 0.411746000
6 13.753818000 6.054136000 1.380078000
6 14.429738000 7.992132000 0.109580000
6 15.013038000 6.029530000 2.051852000
1 13.038996000 5.279460000 1.652410000
6 15.658315000 8.008696000 0.743208000
1 14.221310000 8.745950000 -0.643072000
6 15.334287000 5.044192000 3.030345000
6 15.987352000 7.034711000 1.729343000
1 16.394744000 8.769910000 0.496648000
6 16.561821000 5.052131000 3.662662000
1 14.595210000 4.284850000 3.269493000
6 17.243121000 7.015996000 2.399824000
6 17.523292000 6.047938000 3.344363000
1 16.798020000 4.297903000 4.406114000
1 17.978604000 7.777069000 2.155523000

1 18.483811000 6.043166000 3.849603000
Sum of electronic and thermal Free Energies= -3353.039583

*Optimized structure and free energy for **VI***
21 11.271707000 7.866752000 0.427292000
26 8.322808000 8.566508000 -0.044155000
14 10.506186000 6.449324000 3.649767000
14 11.875109000 11.346800000 1.158119000
7 10.230792000 6.988453000 1.946292000
7 11.142922000 9.918412000 0.329168000
6 8.915985000 7.105282000 1.418120000
6 7.842532000 7.954084000 1.896215000
1 7.902133000 8.605048000 2.753808000
6 6.705954000 7.789398000 1.037372000
1 5.756100000 8.291973000 1.140079000
6 7.063817000 6.870601000 -0.006633000
1 6.431111000 6.562312000 -0.825111000
6 8.412203000 6.452243000 0.216832000
1 8.971211000 5.752529000 -0.381193000
6 9.899356000 10.019712000 -0.331500000
6 8.663203000 10.623998000 0.125292000
1 8.534014000 11.161142000 1.049845000
6 7.639793000 10.375802000 -0.850596000
1 6.615159000 10.710392000 -0.789985000
6 8.199335000 9.569232000 -1.895169000
1 7.678309000 9.199202000 -2.764686000
6 9.580943000 9.348610000 -1.582855000
6 8.954820000 6.678298000 4.753512000
1 8.720718000 7.736186000 4.912476000
1 9.147860000 6.223567000 5.732949000
1 8.074195000 6.194015000 4.319286000
6 11.931849000 7.480422000 4.406071000
1 11.647610000 8.537521000 4.462395000
1 12.854587000 7.403454000 3.821952000
1 12.145464000 7.130075000 5.423515000
6 10.968647000 4.587266000 3.715156000
6 10.673072000 12.228633000 2.376635000
1 9.892943000 12.792371000 1.854931000
1 11.247524000 12.937368000 2.986495000
1 10.193511000 11.511098000 3.052466000
6 13.366420000 10.761422000 2.199860000
1 13.077481000 9.980645000 2.912269000
1 13.750281000 11.612625000 2.776102000
1 14.179031000 10.379463000 1.577846000
6 12.443667000 12.640849000 -0.136684000
21 12.964925000 5.845478000 -1.600692000
26 15.624721000 4.554036000 -2.971154000
14 12.057874000 7.256451000 -4.724651000
14 12.008197000 2.530817000 -0.630877000
7 13.167203000 6.481748000 -3.523768000
7 13.111686000 3.862471000 -1.153270000
6 14.474414000 6.090809000 -3.915787000
6 14.836200000 5.040593000 -4.844221000
1 14.135002000 4.417745000 -5.377027000
6 16.266516000 4.969486000 -4.921455000
1 16.835569000 4.279333000 -5.525929000
6 16.812021000 5.946942000 -4.021728000

1	17.861043000	6.121243000	1	13.238896000	12.229671000
-3.835350000			-0.767061000		
6	15.720686000	6.635708000	1	11.609646000	12.935034000
-3.402692000			-0.784110000		
1	15.793761000	7.449776000	1	12.825764000	13.540665000
-2.699031000			0.360722000		
6	14.447958000	3.528432000	1	15.663536000	4.759734000
-1.504953000			-0.059094000		
6	14.893814000	2.639664000	1	14.246648000	2.097726000
-2.558364000			-3.229062000		
6	16.328144000	2.620870000	1	13.720078000	1.273916000
-2.566898000			0.730348000		
1	16.949992000	2.053703000	1	12.766997000	2.349299000
-3.243069000			1.771736000		
6	16.793798000	3.521286000	1	12.073422000	0.813037000
-1.551210000			1.211506000		
1	17.825516000	3.745367000	1	13.225091000	9.473998000
-1.325958000			-4.925423000		
6	15.648517000	4.078840000	1	11.509220000	9.639219000
-0.896053000			-5.353204000		
6	12.471835000	6.736067000	1	11.998712000	9.563861000
-6.523108000			-3.649673000		
1	12.303080000	5.665534000	1	11.126745000	4.273031000
-6.682037000			4.754285000		
1	11.823394000	7.288044000	1	10.163726000	3.976520000
-7.214815000			3.291177000		
1	13.512829000	6.959963000	1	11.884053000	4.374151000
-6.777780000			3.152708000		
6	10.262532000	6.704506000	1	10.297449000	8.838091000
-4.349279000			-2.207909000		
1	10.143832000	5.641227000	1	11.212922000	6.608926000
-4.590225000			-1.140948000		
1	9.994736000	6.842358000	6	13.584894000	7.238685000
-3.297401000			0.303877000		
1	9.555192000	7.273596000	6	14.641445000	8.181058000
-4.965020000			-0.027000000		
6	12.208190000	9.170094000	6	13.850601000	6.353700000
-4.649949000			1.362755000		
6	11.760231000	1.201586000	6	14.481760000	9.143233000
-1.995876000			-1.068729000		
1	12.675212000	0.626857000	6	15.890281000	8.176977000
-2.173014000			0.694100000		
1	10.975234000	0.499816000	6	15.069424000	6.358440000
-1.687138000			2.096313000		
1	11.452429000	1.664137000	1	13.102804000	5.615196000
-2.940807000			1.643623000		
6	10.302366000	3.293222000	6	15.488282000	10.037589000
-0.243903000			-1.386051000		
1	9.850705000	3.720573000	1	13.542544000	9.169515000
-1.146627000			-1.609917000		
1	9.627461000	2.514811000	6	16.911400000	9.104926000
0.132319000			0.340927000		
1	10.371329000	4.078703000	6	16.067932000	7.248591000
0.514726000			1.760377000		
6	12.711843000	1.657269000	1	15.212564000	5.653868000
0.924302000			2.910160000		

6 16.717375000 10.016636000 -0.678289000
1 15.339918000 10.759550000 -2.182586000
1 17.846945000 9.086966000 0.893363000
1 17.007562000 7.255421000 2.306535000
1 17.500284000 10.721620000 -0.938168000
Sum of electronic and thermal Free Energies= -3353.035689

*Optimized structure and free energy for **VII***
71 12.864794000 5.085326000 -2.388415000
26 15.895426000 5.497053000 -2.895700000
14 13.479374000 1.438906000 -2.512368000
14 12.337308000 5.608964000 -6.035746000
7 13.851812000 3.165813000 -2.196726000
7 13.112599000 5.796462000 -4.429159000
6 15.172930000 3.628977000 -2.031382000
6 16.325145000 3.436147000 -2.886885000
1 16.337045000 2.834750000 -3.782250000
6 17.432471000 4.179263000 -2.354830000
1 18.427457000 4.218553000 -2.771851000
6 16.979183000 4.890537000 -1.194715000
1 17.573662000 5.544579000 -0.575291000
6 15.597178000 4.564886000 -0.997558000
1 14.988070000 4.872374000 -0.158726000
6 14.403849000 6.334713000 -4.272091000
6 15.640608000 5.968916000 -4.931257000
1 15.729026000 5.237659000 -5.718851000
6 16.716432000 6.735999000 -4.368673000
1 17.751000000 6.692811000 -4.673843000
6 16.187448000 7.537184000 -3.304102000
1 16.745364000 8.219725000 -2.681532000
6 14.775535000 7.286552000 -3.231734000
6 14.120579000 0.819366000 -4.216699000
1 13.769710000 1.472090000 -5.024238000
1 13.752129000 -0.195576000 -4.411464000
1 15.215352000 0.790381000 -4.250623000
6 11.572153000 1.274577000 -2.500556000
1 11.107251000 1.949345000 -3.229217000
1 11.165852000 1.506204000 -1.510086000
1 11.280070000 0.249475000 -2.757101000
6 14.231443000 0.322753000 -1.145946000
6 13.327683000 4.490885000 -7.247977000
1 14.264212000 4.963972000 -7.562953000
1 12.729798000 4.299450000 -8.147777000
1 13.566665000 3.526569000 -6.785126000
6 10.627379000 4.795134000 -5.758233000
1 10.727170000 3.804199000 -5.300720000
1 10.115352000 4.673651000 -6.720295000
1 9.993210000 5.407738000 -5.109183000
6 12.100164000 7.319984000 -6.873434000
71 10.858090000 8.044608000 0.915908000
26 8.369279000 9.738241000 1.151052000
14 13.033324000 10.950681000 1.574301000
14 10.097836000 6.536696000 4.224900000
7 11.542340000 10.064628000 1.114330000
7 9.760013000 7.265088000 2.623386000
6 10.303381000 10.708254000 0.875822000
6 9.462433000 11.420555000 1.813311000

1	9.707354000	11.599763000	1	12.579537000	7.002510000
2.848752000			4.083642000		
6	8.263740000	11.833048000	1	12.252254000	5.638428000
1.141263000			5.163075000		
1	7.450288000	12.389574000	1	12.201170000	5.399293000
1.581528000			3.409403000		
6	8.316013000	11.347989000	6	9.060649000	4.945150000
-0.208848000			4.481574000		
1	7.555375000	11.482348000	1	11.445801000	7.958876000
-0.962884000			-6.269950000		
6	9.555060000	10.651063000	1	13.062137000	7.832944000
-0.374959000			-6.986960000		
1	9.923216000	10.218378000	1	11.652499000	7.208636000
-1.293984000			-7.868439000		
6	8.528858000	7.814938000	1	8.286101000	6.925045000
2.237712000			0.172271000		
6	7.690901000	8.782746000	1	7.871291000	9.172846000
2.912422000			3.901582000		
6	6.586666000	9.122336000	1	7.988631000	5.169263000
2.058394000			4.436700000		
1	5.782774000	9.799876000	1	9.285224000	4.209720000
2.303534000			3.701560000		
6	6.759446000	8.444450000	1	9.274261000	4.492651000
0.808405000			5.457392000		
1	6.097779000	8.495883000	1	12.918601000	12.749189000
-0.042685000			-0.192057000		
6	7.958511000	7.655478000	1	14.581809000	12.565597000
0.902738000			0.401232000		
6	12.774351000	12.096716000	1	13.910582000	11.389674000
3.092366000			-0.749920000		
1	12.436875000	11.523194000	1	14.025860000	-0.735215000
3.962991000			-1.348668000		
1	13.715776000	12.594558000	1	15.318001000	0.454756000
3.354718000			-1.089635000		
1	12.029505000	12.871939000	1	13.808584000	0.576179000
2.881321000			-0.167529000		
6	14.329453000	9.611034000	1	14.074399000	7.818495000
2.012682000			-2.603357000		
1	14.022090000	9.038363000	1	13.402964000	6.836411000
2.895936000			-0.343197000		
1	14.472743000	8.912108000	6	12.320297000	6.650524000
1.180588000			-0.320934000		
1	15.297918000	10.074110000	6	11.827585000	5.295836000
2.235184000			0.106758000		
6	13.675193000	12.018407000	6	11.427478000	7.268545000
0.116024000			-1.414526000		
6	9.759575000	7.721192000	6	10.889353000	4.598773000
5.700555000			-0.610140000		
1	8.690582000	7.935430000	1	12.229001000	4.859205000
5.809538000			1.017603000		
1	10.105362000	7.261248000	6	10.532990000	6.486547000
6.634655000			-2.147355000		
1	10.290599000	8.670848000	1	11.646287000	8.281179000
5.570495000			-1.750748000		
6	11.963227000	6.104320000	6	10.384616000	5.087124000
4.213815000			-1.910943000		

1 10.538772000 3.638143000 -0.246379000
1 9.977556000 6.949421000 -2.960500000
1 9.592487000 4.539654000 -2.404523000
Sum of electronic and thermal Free Energies= -5578.50711

*Optimized structure and free energy for **VIII***
71 -0.738920000 0.032079000 2.849298000
26 1.003738000 0.792202000 5.218126000
14 -3.714295000 0.135694000 5.046789000
14 0.338841000 -3.514774000 3.259860000
7 -2.075476000 0.568711000 4.465902000
7 0.414689000 -1.724194000 3.355848000
6 -0.012289000 1.658911000 0.895706000
1 0.668401000 2.484662000 1.079029000
6 -1.437230000 1.882572000 1.043046000
1 -1.802046000 2.857290000 1.349076000
6 -2.306291000 0.827546000 0.836848000
1 -3.375425000 0.946242000 0.971615000
6 -1.764874000 -0.468456000 0.473786000
1 -2.447846000 -1.300161000 0.331412000
6 -0.457358000 -0.557456000 -0.108954000
6 -1.133592000 1.276967000 5.234817000
6 -0.616663000 0.980960000 6.554270000
1 -0.957042000 0.174815000 7.184583000
6 0.413197000 1.928072000 6.875915000
1 0.970732000 1.966688000 7.799573000
6 0.604199000 2.787168000 5.744011000
1 1.313214000 3.597537000 5.670730000
6 -0.329658000 2.386131000 4.731351000
1 -0.502985000 2.899599000 3.795533000
6 1.398791000 -1.054073000 4.113148000
6 1.705400000 -1.167816000 5.523716000
1 1.236460000 -1.860146000 6.204762000
6 2.724587000 -0.213173000 5.857169000
1 3.166560000 -0.073823000 6.832259000
6 3.024800000 0.552645000 4.682084000
1 3.742517000 1.355641000 4.611404000
6 2.210943000 0.050308000 3.614141000
6 -3.709573000 -0.835384000 6.705092000
1 -3.075602000 -1.726498000 6.634754000
1 -4.728724000 -1.158607000 6.950717000
1 -3.345526000 -0.216548000 7.532589000
6 -4.481610000 -0.985021000 3.696551000
1 -3.886890000 -1.895444000 3.553622000
1 -4.552663000 -0.462470000 2.736228000
1 -5.493371000 -1.290226000 3.988175000
6 -4.797329000 1.702547000 5.276018000
6 0.119915000 -4.354005000 4.976068000
1 1.005207000 -4.218175000 5.607040000
1 -0.037085000 -5.432080000 4.846338000
1 -0.747810000 -3.943619000 5.505150000
6 -1.181911000 -3.952444000 2.184446000
1 -2.106122000 -3.556729000 2.621700000
1 -1.286557000 -5.041207000 2.107918000
1 -1.073787000 -3.547904000 1.173077000
6 1.929646000 -4.218730000 2.452016000
6 0.013430000 -1.659925000 -0.895497000

1	-0.667255000	-2.485604000	-1.078753000	1	-3.744383000	-1.352937000	-4.605833000
6	1.438282000	-1.883451000	-1.043392000	6	-2.210737000	-0.048559000	-3.610572000
1	1.803069000	-2.858055000	-1.349715000	6	3.706359000	0.836004000	-6.706189000
6	2.307339000	-0.828383000	-0.837404000	1	3.073076000	1.727461000	-6.633895000
1	3.376460000	-0.946983000	-0.972543000	1	4.725429000	1.158865000	-6.952678000
6	1.766044000	0.467535000	-0.473871000	1	3.340866000	0.218510000	-7.534040000
1	2.449087000	1.299245000	-0.331501000	6	4.482276000	0.981257000	-3.698478000
6	0.458586000	0.556440000	0.109091000	1	3.887898000	1.891530000	-3.553067000
71	0.739065000	-0.032603000	-2.849011000	1	4.554898000	0.457120000	-2.739112000
26	-1.005979000	-0.791248000	-5.216053000	1	5.493582000	1.286802000	-3.991350000
14	3.712491000	-0.137227000	-5.049154000	6	4.794063000	-1.704577000	-5.281821000
14	-0.334974000	3.515496000	-3.259658000	6	-0.115479000	4.353664000	-4.976340000
7	2.074073000	-0.569728000	-4.466819000	1	-1.001287000	4.219031000	-5.606851000
7	-0.413142000	1.724966000	-3.354614000	1	0.043317000	5.431544000	-4.847116000
6	1.131039000	-1.277338000	-5.235051000	1	0.751348000	3.941668000	-5.505649000
6	0.612876000	-0.980688000	-6.553864000	6	1.186722000	3.951729000	-2.184963000
1	0.953011000	-0.174617000	-7.184370000	1	2.110272000	3.554486000	-2.622264000
6	-0.417877000	-1.927147000	-6.874668000	1	1.292866000	5.040405000	-2.109082000
1	-0.976352000	-1.965242000	-7.797728000	1	1.078350000	3.547884000	-1.173286000
6	-0.608233000	-2.786366000	-5.742699000	6	-1.924570000	4.221957000	-2.451600000
1	-1.317588000	-3.596307000	-5.668906000	1	2.060223000	-3.804686000	1.446425000
6	0.326998000	-2.386167000	-4.730977000	1	2.813940000	-3.955355000	3.043873000
1	0.501092000	-2.900009000	-3.795561000	1	1.881443000	-5.311939000	2.378032000
6	-1.398634000	1.055477000	-4.110651000	1	-2.271417000	-0.345670000	-2.572509000
6	-1.706937000	1.169219000	-5.520877000	1	-1.238573000	1.861332000	-6.202505000
6	-2.727149000	0.215190000	-5.852964000	1	-2.809420000	3.959658000	-3.043125000
1	-3.170512000	0.076180000	-6.827425000	1	-2.055460000	3.808362000	-1.445836000
6	-3.026224000	-0.550491000	-4.677486000	1	-1.874791000	5.315126000	-2.377943000

1 4.340805000 -2.382619000 -6.014168000
1 5.797095000 -1.439126000 -5.637288000
1 4.895420000 -2.247568000 -4.335712000
1 -5.800425000 1.436834000 5.631105000
1 -4.345263000 2.382217000 6.007587000
1 -4.898370000 2.243843000 4.328914000
1 2.272548000 0.347757000 2.576108000
Sum of electronic and thermal Free Energies= -5732.099907

*Optimized structure and free energy for **IX***
71 2.312124000 -0.194001000 1.267226000
26 2.645637000 0.525892000 4.243811000
14 1.479103000 -3.683432000 2.254772000
14 6.054315000 -0.191446000 1.171951000
7 1.736817000 -1.904088000 2.408625000
7 4.390874000 0.366362000 1.584277000
6 1.255308000 3.327765000 -0.328858000
1 1.889938000 4.076921000 -0.792564000
6 0.342078000 3.709235000 0.676226000
1 0.273935000 4.751871000 0.969076000
6 -0.463732000 2.752811000 1.289688000
1 -1.169488000 3.039198000 2.062203000
6 -0.361371000 1.399285000 0.904614000
1 -1.012098000 0.656457000 1.359742000
6 0.486686000 1.007215000 -0.155379000
6 1.676126000 -1.315159000 3.703642000
6 2.587568000 -1.497226000 4.812901000
1 3.455893000 -2.137233000 4.800376000
6 2.160543000 -0.667296000 5.901785000
1 2.645633000 -0.582621000 6.862403000
6 0.994851000 0.059226000 5.482445000
1 0.450247000 0.779915000 6.073354000
6 0.695033000 -0.329976000 4.140946000
1 -0.143442000 0.008034000 3.551269000
6 4.142885000 1.117176000 2.744490000
6 4.695502000 0.984872000 4.075298000
1 5.480505000 0.301089000 4.357188000
6 4.042102000 1.919354000 4.949553000
1 4.262053000 2.064304000 5.996426000
6 3.016351000 2.586254000 4.207533000
1 2.345545000 3.343926000 4.581765000
6 3.060611000 2.090653000 2.857339000
6 2.827893000 -4.691729000 3.176668000
1 3.829489000 -4.405068000 2.836181000
1 2.694683000 -5.763631000 2.985718000
1 2.774471000 -4.532623000 4.259060000
6 1.555692000 -4.136493000 0.396981000
1 2.534027000 -3.898955000 -0.036285000
1 0.780940000 -3.615917000 -0.176628000
1 1.393393000 -5.213907000 0.275455000
6 -0.234596000 -4.166292000 2.965208000
6 6.659429000 -1.631980000 2.295548000
1 6.803597000 -1.310204000 3.332774000
1 7.618769000 -2.016336000 1.927346000
1 5.937291000 -2.456586000 2.293836000
6 6.038718000 -0.831647000 -0.629319000
1 5.290764000 -1.619022000 -0.774501000

1	7.020557000	-1.249472000	6	-3.200728000	0.365971000
-0.881670000			-4.794490000		
1	5.824024000	-0.017438000	6	-4.164886000	-0.624687000
-1.328837000			-4.408854000		
6	7.290020000	1.266064000	1	-4.891182000	-1.089194000
1.318845000			-5.058719000		
6	0.575613000	-0.378936000	6	-3.970692000	-0.919825000
-0.691375000			-3.017043000		
1	-0.057433000	-1.135837000	1	-4.530326000	-1.636927000
-0.236259000			-2.435698000		
6	1.935448000	-0.784315000	6	-2.900661000	-0.096231000
-1.186322000			-2.540786000		
1	2.191962000	-1.834709000	6	1.431259000	-0.823560000
-1.278156000			-7.804131000		
6	2.702243000	0.202223000	1	0.784820000	0.057101000
-1.804275000			-7.890714000		
1	3.639583000	-0.058597000	1	2.254169000	-0.716327000
-2.283793000			-8.521801000		
6	2.188151000	1.550690000	1	0.850343000	-1.707724000
-1.909185000			-8.087842000		
1	2.842246000	2.302459000	6	3.261521000	0.534225000
-2.339571000			-5.698733000		
6	1.328007000	2.002123000	1	2.686921000	1.467864000
-0.781021000			-5.722307000		
71	0.293229000	0.312943000	1	3.764963000	0.464573000
-3.102996000			-4.728490000		
26	-2.233234000	-1.374898000	1	4.034219000	0.596638000
-4.118889000			-6.474212000		
14	2.136364000	-0.982821000	6	3.192158000	-2.584440000
-6.023038000			-5.947464000		
14	-1.571558000	3.394171000	6	-2.494450000	3.706025000
-3.908449000			-5.564675000		
7	0.877472000	-0.981268000	1	-3.511823000	3.301108000
-4.747276000			-5.539718000		
7	-1.338965000	1.648482000	1	-2.562898000	4.784389000
-3.557226000			-5.754481000		
6	-0.203501000	-1.886973000	1	-1.960002000	3.244625000
-4.756480000			-6.402919000		
6	-1.190324000	-2.113382000	6	0.169200000	4.180544000
-5.791844000			-4.035609000		
1	-1.199301000	-1.626866000	1	0.724784000	3.769792000
-6.754215000			-4.886659000		
6	-2.140614000	-3.083255000	1	0.083674000	5.264292000
-5.325132000			-4.179812000		
1	-2.983435000	-3.463740000	1	0.749147000	4.003992000
-5.882421000			-3.124047000		
6	-1.802374000	-3.428087000	6	-2.563571000	4.252966000
-3.974633000			-2.507518000		
1	-2.333101000	-4.124115000	1	7.026734000	2.061603000
-3.342944000			0.613244000		
6	-0.624469000	-2.691071000	1	7.282465000	1.692905000
-3.619016000			2.327713000		
1	-0.071398000	-2.788224000	1	8.310209000	0.931034000
-2.695408000			1.097074000		
6	-2.420187000	0.737235000	1	-2.540638000	-0.041331000
-3.633202000			-1.523751000		

1 -3.065451000 0.773061000 -5.784116000
1 -3.543340000 3.777467000 -2.382339000
1 -2.025465000 4.177846000 -1.556301000
1 -2.724680000 5.313938000 -2.734959000
1 2.560119000 -3.469928000 -6.081377000
1 3.956358000 -2.587630000 -6.734246000
1 3.694449000 -2.671350000 -4.977510000
1 -0.387788000 -5.250621000 2.909355000
1 -0.317009000 -3.864053000 4.015378000
1 -1.039614000 -3.675478000 2.407099000
1 2.509215000 2.516995000 2.027369000
Sum of electronic and thermal Free Energies= -5732.099480

Optimized structure and free energy for ***TS**$_{IX\text{-}XI}$*
71 12.206935000 5.747774000 -2.788493000
26 15.395516000 6.117802000 -2.439865000
14 12.699107000 2.267276000 -1.589917000
14 13.176864000 5.353953000 -6.385853000
7 13.065068000 4.015856000 -1.846456000
7 13.202131000 6.055106000 -4.729474000
6 14.387851000 4.453281000 -1.536611000
6 15.628499000 4.048124000 -2.161857000
1 15.709734000 3.354991000 -2.984467000
6 16.714738000 4.752476000 -1.542200000
1 17.758592000 4.664039000 -1.803557000
6 16.167238000 5.618116000 -0.535858000
1 16.725239000 6.294942000 0.093081000
6 14.749791000 5.443087000 -0.532049000
1 14.047064000 5.933938000 0.121461000
6 14.340353000 6.724155000 -4.264623000
6 15.743354000 6.439936000 -4.486783000
1 16.125905000 5.675521000 -5.143967000
6 16.536727000 7.341203000 -3.697003000
1 17.615470000 7.379471000 -3.674641000
6 15.651274000 8.144147000 -2.910010000
1 15.939182000 8.916381000 -2.213650000
6 14.303136000 7.765357000 -3.247080000
6 13.676794000 1.129525000 -2.792025000
1 13.539100000 1.452704000 -3.830370000
1 13.321450000 0.095332000 -2.704435000
1 14.748957000 1.138319000 -2.569202000
6 10.833340000 1.967258000 -1.900266000
1 10.543237000 2.224679000 -2.925241000
1 10.217407000 2.547108000 -1.205440000
1 10.609319000 0.905016000 -1.745936000
6 13.117701000 1.746608000 0.207344000
6 14.351611000 3.838124000 -6.584975000
1 15.403177000 4.135871000 -6.660685000
1 14.093795000 3.283958000 -7.496124000
1 14.250046000 3.159200000 -5.730369000
6 11.414595000 4.724171000 -6.783320000
1 11.079467000 3.971803000 -6.061009000
1 11.415525000 4.261115000 -7.777511000
1 10.690398000 5.543862000 -6.789586000
6 13.671133000 6.684458000 -7.676374000
71 11.047162000 8.011128000 0.850259000
26 9.045015000 9.494028000 2.411444000

14	13.527014000	10.776492000	1.007371000	6	13.656846000	11.876294000	-0.558740000
14	11.402139000	5.536461000	3.655478000	6	11.637909000	6.224043000	5.435610000
7	11.930622000	9.954517000	1.090368000	1	10.683771000	6.320150000	5.965200000
7	10.613650000	6.698174000	2.533049000	1	12.272071000	5.539053000	6.011976000
6	10.765708000	10.574619000	1.604834000	1	12.126363000	7.204889000	5.417835000
6	10.482996000	10.940624000	2.976563000	6	13.126615000	5.175405000	2.916693000
1	11.169903000	10.817583000	3.799529000	1	13.737978000	6.084833000	2.864858000
6	9.161006000	11.490766000	3.047295000	1	13.663036000	4.453393000	3.543588000
1	8.673606000	11.860819000	3.936520000	1	13.051592000	4.747451000	1.911592000
6	8.582614000	11.434835000	1.733259000	6	10.384238000	3.916823000	3.770608000
1	7.587895000	11.756480000	1.464387000	1	12.928252000	7.489287000	-7.695931000
6	9.549775000	10.862262000	0.850375000	1	14.642017000	7.127574000	-7.429041000
1	9.432720000	10.720821000	-0.213959000	1	13.738359000	6.248203000	-8.680221000
6	9.390464000	7.336285000	2.800597000	1	8.321490000	7.100584000	0.817279000
6	8.966587000	8.068456000	3.976685000	1	9.533043000	8.152716000	4.890282000
6	7.668286000	8.629509000	3.734335000	1	9.367393000	4.120320000	4.125471000
1	7.087160000	9.204202000	4.439654000	1	10.311630000	3.434854000	2.789487000
6	7.297175000	8.343865000	2.382104000	1	10.854309000	3.211781000	4.466706000
1	6.380998000	8.638334000	1.893998000	1	12.900924000	12.669980000	-0.538212000
6	8.356458000	7.570593000	1.792464000	1	14.644619000	12.348660000	-0.622743000
6	13.852895000	11.876145000	2.545532000	1	13.500857000	11.282282000	-1.466258000
1	13.902960000	11.273632000	3.459490000	1	12.964613000	0.669371000	0.344563000
1	14.807878000	12.403425000	2.432683000	1	14.161701000	1.977447000	0.445983000
1	13.064730000	12.626341000	2.672478000	1	12.480357000	2.278704000	0.922392000
6	14.843162000	9.388838000	0.929431000	1	13.412946000	8.297946000	-2.933064000
1	14.823607000	8.786724000	1.845989000	1	11.922258000	7.132439000	-1.077775000
1	14.686291000	8.722917000	0.072493000	6	10.490847000	7.252029000	-1.297555000
1	15.847018000	9.820408000	0.834497000	6	9.954371000	5.884766000	-1.354941000

1 9.841123000 5.323385000 -0.430244000
6 10.024168000 7.335383000 -3.809547000
6 9.749572000 5.911115000 -3.795955000
6 9.575445000 5.271893000 -2.553237000
1 9.179456000 4.261327000 -2.529806000
1 9.420214000 5.433981000 -4.709298000
6 10.369538000 8.007900000 -2.586621000
6 10.647844000 9.394928000 -2.635800000
6 9.949986000 8.093941000 -5.008771000
6 10.572272000 10.113720000 -3.823037000
1 10.946508000 9.897582000 -1.719490000
6 10.211850000 9.454474000 -5.016607000
1 9.683112000 7.584374000 -5.929570000
1 10.792894000 11.176108000 -3.832907000
1 10.146871000 10.013374000 -5.944827000
Sum of electronic and thermal Free Energies= -5732.06976

*Optimized structure and free energy for **X***
71 1.822317000 0.020169000 0.118398000
26 4.235986000 -0.777921000 -1.679121000
14 3.038159000 3.521498000 0.105413000
14 3.629303000 -1.772746000 2.881612000
7 2.822502000 1.830216000 -0.481828000
7 3.006745000 -1.429970000 1.218481000
6 3.617141000 1.301514000 -1.531316000
6 5.056441000 1.152202000 -1.574265000
1 5.733012000 1.468786000 -0.796766000
6 5.420204000 0.523272000 -2.811325000
1 6.423986000 0.288646000 -3.131894000
6 4.215444000 0.222585000 -3.531525000
1 4.153297000 -0.270201000 -4.489904000
6 3.109597000 0.687229000 -2.750097000
1 2.069876000 0.655752000 -3.037411000
6 3.738484000 -1.926165000 0.111489000
6 5.163701000 -1.866335000 -0.138022000
1 5.895761000 -1.442864000 0.531990000
6 5.438399000 -2.469160000 -1.411364000
1 6.413514000 -2.583654000 -1.860227000
6 4.190088000 -2.853323000 -2.002899000
1 4.058601000 -3.320119000 -2.966972000
6 3.146083000 -2.515961000 -1.079934000
6 4.806127000 4.202648000 -0.199488000
1 5.553779000 3.658522000 0.387760000
1 4.839834000 5.256406000 0.103307000
1 5.088774000 4.142192000 -1.255569000
6 2.706819000 3.552541000 1.991442000
1 3.415754000 2.898662000 2.513219000
1 1.691116000 3.229380000 2.240896000
1 2.837796000 4.570163000 2.378971000
6 1.811442000 4.703264000 -0.782826000
6 4.994625000 -0.528140000 3.417433000
1 5.879791000 -0.594181000 2.775477000
1 5.308730000 -0.730283000 4.448960000
1 4.619286000 0.500935000 3.370197000
6 2.194657000 -1.622801000 4.136015000
1 1.738311000 -0.627949000 4.124167000
1 2.577356000 -1.807631000 5.147106000

1	1.415369000	-2.363045000	6	-0.624994000	-4.268136000
3.925572000			-1.884111000		
6	4.335589000	-3.552464000	1	-1.393227000	-4.318534000
2.964047000			-2.664405000		
71	-1.530030000	-0.426814000	1	0.045285000	-3.435404000
-0.586960000			-2.127400000		
26	-4.871318000	-0.583455000	1	-0.041536000	-5.196173000
-0.065712000			-1.914883000		
14	-1.442929000	-4.031759000	6	-0.098293000	-4.189756000
-0.164440000			1.196625000		
14	-2.276137000	2.111731000	6	-3.312998000	1.713293000
-3.136344000			-4.701047000		
7	-2.216667000	-2.397473000	1	-4.384690000	1.828885000
-0.104885000			-4.507020000		
7	-2.632320000	0.977746000	1	-3.039585000	2.391562000
-1.778743000			-5.518578000		
6	-3.570161000	-2.269481000	1	-3.133035000	0.684725000
0.297115000			-5.033645000		
6	-4.749447000	-2.647118000	6	-0.422209000	1.926164000
-0.449966000			-3.568531000		
1	-4.739540000	-3.077672000	1	-0.190922000	0.900538000
-1.439838000			-3.878638000		
6	-5.908895000	-2.356335000	1	-0.164613000	2.594241000
0.341626000			-4.398942000		
1	-6.934997000	-2.526174000	1	0.220248000	2.187077000
0.051968000			-2.720097000		
6	-5.470505000	-1.758375000	6	-2.633715000	3.925160000
1.571854000			-2.619952000		
1	-6.109374000	-1.404880000	1	3.548230000	-4.283583000
2.367083000			2.750204000		
6	-4.039915000	-1.696844000	1	5.140634000	-3.699672000
1.546364000			2.236830000		
1	-3.398872000	-1.320137000	1	4.734639000	-3.757971000
2.329273000			3.964472000		
6	-3.965534000	0.946107000	1	-3.782628000	2.012686000
-1.284918000			0.688677000		
6	-5.131645000	0.372296000	1	-5.126426000	-0.143770000
-1.921160000			-2.868852000		
6	-6.271110000	0.599857000	1	-3.661761000	4.029245000
-1.080785000			-2.255209000		
1	-7.283187000	0.283814000	1	-1.954964000	4.243170000
-1.284476000			-1.820335000		
6	-5.826157000	1.285548000	1	-2.501253000	4.604064000
0.100131000			-3.470855000		
1	-6.445095000	1.576525000	1	-0.553867000	-4.092598000
0.935386000			2.189452000		
6	-4.414997000	1.495550000	1	0.387382000	-5.172014000
-0.017664000			1.140327000		
6	-2.731606000	-5.421157000	1	0.681558000	-3.424711000
0.114443000			1.103431000		
1	-3.492381000	-5.432100000	1	1.919965000	5.728765000
-0.672617000			-0.409096000		
1	-2.227171000	-6.394903000	1	2.001729000	4.709826000
0.117695000			-1.862189000		
1	-3.242779000	-5.296832000	1	0.772743000	4.390452000
1.075214000			-0.627280000		

1 2.098792000 -2.751348000 -1.199138000
1 0.405683000 -0.707172000 -1.282209000
6 -0.300655000 0.622500000 1.312025000
6 -0.668740000 1.980633000 1.296006000
6 -0.600634000 -0.088434000 2.537742000
6 -1.286191000 2.645618000 2.398033000
1 -0.477602000 2.583891000 0.408948000
6 -1.187339000 0.521118000 3.631069000
1 -0.352851000 -1.143909000 2.606143000
6 -1.649056000 4.022779000 2.349187000
6 -1.546618000 1.898730000 3.597238000
1 -1.383461000 -0.046641000 4.537375000
6 -2.240636000 4.634747000 3.436267000
1 -1.450968000 4.583769000 1.440283000
6 -2.156608000 2.559262000 4.700750000
6 -2.495337000 3.895854000 4.622128000
1 -2.513631000 5.683924000 3.390228000
1 -2.351996000 1.993457000 5.607065000
1 -2.960110000 4.389844000 5.469372000

Sum of electronic and thermal Free Energies= -5732.124235

*Optimized structure and free energy for **XI***

71 11.237277000 7.906686000 0.490856000
26 8.236849000 8.545963000 0.128190000
14 10.504466000 6.446319000 3.831806000
14 11.799567000 11.546564000 1.004102000
7 10.198301000 7.010796000 2.147070000
7 11.034729000 10.062994000 0.327019000
6 8.877576000 7.112271000 1.632772000
6 7.802907000 7.962583000 2.100131000
1 7.867680000 8.631513000 2.943634000
6 6.657404000 7.766622000 1.259536000
1 5.702465000 8.258999000 1.364457000
6 7.013904000 6.831835000 0.229538000
1 6.373676000 6.494463000 -0.571384000
6 8.371038000 6.435578000 0.445787000
1 8.923690000 5.713386000 -0.134271000
6 9.759371000 10.075202000 -0.273435000
6 8.515590000 10.629774000 0.219617000
1 8.405686000 11.197984000 1.128511000
6 7.463246000 10.303675000 -0.701645000
1 6.428611000 10.597561000 -0.608562000
6 8.012360000 9.481775000 -1.739065000
1 7.474015000 9.062612000 -2.575070000
6 9.414933000 9.328176000 -1.475744000
6 8.985751000 6.686122000 4.978200000
1 8.763493000 7.746726000 5.136911000
1 9.195542000 6.233959000 5.955222000
1 8.091380000 6.207892000 4.565472000
6 11.970966000 7.447649000 4.550922000
1 11.707611000 8.509664000 4.617353000
1 12.873361000 7.357213000 3.937014000
1 12.213429000 7.093171000 5.560122000
6 10.943877000 4.575974000 3.849459000
6 10.599894000 12.637147000 2.038739000
1 9.819662000 13.089138000 1.417536000
1 11.169766000 13.450151000 2.505871000

1 10.120026000 12.059000000 2.836451000
6 13.215153000 10.993477000 2.165758000
1 12.835811000 10.367885000 2.982485000
1 13.686449000 11.876670000 2.613975000
1 13.989490000 10.435826000 1.631193000
6 12.499973000 12.644328000 -0.404730000
71 13.067017000 5.817931000 -1.624852000
26 15.640677000 4.516187000 -3.008721000
14 12.134033000 7.305745000 -4.855886000
14 11.978401000 2.371908000 -0.783979000
7 13.217264000 6.507847000 -3.656495000
7 13.110985000 3.704345000 -1.212112000
6 14.523261000 6.085210000 -4.007861000
6 14.897172000 5.017899000 -4.910402000
1 14.201232000 4.404956000 -5.461703000
6 16.327557000 4.920823000 -4.943830000
1 16.902484000 4.218747000 -5.528684000
6 16.863091000 5.891562000 -4.031178000
1 17.908971000 6.051152000 -3.816409000
6 15.764408000 6.601253000 -3.449418000
1 15.833015000 7.429451000 -2.760042000
6 14.454055000 3.410765000 -1.557561000
6 14.947522000 2.567783000 -2.625705000
6 16.381986000 2.598266000 -2.614375000
1 17.031739000 2.061957000 -3.289493000
6 16.803036000 3.500798000 -1.582220000
1 17.822996000 3.752937000 -1.335000000
6 15.627781000 4.007159000 -0.936031000
6 12.589377000 6.844493000 -6.660543000
1 12.426405000 5.778442000 -6.852577000
1 11.959184000 7.414451000 -7.354052000
1 13.636770000 7.074681000 -6.882504000
6 10.334883000 6.742785000 -4.514770000
1 10.218912000 5.679778000 -4.756382000
1 10.058395000 6.879658000 -3.463879000
1 9.631028000 7.312554000 -5.133519000
6 12.245736000 9.216757000 -4.692337000
6 11.717243000 1.118592000 -2.217390000
1 12.630998000 0.553979000 -2.431441000
1 10.933886000 0.400191000 -1.945464000
1 11.405962000 1.633244000 -3.133543000
6 10.290792000 3.171914000 -0.377924000
1 9.893160000 3.715362000 -1.242901000
1 9.565362000 2.396051000 -0.105782000
1 10.371061000 3.868884000 0.462892000
6 12.622912000 1.407293000 0.743339000
1 13.285755000 12.114157000 -0.952561000
1 11.708376000 12.911525000 -1.114261000
1 12.925260000 13.571245000 -0.000908000
1 15.610662000 4.651451000 -0.068997000
1 14.329242000 2.012606000 -3.313111000
1 13.626520000 1.008438000 0.556747000
1 12.673604000 2.061634000 1.620665000
1 11.959129000 0.566805000 0.978996000
1 13.271281000 9.555432000 -4.880467000
1 11.584439000 9.709555000 -5.415473000

1 11.957559000 9.550587000 -3.688772000
1 11.138735000 4.233488000 4.873169000
1 10.113998000 3.986563000 3.443173000
1 11.833061000 4.364324000 3.244616000
1 10.126422000 8.843309000 -2.129092000
1 11.202083000 6.578188000 -1.145573000
6 13.660004000 7.248206000 0.384836000
6 14.733731000 8.180470000 0.077353000
6 13.902096000 6.356747000 1.446367000
6 14.607828000 9.136331000 -0.975649000
6 15.966838000 8.168893000 0.825180000
6 15.108732000 6.347431000 2.200112000
1 13.142571000 5.624896000 1.719075000
6 15.629855000 10.018780000 -1.276838000
1 13.681852000 9.169695000 -1.541727000
6 17.001537000 9.088323000 0.492253000
6 16.117910000 7.234318000 1.889866000
1 15.231255000 5.638140000 3.012928000
6 16.839622000 9.994157000 -0.537637000
1 15.507298000 10.735441000 -2.082370000
1 17.923881000 9.066341000 1.066209000
1 17.046382000 7.233050000 2.454577000
1 17.634037000 10.691464000 -0.782685000
Sum of electronic and thermal Free Energies= -5732.119893

Optimized structure and free energy for benzene
6 -2.192223000 1.204422000 0.000059000
6 -0.791749000 1.204354000 0.000481000
6 -0.091466000 2.417068000 -0.000022000
6 -0.791678000 3.629937000 -0.001050000
6 -2.192062000 3.630005000 -0.001514000
6 -2.892390000 2.417213000 -0.000923000
1 -2.735087000 0.264140000 0.000493000
1 -0.248985000 0.264012000 0.001258000
1 0.994271000 2.417090000 0.000326000
1 -0.248691000 4.570148000 -0.001477000
1 -2.734944000 4.570279000 -0.002286000
1 -3.978126000 2.417332000 -0.001258000
Sum of electronic and thermal Free Energies= -232.124315

Optimized structure and free energy for benzene
6 -4.637994000 -0.740251000 0.000332000
6 -3.257556000 -0.738616000 0.000150000
6 -2.528130000 0.484713000 0.000236000
6 -3.254742000 1.725593000 0.000515000
6 -4.678520000 1.688129000 0.000695000
6 -5.355516000 0.485091000 0.000608000
1 -0.557610000 -0.416780000 -0.000163000
1 -5.182334000 -1.679326000 0.000265000
1 -2.706144000 -1.674832000 -0.000060000
6 -1.104347000 0.522178000 0.000056000
6 -2.525321000 2.948932000 0.000603000
1 -5.225265000 2.627084000 0.000910000
1 -6.440838000 0.469904000 0.000749000
6 -1.144886000 2.950560000 0.000424000
6 -0.427363000 1.725219000 0.000150000
1 -3.076746000 3.885137000 0.000810000

1 -0.600521000 3.889622000 0.000498000
1 0.657960000 1.740415000 0.000011000
Sum of electronic and thermal Free Energies= -385.689418

*Optimized structure and free energy for **XII***
21 10.968325000 8.005906000 0.922114000
26 8.448728000 9.672087000 1.052797000
14 10.225415000 6.409770000 4.035581000
14 13.128165000 10.831040000 1.333245000
7 9.867543000 7.227690000 2.484203000
7 11.613757000 9.940229000 0.970883000
6 11.998148000 5.243541000 0.247138000
6 8.623954000 7.774661000 2.124544000
6 7.810454000 8.743445000 2.829919000
1 8.025580000 9.135357000 3.811243000
6 6.681526000 9.084206000 2.010702000
1 5.891671000 9.770810000 2.275629000
6 6.806572000 8.391081000 0.761386000
1 6.121629000 8.450695000 -0.070748000
6 7.996968000 7.591440000 0.821605000
1 8.329168000 6.884473000 0.073595000
6 10.379457000 10.593125000 0.732835000
6 9.570333000 11.341381000 1.672156000
1 9.835780000 11.532331000 2.700414000
6 8.371305000 11.767887000 1.010327000
1 7.573677000 12.344948000 1.453196000
6 8.397140000 11.264361000 -0.334446000
1 7.626030000 11.399520000 -1.077856000
6 9.618684000 10.540864000 -0.509019000
6 9.583807000 7.366369000 5.572774000
1 9.985475000 8.385733000 5.598606000
1 9.902024000 6.850907000 6.487471000
1 8.489923000 7.424489000 5.582890000
6 12.134956000 6.298810000 4.151742000
1 12.580901000 7.297219000 4.234947000
1 12.563091000 5.800155000 3.274882000
1 12.427914000 5.725284000 5.039290000
6 9.472134000 4.646541000 4.082148000
6 12.928637000 12.041280000 2.809752000
1 12.176094000 12.807550000 2.593239000
1 13.879799000 12.548027000 3.014004000
1 12.623343000 11.506416000 3.716398000
6 14.443476000 9.512912000 1.779792000
1 14.137524000 8.930064000 2.656771000
1 15.399102000 9.996984000 2.014365000
1 14.610546000 8.820440000 0.947234000
6 13.716614000 11.837680000 -0.189830000
6 12.354617000 6.618275000 -0.200607000
1 13.412091000 6.899234000 -0.233690000
6 11.393729000 7.178806000 -1.254171000
1 11.606667000 8.155820000 -1.681739000
6 10.506284000 6.325339000 -1.924395000
1 9.918906000 6.726601000 -2.745989000
6 10.421989000 4.946375000 -1.628501000
1 9.663020000 4.334603000 -2.100413000
6 11.044425000 4.471480000 -0.369888000
21 12.814755000 5.086424000 -2.223919000

26	15.778299000	5.662293000	1	9.863680000	4.942220000
-2.727306000			-6.429470000		
14	12.159655000	5.660154000	6	12.233903000	7.314418000
-5.737342000			-6.703898000		
14	13.447412000	1.581905000	6	14.677526000	0.817822000
-2.575463000			-3.838174000		
7	12.950428000	5.849212000	1	15.687414000	0.732242000
-4.132515000			-3.423670000		
7	13.813454000	3.288822000	1	14.336485000	-0.190383000
-2.147642000			-4.104954000		
6	14.229410000	6.437599000	1	14.726657000	1.413279000
-4.025012000			-4.756897000		
6	15.443237000	6.107310000	6	11.712849000	1.549238000
-4.745129000			-3.387322000		
1	15.519297000	5.367732000	1	11.728370000	2.079278000
-5.526516000			-4.346377000		
6	16.519066000	6.910988000	1	11.411382000	0.511816000
-4.237712000			-3.577314000		
1	17.541450000	6.891599000	1	10.948817000	2.013591000
-4.583611000			-2.756276000		
6	16.009545000	7.716766000	6	13.466418000	0.469629000
-3.165795000			-1.012608000		
1	16.574865000	8.419551000	1	13.914124000	11.176503000
-2.572859000			-1.041307000		
6	14.612810000	7.431076000	1	12.952707000	12.562323000
-3.030059000			-0.494555000		
1	13.925987000	7.929701000	1	14.636895000	12.388282000
-2.362907000			0.040036000		
6	15.119082000	3.767088000	1	14.861419000	4.951666000
-1.920109000			-0.017822000		
6	16.293516000	3.634700000	1	16.344250000	3.059211000
-2.759954000			-3.669712000		
6	17.363953000	4.400542000	1	14.457634000	0.486496000
-2.187183000			-0.544557000		
1	18.363295000	4.487371000	1	12.738003000	0.817780000
-2.586234000			-0.272989000		
6	16.866591000	5.062748000	1	13.228310000	-0.569031000
-1.016687000			-1.272719000		
1	17.426267000	5.721828000	1	13.269624000	7.648181000
-0.370617000			-6.832597000		
6	15.495896000	4.680431000	1	11.785063000	7.200757000
-0.848665000			-7.697962000		
6	12.962353000	4.291393000	1	11.690013000	8.099684000
-6.826502000			-6.166867000		
1	12.990633000	3.332649000	1	9.708920000	4.148269000
-6.296373000			5.030141000		
1	12.375952000	4.157728000	1	8.381389000	4.689139000
-7.744337000			3.981402000		
1	13.986027000	4.551111000	1	9.864346000	4.036504000
-7.117477000			3.261212000		
6	10.330029000	5.168775000	1	9.958252000	10.070884000
-5.462941000			-1.419779000		
1	10.240714000	4.282378000	1	12.514810000	4.835571000
-4.826246000			1.112959000		
1	9.766282000	5.984842000	6	10.622062000	3.133546000
-4.998742000			0.179809000		

1 9.583957000 3.175047000 0.538497000
1 10.665567000 2.350778000 -0.585973000
1 11.256948000 2.826190000 1.016749000
Sum of electronic and thermal Free Energies= -3238.718524

Optimized structure and free energy for ***TS$_{XII-XVI}$***
21 1.977316000 -0.013990000 -0.605903000
26 3.047887000 -0.124747000 2.224130000
14 4.841641000 -1.888555000 -1.759497000
14 3.309357000 3.237633000 -1.078189000
7 3.542908000 -1.357588000 -0.636262000
7 2.542332000 1.896843000 -0.150739000
6 3.547501000 -1.641624000 0.739800000
6 4.597274000 -1.444081000 1.719452000
1 5.598212000 -1.111184000 1.498162000
6 4.082299000 -1.760270000 3.022074000
1 4.637105000 -1.722844000 3.947556000
6 2.693963000 -2.090751000 2.889407000
1 2.024411000 -2.363614000 3.690635000
6 2.358120000 -2.016554000 1.495052000
1 1.414851000 -2.308042000 1.052373000
6 2.691464000 1.767711000 1.248964000
6 3.907372000 1.783998000 2.035898000
1 4.899601000 1.944115000 1.643624000
6 3.574740000 1.524439000 3.407868000
1 4.272519000 1.475428000 4.230137000
6 2.157860000 1.310727000 3.493863000
1 1.601650000 1.075858000 4.388645000
6 1.615265000 1.452091000 2.178063000
6 6.614836000 -1.609907000 -1.070181000
1 6.770795000 -0.564203000 -0.781634000
1 7.345009000 -1.859173000 -1.850310000
1 6.821266000 -2.245646000 -0.202672000
6 4.690770000 -0.869934000 -3.373002000
1 4.785834000 0.204137000 -3.175338000
1 3.733614000 -1.049925000 -3.869615000
1 5.494547000 -1.156931000 -4.061907000
6 4.664187000 -3.754838000 -2.161721000
6 5.211268000 3.012200000 -1.254374000
1 5.720323000 3.144952000 -0.293106000
1 5.616170000 3.753327000 -1.954818000
1 5.452978000 2.012537000 -1.632280000
6 2.533916000 3.198315000 -2.827741000
1 2.709768000 2.238295000 -3.327239000
1 2.972868000 3.984546000 -3.453370000
1 1.452838000 3.365606000 -2.772950000
6 2.992401000 4.933762000 -0.249317000
21 -2.155844000 -0.041347000 -0.023347000
26 -4.759872000 -0.297969000 -1.137876000
14 -2.467855000 3.534593000 0.622498000
14 -2.736897000 -2.195586000 2.829838000
7 -2.708821000 1.942991000 -0.176399000
7 -2.959807000 -1.461735000 1.209082000
6 -3.746914000 1.649776000 -1.078451000
6 -5.181001000 1.749783000 -0.886075000
1 -5.658823000 2.161785000 -0.011445000
6 -5.841776000 1.245154000 -2.055095000

1	-6.909035000	1.207357000	1	-0.403657000	-1.236701000
-2.212009000			3.039270000		
6	-4.843206000	0.747391000	6	-2.278337000	-4.052613000
-2.956920000			2.686009000		
1	-5.024583000	0.284405000	1	1.925969000	5.178923000
-3.914684000			-0.250103000		
6	-3.558756000	0.979390000	1	3.342332000	4.931748000
-2.363001000			0.789094000		
1	-2.598351000	0.785505000	1	3.530620000	5.722441000
-2.821428000			-0.788897000		
6	-4.086563000	-1.692891000	1	-3.177160000	-2.739271000
0.386718000			-1.393378000		
6	-5.454454000	-1.262597000	1	-5.805292000	-0.740095000
0.602653000			1.479137000		
6	-6.242888000	-1.653126000	1	-3.067028000	-4.608975000
-0.528353000			2.166151000		
1	-7.299755000	-1.474560000	1	-1.346649000	-4.180018000
-0.656382000			2.123040000		
6	-5.377267000	-2.284971000	1	-2.144110000	-4.498343000
-1.485115000			3.679254000		
1	-5.671063000	-2.664601000	1	-1.145859000	4.631932000
-2.451788000			-1.213888000		
6	-4.056326000	-2.306892000	1	-0.719363000	5.337054000
-0.938000000			0.362410000		
6	-3.993758000	4.680869000	1	-0.072985000	3.747909000
0.434435000			-0.111024000		
1	-4.850653000	4.319559000	1	5.474386000	-4.089723000
1.013186000			-2.820801000		
1	-3.738892000	5.683525000	1	4.698355000	-4.353583000
0.798872000			-1.244207000		
1	-4.300161000	4.768071000	1	3.708600000	-3.948994000
-0.613633000			-2.659647000		
6	-2.136538000	3.240732000	1	0.573879000	1.392473000
2.487143000			1.903497000		
1	-2.985828000	2.725409000	1	0.033382000	-0.428757000
2.950713000			0.012397000		
1	-1.236024000	2.637231000	6	-0.453133000	-0.761413000
2.648895000			-1.233066000		
1	-1.989256000	4.197181000	6	-0.302378000	-2.218512000
3.003479000			-1.413096000		
6	-0.951561000	4.400871000	6	0.364111000	-2.799840000
-0.159885000			-2.470191000		
6	-4.311044000	-2.047872000	6	1.001603000	-1.971342000
3.917930000			-3.461267000		
1	-5.162282000	-2.564784000	6	0.279835000	0.038942000
3.460729000			-2.239711000		
1	-4.130397000	-2.497672000	1	0.047295000	1.101646000
4.901992000			-2.332259000		
1	-4.586400000	-0.997576000	6	0.927578000	-0.598188000
4.068197000			-3.344227000		
6	-1.305331000	-1.238465000	1	1.511982000	-2.434192000
3.663026000			-4.299404000		
1	-1.593304000	-0.197734000	1	1.370902000	0.033785000
3.855064000			-4.111615000		
1	-1.050078000	-1.699402000	1	-0.799275000	-2.870842000
4.625099000			-0.695311000		

6 0.406414000 -4.301956000 -2.635578000
1 -0.165970000 -4.809799000 -1.852795000
1 -0.001223000 -4.607061000 -3.608333000
1 1.439081000 -4.671684000 -2.590475000
Sum of electronic and thermal Free Energies= -3238.695310

*Optimized structure and free energy for **XVI***
21 1.662383000 0.082113000 0.253553000
26 3.964023000 -0.450883000 -1.772029000
14 3.051649000 3.307951000 0.999282000
14 3.322952000 -2.259610000 2.492165000
7 2.699092000 1.828572000 0.023470000
7 2.708676000 -1.548764000 0.939963000
6 3.426888000 1.539002000 -1.159599000
6 4.859768000 1.378444000 -1.309287000
1 5.585095000 1.498448000 -0.520938000
6 5.144576000 1.027951000 -2.670814000
1 6.124521000 0.845422000 -3.085487000
6 3.899025000 0.920087000 -3.375745000
1 3.777348000 0.647842000 -4.413170000
6 2.845919000 1.230433000 -2.458058000
1 1.793057000 1.269254000 -2.684552000
6 3.424177000 -1.868242000 -0.244214000
6 4.855020000 -1.822350000 -0.470952000
1 5.594176000 -1.544014000 0.263694000
6 5.118899000 -2.197147000 -1.830598000
1 6.092419000 -2.258205000 -2.293064000
6 3.862185000 -2.434884000 -2.480959000
1 3.723099000 -2.712979000 -3.514549000
6 2.823366000 -2.235385000 -1.515984000
6 4.868606000 3.904830000 0.841141000
1 5.571213000 3.176910000 1.261410000
1 4.978723000 4.841861000 1.401300000
1 5.149405000 4.095872000 -0.199508000
6 2.739592000 2.912877000 2.846374000
1 3.443157000 2.146931000 3.193517000
1 1.722805000 2.554264000 3.031137000
1 2.897929000 3.815212000 3.449986000
6 1.938331000 4.768181000 0.437329000
6 4.756195000 -1.215772000 3.238155000
1 5.637592000 -1.206256000 2.587855000
1 5.055612000 -1.627637000 4.209949000
1 4.436376000 -0.178020000 3.389406000
6 1.939228000 -2.328512000 3.808972000
1 1.548980000 -1.338059000 4.059963000
1 2.351788000 -2.772258000 4.723736000
1 1.106927000 -2.955915000 3.473122000
6 3.935044000 -4.049369000 2.186451000
21 -1.553620000 -0.140922000 -0.432887000
26 -4.847159000 -0.460747000 0.247452000
14 -1.443477000 -3.577591000 -1.143713000
14 -2.368132000 2.827043000 -2.218406000
7 -2.199998000 -2.065194000 -0.484919000
7 -2.661449000 1.416941000 -1.124003000
6 -3.520887000 -2.119846000 0.029203000
6 -4.745717000 -2.314687000 -0.716606000
1 -4.804630000 -2.439674000 -1.786996000

6	-5.847937000	-2.302737000	1	-0.344255000	3.612548000
0.200710000			-3.460052000		
1	-6.889975000	-2.417615000	1	0.149362000	2.806100000
-0.057188000			-1.961811000		
6	-5.328618000	-2.070998000	6	-2.692441000	4.473182000
1.519622000			-1.289279000		
1	-5.912336000	-1.980720000	1	3.112501000	-4.675134000
2.423348000			1.822822000		
6	-3.904578000	-1.956987000	1	4.739379000	-4.083037000
1.419618000			1.445058000		
1	-3.214634000	-1.786868000	1	4.310051000	-4.481823000
2.231668000			3.121898000		
6	-3.965026000	1.303312000	1	-3.614009000	1.778097000
-0.564262000			1.607154000		
6	-5.192142000	0.960524000	1	-5.266768000	0.717604000
-1.251264000			-2.299641000		
6	-6.267972000	0.981381000	1	-3.711250000	4.497627000
-0.303205000			-0.886789000		
1	-7.303229000	0.758684000	1	-1.993238000	4.596766000
-0.513515000			-0.454593000		
6	-5.723557000	1.310057000	1	-2.571353000	5.326323000
0.984410000			-1.967642000		
1	-6.278394000	1.377574000	1	-0.561672000	-4.558643000
1.908023000			0.987345000		
6	-4.313544000	1.508698000	1	0.432335000	-5.082190000
0.830522000			-0.388153000		
6	-2.739819000	-4.972329000	1	0.648997000	-3.459482000
-1.353540000			0.300272000		
1	-3.498329000	-4.715479000	1	2.150860000	5.664222000
-2.099762000			1.033484000		
1	-2.231145000	-5.886615000	1	2.128058000	5.005242000
-1.683533000			-0.615947000		
1	-3.251810000	-5.187558000	1	0.874431000	4.531012000
-0.409658000			0.541830000		
6	-0.702472000	-3.181005000	1	1.768213000	-2.385318000
-2.868293000			-1.676637000		
1	-1.515291000	-3.019933000	1	0.274976000	-0.238763000
-3.586628000			-1.177565000		
1	-0.088201000	-2.274238000	6	-0.318990000	0.495349000
-2.849846000			1.521948000		
1	-0.083629000	-4.010963000	6	-0.599163000	1.867965000
-3.230345000			1.773766000		
6	-0.092963000	-4.225976000	6	-0.656387000	-0.408147000
0.053018000			2.570495000		
6	-3.497802000	2.785645000	6	-1.158730000	2.339039000
-3.769882000			2.978611000		
1	-4.554983000	2.878689000	1	-0.371741000	2.602247000
-3.500257000			1.003316000		
1	-3.241746000	3.619657000	6	-1.208058000	0.035079000
-4.435166000			3.779961000		
1	-3.364711000	1.850761000	1	-0.478071000	-1.471092000
-4.326255000			2.436847000		
6	-0.551476000	2.760252000	6	-1.454060000	1.399053000
-2.801701000			3.980193000		
1	-0.355620000	1.842709000	1	-1.882242000	1.738163000
-3.368132000			4.919735000		

6 -1.432731000 3.814009000 3.180172000
1 -2.142406000 4.192831000 2.433761000
1 -1.853749000 4.010634000 4.171110000
1 -0.514995000 4.406801000 3.082350000
1 -1.444065000 -0.676338000 4.566545000
Sum of electronic and thermal Free Energies= -3238.760159

Optimized structure and free energy for ***TS****$_{XII\text{-}XV}$*
21 -2.081250000 0.227010000 -0.938843000
26 -3.183520000 -0.740262000 2.021523000
14 -3.116908000 3.549493000 -0.139802000
14 -4.927170000 -1.654459000 -2.134208000
7 -2.705642000 1.818214000 0.193863000
7 -3.497023000 -1.297079000 -1.084721000
6 -2.915480000 1.311316000 1.506329000
6 -4.178602000 1.091492000 2.177986000
1 -5.149266000 1.274980000 1.744167000
6 -3.920436000 0.564586000 3.487810000
1 -4.664890000 0.290585000 4.220150000
6 -2.498373000 0.431019000 3.642684000
1 -1.988181000 0.038183000 4.509129000
6 -1.881740000 0.882597000 2.433987000
1 -0.824642000 0.921787000 2.228341000
6 -3.478039000 -1.866662000 0.205888000
6 -4.572903000 -2.023435000 1.143709000
1 -5.597464000 -1.740595000 0.959866000
6 -4.069814000 -2.608870000 2.354314000
1 -4.652364000 -2.852065000 3.230177000
6 -2.652423000 -2.769621000 2.215703000
1 -1.980952000 -3.168350000 2.960201000
6 -2.286213000 -2.318095000 0.902799000
6 -4.212232000 4.299610000 1.244090000
1 -5.199174000 3.827416000 1.281843000
1 -4.353430000 5.369644000 1.047665000
1 -3.746809000 4.189455000 2.229031000
6 -4.091503000 3.687995000 -1.787751000
1 -5.019811000 3.108757000 -1.722519000
1 -3.522194000 3.315498000 -2.645012000
1 -4.353005000 4.735770000 -1.981421000
6 -1.540969000 4.646440000 -0.245600000
6 -6.376046000 -0.436791000 -1.787368000
1 -6.730204000 -0.511297000 -0.753431000
1 -7.220927000 -0.645623000 -2.455326000
1 -6.050043000 0.596645000 -1.955819000
6 -4.526627000 -1.500273000 -4.002225000
1 -4.192126000 -0.498460000 -4.285668000
1 -5.444929000 -1.716653000 -4.562639000
1 -3.767944000 -2.227549000 -4.309995000
6 -5.526653000 -3.456757000 -1.862242000
21 2.189585000 -0.083841000 -0.210830000
26 4.855968000 -0.386320000 -1.192274000
14 2.319178000 -2.857627000 2.101454000
14 3.058809000 2.988180000 1.554297000
7 2.746038000 -1.829934000 0.687748000
7 3.020138000 1.743145000 0.254626000
6 3.931341000 -1.992321000 -0.066144000
6 5.298194000 -1.747147000 0.352291000

1	5.594562000	-1.447705000	1.345453000	1	1.440326000	1.758333000	3.050632000
6	6.168992000	-1.967913000	-0.764326000	1	1.418076000	3.496734000	3.378996000
1	7.243611000	-1.865220000	-0.760521000	1	0.573838000	2.861119000	1.957091000
6	5.363264000	-2.310810000	-1.902778000	6	3.093845000	4.740520000	0.781962000
1	5.726540000	-2.512074000	-2.899179000	1	-4.731172000	-4.162870000	-2.127191000
6	3.996433000	-2.320979000	-1.486525000	1	-5.812452000	-3.646547000	-0.823791000
1	3.144200000	-2.583101000	-2.093366000	1	-6.393765000	-3.660246000	-2.502276000
6	4.050445000	1.585536000	-0.690190000	1	2.865409000	1.289859000	-2.595546000
6	5.482056000	1.493644000	-0.483284000	1	5.981751000	1.632608000	0.461982000
6	6.114630000	1.202178000	-1.737925000	1	3.958654000	4.859352000	0.119173000
1	7.176288000	1.091684000	-1.899580000	1	2.187373000	4.921809000	0.194361000
6	5.093894000	1.029783000	-2.728362000	1	3.156406000	5.505910000	1.564846000
1	5.249012000	0.787934000	-3.768608000	1	2.138286000	-5.059916000	0.882879000
6	3.824558000	1.252700000	-2.095947000	1	1.228346000	-5.110887000	2.406484000
6	3.863828000	-3.314726000	3.143772000	1	0.548531000	-4.280342000	0.992159000
1	4.336390000	-2.421326000	3.567516000	1	-1.817861000	5.684460000	-0.468389000
1	3.566703000	-3.967415000	3.973748000	1	-1.008928000	4.633400000	0.712851000
1	4.610211000	-3.847832000	2.544803000	1	-0.848621000	4.302979000	-1.020580000
6	1.116229000	-1.838603000	3.183184000	1	-1.298685000	-2.366724000	0.467454000
1	1.610888000	-0.936448000	3.563095000	1	-0.051167000	-0.174664000	-0.290600000
1	0.219357000	-1.537252000	2.630748000	6	0.425209000	0.106673000	-1.581662000
1	0.791624000	-2.431474000	4.047151000	6	0.045948000	1.504275000	-1.885332000
6	1.475087000	-4.485308000	1.539875000	6	-0.221387000	-0.874290000	-2.489589000
6	4.567941000	2.812599000	2.732938000	6	-1.001642000	1.838090000	-2.728857000
1	5.507571000	3.079066000	2.236722000	1	0.574454000	2.302694000	-1.371544000
1	4.442755000	3.483774000	3.591805000	6	-1.273601000	-0.502728000	-3.315756000
1	4.654281000	1.787889000	3.112214000	6	-1.784977000	0.831140000	-3.360837000
6	1.467469000	2.748051000	2.579404000	1	-1.253524000	2.883011000	-2.878027000

1 -1.756470000 -1.265856000 -3.914905000
1 -2.574967000 1.095035000 -4.051023000
6 0.230847000 -2.312820000 -2.443710000
1 1.210574000 -2.430178000 -2.926293000
1 0.342267000 -2.668322000 -1.409662000
1 -0.473616000 -2.976037000 -2.956050000
Sum of electronic and thermal Free Energies= -3238.695405

*Optimized structure and free energy for **XV***
21 11.346799000 7.873758000 0.357946000
26 8.459145000 8.661034000 -0.117301000
14 10.572609000 6.449271000 3.571408000
14 11.873248000 11.267707000 1.450438000
7 10.301367000 7.019068000 1.876599000
7 11.283912000 9.946274000 0.369988000
6 8.989028000 7.185176000 1.353365000
6 7.955480000 8.083132000 1.828958000
1 8.048370000 8.738150000 2.680544000
6 6.810326000 7.963670000 0.974015000
1 5.883326000 8.507253000 1.076649000
6 7.123286000 7.020872000 -0.063193000
1 6.474535000 6.734432000 -0.877034000
6 8.451780000 6.544936000 0.158937000
1 8.979005000 5.818208000 -0.436234000
6 10.085030000 10.081832000 -0.352929000
6 8.840052000 10.718697000 0.026813000
1 8.674842000 11.280408000 0.931383000
6 7.860448000 10.469559000 -0.993613000
1 6.842753000 10.829694000 -0.992471000
6 8.451618000 9.626260000 -1.988909000
1 7.969828000 9.251769000 -2.878796000
6 9.812478000 9.383039000 -1.601559000
6 9.015152000 6.669455000 4.667158000
1 8.783760000 7.725761000 4.839397000
1 9.197016000 6.199372000 5.641376000
1 8.136230000 6.196013000 4.217548000
6 12.006844000 7.454096000 4.347315000
1 11.736214000 8.513020000 4.427346000
1 12.927514000 7.378129000 3.759367000
1 12.218906000 7.079114000 5.356299000
6 11.031340000 4.586702000 3.600018000
6 10.684882000 11.654919000 2.915176000
1 9.805555000 12.226159000 2.599305000
1 11.218605000 12.251372000 3.665726000
1 10.343016000 10.729946000 3.393590000
6 13.536523000 10.725633000 2.216944000
1 13.431278000 9.816519000 2.818783000
1 13.901467000 11.522409000 2.876925000
1 14.296334000 10.539804000 1.453575000
6 12.122280000 12.870778000 0.429607000
21 12.990872000 5.798060000 -1.638660000
26 15.649924000 4.447913000 -2.969670000
14 12.106877000 7.107228000 -4.812955000
14 11.972997000 2.516550000 -0.641562000
7 13.221197000 6.401779000 -3.573338000
7 13.111089000 3.820238000 -1.161946000
6 14.532236000 5.998446000 -3.938430000

6	14.904832000	4.944097000	6	10.283759000	3.323392000
-4.858116000			-0.270330000		
1	14.209848000	4.328128000	1	9.845891000	3.751663000
-5.406148000			-1.179458000		
6	16.335697000	4.859412000	1	9.589046000	2.565446000
-4.906645000			0.111622000		
1	16.910108000	4.165257000	1	10.369347000	4.115292000
-5.501331000			0.479637000		
6	16.872154000	5.828666000	6	12.645044000	1.628980000
-3.993610000			0.919160000		
1	17.918569000	5.992875000	1	12.902248000	12.729163000
-3.784858000			-0.326728000		
6	15.774084000	6.527212000	1	11.198028000	13.154590000
-3.396568000			-0.086140000		
1	15.847434000	7.332252000	1	12.419831000	13.700732000
-2.682750000			1.081714000		
6	14.441303000	3.454428000	1	15.676363000	4.666317000
-1.506332000			-0.062828000		
6	14.870637000	2.551925000	1	14.213739000	2.022529000
-2.554992000			-3.226321000		
6	16.304175000	2.499743000	1	13.643504000	1.218215000
-2.557139000			0.730897000		
1	16.915683000	1.916329000	1	12.714357000	2.320966000
-3.228895000			1.765276000		
6	16.785954000	3.391522000	1	11.982780000	0.802617000
-1.541037000			1.204403000		
1	17.821562000	3.592322000	1	13.304970000	9.295645000
-1.311807000			-5.153766000		
6	15.651196000	3.978063000	1	11.601794000	9.435841000
-0.893483000			-5.635601000		
6	12.476099000	6.453567000	1	12.048807000	9.490095000
-6.578247000			-3.919676000		
1	12.288847000	5.377213000	1	11.196636000	4.252539000
-6.657781000			4.631720000		
1	11.819384000	6.965631000	1	10.224634000	3.983672000
-7.292520000			3.168913000		
1	13.513619000	6.643444000	1	11.943509000	4.386835000
-6.871576000			3.027389000		
6	10.309236000	6.617679000	1	10.547702000	8.857786000
-4.369893000			-2.193173000		
1	10.172398000	5.537832000	1	11.254421000	6.593040000
-4.503815000			-1.194332000		
1	10.052258000	6.864832000	6	13.655259000	7.260329000
-3.335497000			0.184507000		
1	9.606481000	7.133940000	6	14.013293000	6.419980000
-5.035507000			1.278400000		
6	12.279756000	9.018754000	6	14.632980000	8.230853000
-4.880829000			-0.221044000		
6	11.700654000	1.188812000	6	15.244572000	6.514496000
-2.003554000			1.943496000		
1	12.601365000	0.588858000	1	13.310620000	5.659039000
-2.169877000			1.613074000		
1	10.894543000	0.509775000	6	15.877346000	8.300305000
-1.698348000			0.432335000		
1	11.413535000	1.654521000	6	16.181729000	7.456508000
-2.953411000			1.507601000		

1 15.472129000 5.856661000 2.777188000
1 16.611672000 9.031954000 0.104318000
1 17.145895000 7.536929000 2.000880000
6 14.329731000 9.222677000 -1.328736000
1 15.228716000 9.767843000 -1.636755000
1 13.911760000 8.729456000 -2.213094000
1 13.583312000 9.952394000 -0.990515000
Sum of electronic and thermal Free Energies= -3238.749739

Optimized structure and free energy for ***TS***$_{XII\text{-}XIV}$
21 1.986272000 -0.115353000 -0.533627000
26 3.022075000 0.353647000 2.277194000
14 4.750804000 -2.317909000 -1.230116000
14 3.346101000 2.969227000 -1.644732000
7 3.508673000 -1.469662000 -0.247263000
7 2.554095000 1.852102000 -0.475388000
6 3.522393000 -1.441377000 1.159875000
6 4.582526000 -1.027101000 2.056520000
1 5.576462000 -0.742082000 1.752081000
6 4.086529000 -1.053803000 3.403714000
1 4.650062000 -0.805604000 4.290541000
6 2.701441000 -1.423518000 3.366405000
1 2.043607000 -1.517185000 4.216733000
6 2.349176000 -1.660740000 1.995921000
1 1.403892000 -2.042902000 1.636416000
6 2.679234000 2.007026000 0.922376000
6 3.876862000 2.189778000 1.716468000
1 4.877695000 2.276336000 1.323179000
6 3.512340000 2.215143000 3.104943000
1 4.191280000 2.340188000 3.934916000
6 2.095113000 2.009744000 3.201969000
1 1.519810000 1.959722000 4.113664000
6 1.582887000 1.877388000 1.872556000
6 6.538106000 -2.088147000 -0.562951000
1 6.810426000 -1.027789000 -0.510511000
1 7.241812000 -2.585902000 -1.241929000
1 6.660754000 -2.529636000 0.431621000
6 4.693983000 -1.578896000 -2.994330000
1 4.946909000 -0.512200000 -2.974277000
1 3.704912000 -1.694454000 -3.446648000
1 5.424519000 -2.087236000 -3.635145000
6 4.391178000 -4.200742000 -1.288471000
6 5.255749000 2.746697000 -1.706937000
1 5.732677000 3.095781000 -0.784217000
1 5.674042000 3.324020000 -2.541053000
1 5.520974000 1.693021000 -1.850614000
6 2.644013000 2.529771000 -3.370237000
1 2.859166000 1.488107000 -3.636816000
1 3.097340000 3.170456000 -4.135993000
1 1.558804000 2.675365000 -3.398851000
6 2.973974000 4.798008000 -1.218896000
21 -2.170249000 -0.091763000 -0.021199000
26 -4.758244000 -0.510640000 -1.076691000
14 -2.498706000 3.525587000 0.142555000
14 -2.753352000 -1.729111000 3.158512000
7 -2.711673000 1.850868000 -0.474801000
7 -2.975225000 -1.276287000 1.437521000

6	-3.738610000	1.422485000	1	-4.651588000	-0.404261000
-1.330529000			4.175877000		
6	-5.174845000	1.553912000	6	-1.362993000	-0.603911000
-1.177456000			3.836567000		
1	-5.665402000	2.106692000	1	-1.684328000	0.444327000
-0.392047000			3.846427000		
6	-5.821740000	0.860565000	1	-1.110792000	-0.888926000
-2.253660000			4.865243000		
1	-6.887062000	0.799757000	1	-0.451152000	-0.678263000
-2.417498000			3.232673000		
6	-4.813801000	0.216477000	6	-2.239849000	-3.570061000
-3.044791000			3.325197000		
1	-4.984001000	-0.399692000	1	1.902882000	5.007216000
-3.914405000			-1.300202000		
6	-3.536145000	0.542756000	1	3.289884000	5.032213000
-2.480082000			-0.195950000		
1	-2.570935000	0.274677000	1	3.512539000	5.464598000
-2.888456000			-1.903213000		
6	-4.100723000	-1.637367000	1	-3.187192000	-2.966747000
0.662215000			-0.916729000		
6	-5.468044000	-1.172374000	1	-5.821627000	-0.512785000
0.794577000			1.571980000		
6	-6.251541000	-1.740771000	1	-3.005087000	-4.227366000
-0.262306000			2.896101000		
1	-7.306600000	-1.581043000	1	-1.296665000	-3.761248000
-0.425958000			2.800916000		
6	-5.382967000	-2.525930000	1	-2.108866000	-3.842357000
-1.094904000			4.379639000		
1	-5.672166000	-3.059667000	1	-1.101033000	4.425153000
-1.987558000			-1.743035000		
6	-4.065725000	-2.461608000	1	-0.713156000	5.269229000
-0.542654000			-0.226095000		
6	-4.009362000	4.642750000	1	-0.075893000	3.636787000
-0.241085000			-0.529809000		
1	-4.886550000	4.360356000	1	5.121518000	-4.719309000
0.350965000			-1.921606000		
1	-3.759614000	5.682901000	1	4.442787000	-4.632038000
0.001181000			-0.281854000		
1	-4.281129000	4.596703000	1	3.387777000	-4.387977000
-1.301153000			-1.684754000		
6	-2.254749000	3.450590000	1	0.547080000	1.765401000
2.042939000			1.593031000		
1	-3.143184000	3.027458000	1	0.029645000	-0.496758000
2.525850000			0.103304000		
1	-1.389669000	2.836501000	6	-0.428598000	-0.991024000
2.317854000			-1.048316000		
1	-2.087079000	4.456354000	6	-0.323412000	-2.465292000
2.447034000			-1.006901000		
6	-0.943688000	4.291468000	6	0.258612000	-3.199015000
-0.666361000			-2.007809000		
6	-4.348623000	-1.457456000	1	-0.793009000	-2.989418000
4.189898000			-0.175668000		
1	-5.179191000	-2.059306000	6	0.881207000	-2.587845000
3.804339000			-3.159500000		
1	-4.175207000	-1.748831000	6	0.336783000	-0.382786000
5.233028000			-2.166384000		

1 0.122410000 0.657079000 -2.428158000
6 0.895489000 -1.208585000 -3.204122000
1 0.223660000 -4.285924000 -1.955521000
1 1.335492000 -0.707664000 -4.065927000
6 1.457270000 -3.451914000 -4.255660000
1 1.812282000 -2.843438000 -5.094786000
1 2.305401000 -4.057654000 -3.905649000
1 0.707942000 -4.153513000 -4.648595000
Sum of electronic and thermal Free Energies= -3238.690453

*Optimized structure and free energy for **XIV***
21 11.202903000 7.700892000 0.371116000
26 8.187236000 8.408906000 0.060947000
14 10.618396000 6.594134000 3.730783000
14 11.822583000 11.285258000 0.601015000
7 10.225883000 6.961912000 2.004288000
7 11.083414000 9.727387000 0.035461000
6 8.881917000 7.026933000 1.552360000
6 7.816853000 7.877195000 2.046158000
1 7.904922000 8.566404000 2.869922000
6 6.641801000 7.651012000 1.255200000
1 5.687640000 8.139042000 1.384951000
6 6.966670000 6.696642000 0.233494000
1 6.299955000 6.337471000 -0.535753000
6 8.334306000 6.313693000 0.407379000
1 8.874799000 5.594428000 -0.185008000
6 9.754697000 9.789771000 -0.462143000
6 8.606327000 10.455111000 0.121008000
1 8.616215000 11.030000000 1.033334000
6 7.462112000 10.215589000 -0.711004000
1 6.463143000 10.585454000 -0.536103000
6 7.866075000 9.362788000 -1.791796000
1 7.228631000 8.983125000 -2.575597000
6 9.266212000 9.100263000 -1.645287000
6 9.207812000 7.074855000 4.939521000
1 9.054974000 8.159041000 4.973184000
1 9.481481000 6.741401000 5.948295000
1 8.258782000 6.600810000 4.669597000
6 12.172255000 7.594475000 4.232299000
1 11.972848000 8.669416000 4.149355000
1 13.041561000 7.355046000 3.612814000
1 12.430036000 7.377088000 5.276334000
6 10.939611000 4.716925000 3.969488000
6 11.287215000 11.734293000 2.393782000
1 10.209259000 11.912906000 2.468939000
1 11.804905000 12.645313000 2.719411000
1 11.546380000 10.927174000 3.088963000
6 13.730741000 11.174354000 0.604310000
1 14.104003000 10.380856000 1.258166000
1 14.134007000 12.129064000 0.964573000
1 14.116320000 11.002326000 -0.405975000
6 11.311678000 12.705051000 -0.579523000
21 12.883067000 5.693427000 -1.628061000
26 15.605830000 4.283305000 -3.071730000
14 12.591907000 7.791632000 -4.428147000
14 11.939475000 2.418325000 -0.583743000
7 13.446616000 6.602382000 -3.354854000

7	13.005114000	3.689405000	1	10.922136000	0.254377000
-1.312172000			-1.350861000		
6	14.708248000	6.094332000	1	11.103380000	1.367152000
-3.758270000			-2.724231000		
6	14.978594000	5.186539000	6	10.277136000	3.225160000
-4.852488000			-0.107131000		
1	14.229988000	4.771601000	1	9.765686000	3.619884000
-5.509928000			-0.992374000		
6	16.389684000	4.937501000	1	9.622268000	2.475126000
-4.903935000			0.352731000		
1	16.895809000	4.294675000	1	10.409246000	4.040067000
-5.608381000			0.611708000		
6	17.009693000	5.659373000	6	12.768289000	1.668480000
-3.828288000			0.975703000		
1	18.061695000	5.653494000	1	11.676711000	12.506777000
-3.585431000			-1.593389000		
6	15.984432000	6.368783000	1	10.224196000	12.819332000
-3.123228000			-0.627529000		
1	16.119527000	7.010238000	1	11.743026000	13.653038000
-2.266092000			-0.236229000		
6	14.283364000	3.249514000	1	15.666244000	4.069744000
-1.758554000			-0.185888000		
6	14.579874000	2.462080000	1	13.848588000	2.127687000
-2.936227000			-3.655496000		
6	15.993213000	2.223560000	1	13.769829000	1.292422000
-2.982188000			0.738757000		
1	16.519447000	1.674698000	1	12.865129000	2.417929000
-3.748632000			1.769372000		
6	16.594013000	2.876057000	1	12.171168000	0.834650000
-1.852379000			1.364099000		
1	17.648825000	2.900760000	1	13.604254000	9.919309000
-1.623118000			-3.570111000		
6	15.551430000	3.506417000	1	11.989798000	10.228641000
-1.099593000			-4.241735000		
6	13.471077000	7.951457000	1	12.159116000	9.533773000
-6.122729000			-2.617787000		
1	13.431707000	7.018817000	1	11.179121000	4.499888000
-6.694122000			5.017765000		
1	12.976672000	8.734348000	1	10.048145000	4.141237000
-6.710978000			3.695372000		
1	14.523347000	8.228786000	1	11.770781000	4.365203000
-5.999583000			3.349351000		
6	10.802362000	7.167858000	1	9.881231000	8.531647000
-4.729994000			-2.323764000		
1	10.827116000	6.276018000	1	11.114535000	6.482922000
-5.367664000			-1.234643000		
1	10.301314000	6.895189000	6	13.457397000	6.912219000
-3.794782000			0.350877000		
1	10.200343000	7.933526000	6	13.821542000	5.974545000
-5.234184000			1.362151000		
6	12.578706000	9.534341000	6	14.469374000	7.857753000
-3.629272000			0.015015000		
6	11.589009000	0.990466000	6	15.072561000	5.987968000
-1.816722000			1.991041000		
1	12.511986000	0.477992000	1	13.106109000	5.215500000
-2.107203000			1.667633000		

6 15.722504000 7.878111000 0.641823000
1 14.268100000 8.600646000 -0.751779000
6 16.045183000 6.941958000 1.639802000
1 15.297877000 5.256754000 2.763730000
1 16.455551000 8.630495000 0.360538000
6 17.406367000 6.943757000 2.297441000
1 17.358709000 6.550694000 3.318218000
1 18.113971000 6.316076000 1.738629000
1 17.829543000 7.952786000 2.338601000
Sum of electronic and thermal Free Energies= -3238.758932

Optimized structure and free energy for ***TS****$_{XII\text{-}XIII}$*
21 -2.472732000 0.392126000 0.916362000
26 -3.024529000 -1.424334000 -1.838825000
14 -3.251805000 -2.457390000 2.884985000
14 -4.270267000 3.075206000 -0.598311000
7 -2.871559000 -1.577569000 1.351649000
7 -3.403826000 1.487284000 -0.553855000
6 -2.912387000 -2.286190000 0.122528000
6 -4.085782000 -2.737674000 -0.593142000
1 -5.103720000 -2.571940000 -0.274506000
6 -3.666015000 -3.420938000 -1.782180000
1 -4.314354000 -3.863230000 -2.523540000
6 -2.231575000 -3.378874000 -1.837692000
1 -1.615677000 -3.787697000 -2.624360000
6 -1.766478000 -2.681941000 -0.675806000
1 -0.737159000 -2.489853000 -0.411457000
6 -3.322662000 0.710539000 -1.735182000
6 -4.401993000 0.038057000 -2.427743000
1 -5.434568000 0.047548000 -2.115794000
6 -3.869097000 -0.627999000 -3.581010000
1 -4.432217000 -1.214701000 -4.291175000
6 -2.448186000 -0.421581000 -3.598620000
1 -1.758234000 -0.816923000 -4.328588000
6 -2.110521000 0.394901000 -2.469992000
6 -4.030347000 -4.171977000 2.530258000
1 -4.997900000 -4.076796000 2.026976000
1 -4.185992000 -4.704872000 3.476135000
1 -3.378497000 -4.781425000 1.895301000
6 -4.482816000 -1.428671000 3.936428000
1 -5.447498000 -1.349912000 3.421741000
1 -4.113822000 -0.413182000 4.116045000
1 -4.649291000 -1.909257000 4.908401000
6 -1.659627000 -2.759166000 3.923568000
6 -5.671661000 3.088543000 -1.909862000
1 -5.291017000 2.871362000 -2.913256000
1 -6.136708000 4.082142000 -1.926507000
1 -6.448925000 2.354039000 -1.672519000
6 -5.064787000 3.392907000 1.113052000
1 -5.791177000 2.605682000 1.348053000
1 -5.594785000 4.353574000 1.103037000
1 -4.316667000 3.428555000 1.911185000
6 -3.056133000 4.497190000 -1.030106000
21 2.154998000 0.020231000 -0.078219000
26 4.672155000 -0.049487000 1.266748000
14 2.894372000 2.948575000 -2.070220000
14 2.652782000 -3.039421000 -1.896563000

7	2.975235000	1.763919000	1	5.039064000	-3.872515000
-0.713707000			-2.078894000		
7	2.803475000	-1.850250000	1	4.172533000	-4.063214000
-0.553670000			-3.612832000		
6	4.017571000	1.755717000	1	4.784052000	-2.466663000
0.244087000			-3.137564000		
6	5.425905000	1.484880000	6	1.449889000	-2.249470000
0.036201000			-3.156233000		
1	5.884348000	1.301992000	1	1.880210000	-1.338937000
-0.923122000			-3.591047000		
6	6.088114000	1.497262000	1	1.250485000	-2.947576000
1.307764000			-3.978336000		
1	7.141807000	1.332917000	1	0.489062000	-1.996274000
1.474557000			-2.693995000		
6	5.104061000	1.728524000	6	1.948512000	-4.696638000
2.327162000			-1.245839000		
1	5.289079000	1.776191000	1	-2.224692000	4.517797000
3.389393000			-0.317979000		
6	3.834495000	1.883719000	1	-2.643714000	4.355554000
1.686472000			-2.036228000		
1	2.901749000	2.139641000	1	-3.566029000	5.468057000
2.168005000			-1.000730000		
6	3.794388000	-1.878910000	1	2.547715000	-1.822521000
0.448642000			2.329744000		
6	5.235769000	-1.837635000	1	5.763807000	-1.862068000
0.303755000			-0.636396000		
6	5.828944000	-1.765195000	1	2.601545000	-5.117903000
1.607859000			-0.472831000		
1	6.886747000	-1.731951000	1	0.954017000	-4.553857000
1.820481000			-0.809762000		
6	4.776332000	-1.695600000	1	1.866504000	-5.428425000
2.580069000			-2.058553000		
1	4.901144000	-1.617809000	1	3.430406000	4.991110000
3.649127000			-0.688605000		
6	3.527837000	-1.759854000	1	2.643568000	5.451541000
1.878663000			-2.211818000		
6	4.487784000	2.925284000	1	1.675854000	4.800406000
-3.139343000			-0.872002000		
1	4.667749000	1.927714000	1	-1.906974000	-3.299546000
-3.556198000			4.845760000		
1	4.389444000	3.630896000	1	-0.944442000	-3.366046000
-3.973366000			3.355224000		
1	5.365885000	3.218118000	1	-1.165785000	-1.822593000
-2.553183000			4.207603000		
6	1.403020000	2.429635000	1	-1.127096000	0.759105000
-3.145675000			-2.213205000		
1	1.506482000	1.398486000	1	0.135676000	0.014445000
-3.504753000			0.429971000		
1	0.464261000	2.512221000	6	0.157689000	0.210973000
-2.587400000			1.655626000		
1	1.325667000	3.080560000	6	-0.637938000	1.340344000
-4.024772000			2.097008000		
6	2.635856000	4.721231000	6	-1.806610000	1.212966000
-1.393782000			3.006540000		
6	4.330135000	-3.390363000	6	-2.329598000	2.407835000
-2.760959000			3.599839000		

6 -1.915473000 3.666385000 3.219339000
1 -2.350574000 4.554470000 3.664204000
6 -0.271226000 2.683462000 1.693353000
6 -0.884371000 3.793381000 2.226240000
1 -1.911650000 0.290415000 3.577146000
1 -3.090612000 2.300071000 4.370045000
1 0.547242000 2.806096000 0.984656000
1 -0.561004000 4.784247000 1.919830000
1 -0.107643000 -0.747036000 2.108002000
1 1.275908000 0.347971000 1.828542000
Sum of electronic and thermal Free Energies= -3238.638309

*Optimized structure and free energy for **XIII***
21 11.709362000 7.728271000 0.867936000
26 8.451634000 8.905030000 1.356572000
14 10.729869000 5.090246000 3.135889000
14 12.306281000 10.874683000 -0.718066000
7 10.531297000 6.565188000 2.084017000
7 11.343346000 9.595654000 0.151305000
6 9.197594000 7.070529000 2.120063000
6 8.596289000 7.865282000 3.173276000
1 9.116692000 8.230813000 4.045405000
6 7.218692000 8.087479000 2.847505000
1 6.512067000 8.659005000 3.430543000
6 6.950905000 7.451795000 1.587265000
1 6.008774000 7.465546000 1.060189000
6 8.160022000 6.828232000 1.137759000
1 8.297901000 6.271759000 0.223375000
6 9.994299000 9.987479000 0.384002000
6 9.486993000 10.728147000 1.520726000
1 10.076303000 11.024398000 2.375404000
6 8.089569000 10.974089000 1.317130000
1 7.427779000 11.488174000 1.997990000
6 7.712148000 10.387469000 0.060682000
1 6.718229000 10.382564000 -0.361293000
6 8.874006000 9.775706000 -0.510434000
6 10.648042000 5.564389000 4.998148000
1 11.442820000 6.270137000 5.267780000
1 10.768147000 4.666137000 5.616477000
1 9.684989000 6.022558000 5.245396000
6 12.417886000 4.231608000 2.847455000
1 13.256501000 4.820380000 3.235418000
1 12.596244000 4.009561000 1.790153000
1 12.410587000 3.279495000 3.393231000
6 9.333372000 3.822429000 2.798474000
6 12.754645000 12.307256000 0.477232000
1 11.847013000 12.751611000 0.900812000
1 13.301941000 13.092847000 -0.058505000
1 13.378859000 11.948808000 1.302656000
6 13.910142000 10.140296000 -1.454510000
1 14.610275000 9.838842000 -0.671751000
1 14.400862000 10.909978000 -2.063991000
1 13.705863000 9.277612000 -2.096866000
6 11.286177000 11.621976000 -2.161444000
21 13.317197000 5.903017000 -1.283284000
26 15.918087000 4.670404000 -2.340921000
14 12.566943000 7.215261000 -4.510579000

14	11.706150000	2.748281000	6	11.721325000	1.885250000
-1.400670000			-3.119047000		
7	13.615774000	6.687493000	1	12.526624000	1.147004000
-3.137558000			-3.198581000		
7	13.093240000	3.881928000	1	10.769698000	1.359932000
-1.172343000			-3.269206000		
6	14.975879000	6.353214000	1	11.837427000	2.615489000
-3.321654000			-3.928239000		
6	15.565481000	5.425035000	6	10.108891000	3.790342000
-4.263992000			-1.280325000		
1	15.023550000	4.878221000	1	10.015893000	4.471928000
-5.018861000			-2.133699000		
6	16.977231000	5.351047000	1	9.234981000	3.127465000
-4.017283000			-1.281552000		
1	17.684213000	4.746378000	1	10.087293000	4.392836000
-4.564918000			-0.367329000		
6	17.282508000	6.187426000	6	11.727289000	1.377365000
-2.892657000			-0.062234000		
1	18.258099000	6.333084000	1	11.056261000	10.867590000
-2.454421000			-2.921586000		
6	16.062670000	6.802702000	1	10.341145000	12.044794000
-2.461934000			-1.806121000		
1	15.964303000	7.556189000	1	11.864255000	12.423295000
-1.694197000			-2.638260000		
6	14.441066000	3.477046000	1	15.390127000	4.370771000
-1.305424000			0.537082000		
6	15.064921000	2.755408000	1	14.548830000	2.363880000
-2.395807000			-3.257525000		
6	16.473422000	2.657738000	1	12.676054000	0.828865000
-2.139961000			-0.085205000		
1	17.198896000	2.170541000	1	11.602626000	1.799341000
-2.773648000			0.939946000		
6	16.757815000	3.353523000	1	10.915146000	0.662028000
-0.918684000			-0.239928000		
1	17.729792000	3.472346000	1	14.342223000	8.533218000
-0.464735000			-5.722039000		
6	15.520639000	3.859083000	1	12.720288000	9.046744000
-0.404370000			-6.230680000		
6	12.349135000	5.841017000	1	13.383436000	9.598031000
-5.837718000			-4.676694000		
1	12.023214000	4.900396000	1	9.398550000	2.999127000
-5.378961000			3.520279000		
1	11.586164000	6.147866000	1	8.348525000	4.290203000
-6.564212000			2.898403000		
1	13.278197000	5.654137000	1	9.408817000	3.401814000
-6.387372000			1.790421000		
6	10.846217000	7.629796000	1	8.928964000	9.239159000
-3.793436000			-1.444842000		
1	10.350471000	6.736425000	1	11.624614000	6.686705000
-3.397762000			-0.777763000		
1	10.921987000	8.355460000	6	14.004883000	6.870524000
-2.978214000			0.900116000		
1	10.210541000	8.051071000	1	14.905265000	6.777828000
-4.581883000			0.269788000		
6	13.328068000	8.750342000	1	13.854866000	5.911243000
-5.367288000			1.414389000		

6 14.237019000 7.969752000 1.884300000
6 15.247817000 8.946739000 1.693663000
6 13.421858000 8.105822000 3.037934000
6 15.421709000 9.998111000 2.590927000
1 15.917750000 8.850874000 0.844395000
6 13.593672000 9.174977000 3.933211000
1 12.688893000 7.342011000 3.282450000
6 14.588110000 10.127748000 3.714803000
1 16.215936000 10.719097000 2.421745000
1 12.954808000 9.241279000 4.808744000
1 14.728083000 10.949103000 4.409285000

Sum of electronic and thermal Free Energies= -3238.748954

*Optimized structure and free energy for **I (triplet state)***

21 11.072094000 7.924890000 0.724632000
26 8.928905000 10.172772000 0.832267000
14 9.209139000 5.962315000 3.044762000
14 13.495078000 10.041904000 2.30709600
7 9.457794000 7.209880000 1.779034000
7 11.988453000 9.595197000 1.428296000
6 12.716698000 6.206227000 0.121718000
6 8.468781000 8.129292000 1.380093000
6 7.749569000 9.091681000 2.189365000
1 7.837157000 9.188530000 3.259720000
6 6.913461000 9.884067000 1.333291000
1 6.254759000 10.678337000 1.650964000
6 7.135704000 9.469345000 -0.021811000
1 6.667989000 9.888254000 -0.899791000
6 8.087333000 8.397754000 -0.000741000
1 8.420435000 7.821083000 -0.850953000
6 11.016942000 10.581520000 1.121245000
6 10.186946000 11.332356000 2.039932000
1 10.216745000 11.241672000 3.114413000
6 9.317109000 12.184077000 1.281295000
1 8.579705000 12.860005000 1.687079000
6 9.568700000 11.955625000 -0.114098000
1 9.058688000 12.433041000 -0.937172000
6 10.606675000 10.977279000 -0.21884600
6 8.163037000 6.589309000 4.528537000
1 8.639369000 7.447603000 5.015813000
1 8.069186000 5.786825000 5.270694000
1 7.154438000 6.882689000 4.218685000
6 10.938141000 5.471780000 3.708913000
1 11.415259000 6.322751000 4.209430000
1 11.599617000 5.128302000 2.906560000
1 10.842855000 4.659040000 4.439201000
6 8.335316000 4.413574000 2.324245000
6 13.135018000 10.781821000 4.040832000
1 12.581810000 11.723966000 3.962500000
1 14.076279000 10.984227000 4.566434000
1 12.545167000 10.085918000 4.648236000
6 14.534602000 8.449358000 2.526501000
1 13.981001000 7.678565000 3.075030000
1 15.443220000 8.678583000 3.096095000
1 14.841948000 8.035054000 1.560122000
6 14.496887000 11.326218000 1.295008000

6	12.811287000	7.254385000	6	17.335977000	5.790657000
-0.896896000			-2.408029000		
1	13.589874000	8.003994000	1	18.010312000	6.611611000
-0.831851000			-2.216110000		
6	11.603812000	7.524284000	6	16.096009000	5.541551000
-1.674940000			-1.736905000		
1	11.595505000	8.356959000	6	12.012929000	4.483057000
-2.368609000			-7.220306000		
6	10.649695000	6.451503000	1	12.534016000	3.537566000
-1.860128000			-7.031941000		
1	9.855869000	6.566802000	1	11.168735000	4.279110000
-2.586823000			-7.890622000		
6	10.754780000	5.252690000	1	12.701741000	5.159336000
-1.094043000			-7.737317000		
1	10.010906000	4.472744000	6	10.173057000	3.986295000
-1.204680000			-4.775685000		
6	11.752442000	5.144901000	1	10.708960000	3.066643000
-0.081431000			-4.512996000		
21	12.920147000	5.317455000	1	9.704018000	4.381314000
-2.39705900			-3.868629000		
26	15.769728000	5.819323000	1	9.374786000	3.723787000
-3.82532100			-5.480649000		
14	11.360379000	5.252773000	6	10.376350000	6.837644000
-5.58736500			-6.046842000		
14	14.070434000	2.142877000	6	15.178496000	0.875730000
-1.27530900			-2.197397000		
7	12.669238000	5.617830000	1	16.238876000	1.137939000
-4.412379000			-2.120156000		
7	14.230942000	3.810213000	1	15.040535000	-0.119653000
-1.927544000			-1.757307000		
6	13.897645000	6.186795000	1	14.914316000	0.818349000
-4.819038000			-3.259425000		
6	14.888443000	5.626250000	6	12.246524000	1.594195000
-5.714556000			-1.485070000		
1	14.793366000	4.683745000	1	11.963078000	1.584955000
-6.230182000			-2.543996000		
6	16.007298000	6.522044000	1	12.118527000	0.578817000
-5.785842000			-1.090486000		
1	16.901708000	6.373143000	1	11.554317000	2.252800000
-6.371734000			-0.950436000		
6	15.750851000	7.630443000	6	14.538928000	2.075810000
-4.910629000			0.586883000		
1	16.412968000	8.463947000	1	14.814148000	10.903072000
-4.730830000			0.335009000		
6	14.463404000	7.430244000	1	13.890151000	12.215139000
-4.315828000			1.088189000		
1	13.962398000	8.103614000	1	15.391598000	11.643093000
-3.636641000			1.844301000		
6	15.490366000	4.340058000	1	15.683376000	6.114702000
-2.291752000			-0.920269000		
6	16.385115000	3.880666000	1	16.208319000	3.025980000
-3.333446000			-3.966769000		
6	17.521201000	4.756043000	1	15.568012000	2.422306000
-3.386020000			0.736977000		
1	18.355913000	4.670929000	1	13.877337000	2.713335000
-4.065451000			1.184662000		

1 14.464035000 1.050416000 0.969334000
1 11.043533000 7.590389000 -6.482509000
1 9.592530000 6.609172000 -6.779335000
1 9.902246000 7.278068000 -5.162181000
1 8.206488000 3.644768000 3.095779000
1 7.345557000 4.676009000 1.933100000
1 8.921023000 3.986292000 1.502950000
1 11.053730000 10.611985000 -1.13140300
1 13.558157000 6.031506000 0.781693000
1 11.788105000 4.268740000 0.552577000
Sum of electronic and thermal Free Energies= -3199.429070

Optimized structure and free energy for ***TS$_{I\text{-}II}$ (triplet state)***
21 2.126155000 0.196178000 0.434589000
26 3.678155000 -1.463122000 -1.506698000
14 4.446886000 2.947581000 0.452385000
14 3.553359000 -1.461820000 3.303534000
7 3.534530000 1.540234000 -0.202750000
7 2.804861000 -1.314718000 1.670954000
6 3.846734000 0.880439000 -1.404171000
6 5.091900000 0.191749000 -1.769125000
1 6.008677000 0.250531000 -1.202150000
6 4.910158000 -0.445738000 -3.031897000
1 5.660819000 -0.975976000 -3.598804000
6 3.525586000 -0.315471000 -3.381812000
1 3.064434000 -0.689371000 -4.284427000
6 2.891501000 0.554726000 -2.420617000
1 1.886228000 0.950122000 -2.486646000
6 2.981800000 -2.227675000 0.630786000
6 4.221186000 -2.837306000 0.130099000
1 5.175733000 -2.781868000 0.632235000
6 3.920504000 -3.601043000 -1.035211000
1 4.604343000 -4.226536000 -1.589406000
6 2.555997000 -3.332027000 -1.382387000
1 2.019716000 -3.768196000 -2.212387000
6 1.959779000 -2.541539000 -0.327995000
6 6.347514000 2.675221000 0.456312000
1 6.619309000 1.779723000 1.026661000
1 6.840700000 3.537690000 0.921590000
1 6.740478000 2.571050000 -0.560783000
6 3.849668000 3.202739000 2.249912000
1 4.163017000 2.370304000 2.890099000
1 2.758525000 3.289536000 2.301535000
1 4.282272000 4.122893000 2.660906000
6 4.067375000 4.507525000 -0.594183000
6 5.424727000 -1.022770000 3.306235000
1 6.008016000 -1.736180000 2.713306000
1 5.814197000 -1.037485000 4.331727000
1 5.588778000 -0.021975000 2.890590000
6 2.625258000 -0.230204000 4.430735000
1 2.719801000 0.800762000 4.072184000
1 3.026115000 -0.270183000 5.450660000
1 1.558179000 -0.473237000 4.467660000
6 3.334094000 -3.248503000 3.956497000
21 -2.035201000 0.121716000 0.172610000
26 -4.725928000 -0.921205000 0.889209000

14	-1.855070000	-2.421730000	6	-1.337097000	-4.263086000
-2.357656000			-2.251477000		
14	-3.305615000	2.945540000	6	-4.632285000	2.790322000
-1.624742000			-3.003267000		
7	-2.118818000	-1.758793000	1	-5.638937000	2.718908000
-0.700143000			-2.576231000		
7	-3.320769000	1.523082000	1	-4.602053000	3.672217000
-0.525720000			-3.654882000		
6	-3.145654000	-2.236347000	1	-4.457573000	1.902016000
0.137158000			-3.621294000		
6	-4.476259000	-2.698602000	6	-1.569508000	3.005221000
-0.203318000			-2.427237000		
1	-4.854406000	-2.830665000	1	-1.395313000	2.128132000
-1.203383000			-3.061125000		
6	-5.203717000	-2.958802000	1	-1.475309000	3.898806000
1.007348000			-3.055963000		
1	-6.215647000	-3.329588000	1	-0.786696000	3.045261000
1.067544000			-1.661898000		
6	-4.374884000	-2.594741000	6	-3.634940000	4.567427000
2.115883000			-0.657549000		
1	-4.637861000	-2.663676000	1	2.273641000	-3.522318000
3.160240000			3.976170000		
6	-3.115073000	-2.145944000	1	3.858896000	-3.970138000
1.591914000			3.320712000		
1	-2.239824000	-1.908824000	1	3.733005000	-3.335889000
2.178271000			4.974148000		
6	-4.497969000	1.076435000	1	-4.072067000	1.564789000
0.125642000			2.280707000		
6	-5.637158000	0.403116000	1	-5.751589000	0.188621000
-0.462386000			-1.513878000		
6	-6.556643000	0.058175000	1	-4.608243000	4.528575000
0.582856000			-0.154807000		
1	-7.496355000	-0.457944000	1	-2.864611000	4.722808000
0.455644000			0.105158000		
6	-5.995411000	0.486457000	1	-3.634398000	5.429686000
1.834456000			-1.335490000		
1	-6.442458000	0.350986000	1	-2.113989000	-4.852409000
2.807790000			-1.751066000		
6	-4.737467000	1.107784000	1	-1.185350000	-4.681348000
1.564128000			-3.253888000		
6	-3.389897000	-2.300377000	1	-0.409640000	-4.378256000
-3.514763000			-1.680995000		
1	-3.855523000	-1.310276000	1	4.610288000	5.377953000
-3.451134000			-0.206360000		
1	-3.066776000	-2.458298000	1	4.364767000	4.355380000
-4.551583000			-1.638111000		
1	-4.148209000	-3.056459000	1	2.995368000	4.733463000
-3.285883000			-0.576601000		
6	-0.482324000	-1.372696000	1	0.899812000	-2.351723000
-3.174376000			-0.204008000		
1	-0.797066000	-0.327234000	1	-0.024096000	0.698903000
-3.275885000			-0.131922000		
1	0.450046000	-1.398545000	6	0.236739000	1.128278000
-2.604076000			1.079835000		
1	-0.277848000	-1.758819000	6	0.129893000	2.601628000
-4.180730000			1.112726000		

6 -0.647824000 0.436465000 2.058160000
6 -0.642075000 3.268524000 2.030812000
1 0.745003000 3.175107000 0.421481000
6 -1.403666000 1.191995000 3.014695000
1 -0.384254000 -0.588119000 2.337135000
6 -1.438454000 2.570941000 3.002261000
1 -0.621647000 4.355889000 2.052491000
1 -1.957736000 0.642185000 3.773840000
1 -2.025213000 3.126037000 3.725757000
Sum of electronic and thermal Free Energies= -3199.397569

Optimized structure and free energy for ***II (triplet state)***
21 11.143805000 7.699836000 0.272916000
26 8.074784000 8.487511000 -0.027252000
14 10.683616000 6.779075000 3.702722000
14 11.710965000 11.202374000 0.98245700
7 10.221525000 7.039844000 1.970357000
7 11.076686000 9.765183000 0.070556000
6 8.861071000 7.017481000 1.566521000
6 7.781353000 7.899211000 2.034869000
1 7.877330000 8.605158000 2.844861000
6 6.582807000 7.566330000 1.337059000
1 5.605536000 7.997902000 1.494372000
6 6.930500000 6.608221000 0.331105000
1 6.249329000 6.163143000 -0.379986000
6 8.303048000 6.221953000 0.518416000
1 8.831736000 5.469131000 -0.043119000
6 9.849016000 9.875441000 -0.605838000
6 8.630727000 10.580045000 -0.176586000
1 8.569324000 11.243952000 0.671596000
6 7.598435000 10.334151000 -1.127962000
1 6.607283000 10.762416000 -1.127555000
6 8.096653000 9.357837000 -2.052799000
1 7.556987000 8.955406000 -2.897770000
6 9.494698000 9.142019000 -1.782651000
6 9.342627000 7.373288000 4.939234000
1 9.197819000 8.458045000 4.889509000
1 9.668738000 7.122764000 5.956461000
1 8.378005000 6.887581000 4.761723000
6 12.287116000 7.754820000 4.078689000
1 12.123808000 8.831437000 3.958134000
1 13.119015000 7.456544000 3.434400000
1 12.584305000 7.573365000 5.119229000
6 10.970607000 4.910782000 4.030278000
6 10.762513000 11.504969000 2.629717000
1 9.761975000 11.917308000 2.462059000
1 11.320087000 12.216036000 3.251888000
1 10.652745000 10.569954000 3.189975000
6 13.547168000 10.918562000 1.425291000
1 13.704935000 10.000950000 2.000204000
1 13.898945000 11.762545000 2.031626000
1 14.165410000 10.865908000 0.523943000
6 11.575773000 12.763628000 -0.11789500
21 12.837752000 5.660424000 -1.70848200
26 15.591204000 4.243181000 -3.15047100
14 12.561560000 7.723065000 -4.53412200

14	11.999855000	2.405233000	6	11.616030000	0.950937000
-0.54071500			-1.731001000		
7	13.402770000	6.530800000	1	12.532481000	0.447276000
-3.451722000			-2.055429000		
7	13.019108000	3.672737000	1	10.982471000	0.213257000
-1.342773000			-1.223220000		
6	14.673236000	6.035192000	1	11.083606000	1.305170000
-3.847278000			-2.621145000		
6	14.957252000	5.126783000	6	10.350309000	3.204521000
-4.937481000			-0.011126000		
1	14.215795000	4.699077000	1	9.803228000	3.584616000
-5.594690000			-0.881196000		
6	16.371654000	4.896611000	1	9.719143000	2.455058000
-4.985273000			0.481439000		
1	16.887405000	4.256982000	1	10.501528000	4.028760000
-5.685633000			0.693389000		
6	16.980100000	5.631949000	6	12.902832000	1.700384000
-3.912275000			0.998259000		
1	18.031528000	5.641063000	1	12.190589000	12.650172000
-3.667174000			-1.01756300		
6	15.944320000	6.331671000	1	10.542632000	12.940920000
-3.212676000			-0.43429800		
1	16.069433000	6.978626000	1	11.924429000	13.647248000
-2.358287000			0.429991000		
6	14.289176000	3.227559000	1	15.704272000	4.053584000
-1.810580000			-0.269823000		
6	14.560060000	2.427960000	1	13.814852000	2.092613000
-2.986172000			-3.690652000		
6	15.971235000	2.181912000	1	13.901138000	1.337735000
-3.055152000			0.729494000		
1	16.481275000	1.625219000	1	13.016478000	2.466122000
-3.826869000			1.774032000		
6	16.594802000	2.838212000	1	12.336015000	0.863807000
-1.939958000			1.424140000		
1	17.653544000	2.859400000	1	13.715364000	9.825909000
-1.729290000			-3.811699000		
6	15.569188000	3.480471000	1	12.078010000	10.194513000
-1.174360000			-4.39223000		
6	13.372894000	7.787826000	1	12.315494000	9.544589000
-6.268239000			-2.760745000		
1	13.262358000	6.839896000	1	11.242872000	4.742898000
-6.804340000			5.079466000		
1	12.888261000	8.573684000	1	10.059150000	4.341171000
-6.860817000			3.816553000		
1	14.441492000	8.017568000	1	11.772927000	4.511487000
-6.203206000			3.400625000		
6	10.740410000	7.160052000	1	10.171589000	8.564917000
-4.753613000			-2.390554000		
1	10.714088000	6.271163000	1	11.055834000	6.424664000
-5.395272000			-1.295037000		
1	10.267812000	6.897838000	6	13.406793000	6.960662000
-3.801337000			0.236191000		
1	10.142424000	7.945403000	6	13.813228000	6.019141000
-5.231238000			1.227613000		
6	12.670935000	9.490985000	6	14.390411000	7.921453000
-3.794977000			-0.140125000		

6 15.089520000 6.040410000 1.808563000
1 13.112973000 5.254888000 1.555251000
6 15.669917000 7.951146000 0.434065000
1 14.144324000 8.667345000 -0.891477000
6 16.018999000 7.010694000 1.411322000
1 15.356442000 5.309240000 2.566344000
1 16.387172000 8.707662000 0.128534000
1 17.007652000 7.033141000 1.859903000
Sum of electronic and thermal Free Energies= -3199.473859

References:

1. Huang, W.; Upton, B. M.; Khan, S. I.; Diaconescu, P. L., *Organometallics* **2013,** *32*, 1379.
2. Becke, A. D., *J. Chem. Phys.* **1993,** *98*, 5648.
3. Lee, C.; Yang, W.; Parr, R. G., *Phys. Rev. B* **1988,** *37*, 785.
4. Cao, X.; Dolg, M., *J. Chem. Phys.* **2001,** *115*, 7348.
5. Cao, X.; Dolg, M., *J. Mol. Struct. (Theochem)* **2002,** *581*, 139.
6. Dolg, M.; Stoll, H.; Preuss, H., *J. Chem. Phys.* **1989,** *90*, 1730.
7. Hay, P. J.; Wadt, W. R., *J. Chem. Phys.* **1985,** *82*, 299.
8. Frisch, M. J. *Gaussian Inc.* , Gaussian Inc.: Wallingford, CT, 2009 (see the SI for the full reference).
9. Reed, A. E.; Curtiss, L. A.; Weinhold, F., *Chem. Rev.* **1988,** *88*, 899.