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Authors

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

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Supporting Information for

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

Wenliang Huang^{1†}, Florian Dulong², Saeed I. Khan¹, Thibault Cantat^{2*}, Paula L. Diaconescu^{1*}

Affiliations:

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

²CEA, 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

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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 (Et₂O), 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 (Me₃SiI) 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^tBu 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 (KC₈) 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^tBuMe₂)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 C₆D₆ or C₇D₈ unless otherwise specified. Chemical shifts are reported with respect to internal solvent (C₆D₆ at 7.16 ppm or C₇D₈ 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/KC₈ 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 KC₈ (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 ¹H NMR spectroscopy (Figures S1-S3). The reaction went to completion after stirring at 25 °C for 4.5 h. The ¹H NMR spectra of the aliquots showed a 1:1 scandium molar ratio formation of [(NN^{fc})Sc(THF)_x]₂(μ-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(μ-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)](μ-H)₂[Sc(NN^{fc})]; however, crystals of **2a** grown from toluene layered with

hexanes had no coordinating THF molecule based on the corresponding ^1H NMR spectrum. Yield: 0.0400 g, 20.7% (maximum 50%, same for the other **2** and **3**). Characterization of **2a**: ^1H 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 CH on Cp), 1.10 (s, 18H, $\text{C}(\text{CH}_3)_3$), and 0.50 and 0.35 (s, 6H each, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6 , 25 °C) δ , ppm: 107.5 (CN), 71.7, 70.0, 69.2, and 66.6 (CH on Cp), 27.6 ($\text{C}(\text{CH}_3)_3$), 21.4 ($\text{C}(\text{CH}_3)_3$), and -1.2 and -2.1 (SiCH_3). Anal. (%): Calcd. for $\text{C}_{44}\text{H}_{78}\text{N}_4\text{Fe}_2\text{Sc}_2\text{Si}_4$, $M_w = 977.082$: 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 ^1H 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**: ^1H NMR (500 MHz, C_6D_6 , 25 °C) δ , ppm: 7.71 (t, 1H, *hydride*), 4.14 (OCH_2CH_2), 4.05, and 3.74 (br s, 4H each, both belong to CH on Cp), 1.47 (OCH_2CH_2), 1.07 (s, 18H, $\text{C}(\text{CH}_3)_3$), and 0.32 (s, 12H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6 , 25 °C) δ , ppm: 107.0 (CN), 71.8 and 67.1 (CH on Cp), 67.1 (OCH_2CH_2), 28.1 ($\text{C}(\text{CH}_3)_3$), 25.5 (OCH_2CH_2), 20.5 ($\text{C}(\text{CH}_3)_3$), and -1.2 (SiCH_3). Anal. (%): Calcd. for $\text{C}_{52}\text{H}_{94}\text{N}_4\text{Fe}_2\text{O}_2\text{Si}_4\text{Y}_2$, $M_w = 1209.196$: 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 ^1H 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**: ^1H NMR (500 MHz, C_6D_6 , 25 °C) δ , ppm: 12.49 (s, 1H, *hydride*), 4.16 (OCH_2CH_2), 4.01, and 3.82 (br s, 4H each, both belong to CH on Cp), 1.47 (OCH_2CH_2), 1.07 (s, 18H, $\text{C}(\text{CH}_3)_3$), and 0.32 (s, 12H, SiCH_3). ^{13}C NMR (126 MHz, C_6D_6 , 25 °C) δ , ppm: 106.3 (CN), 72.1, 68.7, and 65.9 (CH on Cp), 67.4 (OCH_2CH_2), 28.2 ($\text{C}(\text{CH}_3)_3$), 25.6 (OCH_2CH_2), 20.6 ($\text{C}(\text{CH}_3)_3$), and -1.2 (SiCH_3). Anal. (%): Calcd. for $\text{C}_{52}\text{H}_{94}\text{N}_4\text{Fe}_2\text{Lu}_2\text{O}_2\text{Si}_4$, $M_w = 1381.318$: 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 $\text{C}_6\text{H}_5\text{Li}(\text{OEt}_2)_{0.31}$ ($M_w = 106.9$ 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 $(NN^{fc})Sc(\mu-Ph)_2Li + (NN^{fc})ScI \leftrightarrow 2 (NN^{fc})ScPh + LiI$ 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%. 1H NMR (500 MHz, C_6D_6 , 25 °C) δ , ppm: 8.15 (m, 2H, *ortho-CH*), 7.44 (t, 2H, *meta-CH*), 7.32 (t, 1H, *para-CH*), 3.99 (br s, 4H) and 3.53 (br s, 4H), both belong to CH on Cp, 3.86 (m, 4H, OCH_2CH_2), 1.29 (m, 4H, OCH_2CH_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-CH*), 126.9 and 126.8 (*meta-* and *para-CH*), 105.3 (CN), 71.5 and 68.7 (CH on Cp), 68.3 (OCH_2CH_2), 27.8 ($C(CH_3)_3$), 25.2 (OCH_2CH_2), 20.4 ($C(CH_3)_3$) and -2.4 ($SiCH_3$). 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%. 1H NMR (with 15% **1b**) (500 MHz, C_6D_6 , 25 °C) δ , ppm: 8.12 (d, 2H, *ortho-CH*), 7.48 (t, 2H, *meta-CH*), 7.36 (m, 1H, *para-CH*), 4.07 (t, 4H) and 3.22 (t, 4H), both belong to CH on Cp, 3.94 (br s, 8H, OCH_2CH_2), 1.33 (br s, 8H, OCH_2CH_2), 1.04 (s, 18H, $C(CH_3)_3$), and 0.30 (s, 12H, $SiCH_3$). ^{13}C

NMR (126 MHz, C₆D₆, 25 °C) δ , ppm: 186.1 (d, *ipso-C*, J_{YC} = 59 Hz), 138.4 (*ortho-CH*), 126.3 and 125.7 (*meta-* and *para-CH*), 104.4 (CN), 71.6 (OCH₂CH₂), 66.8 and 66.2 (CH on Cp), 28.0 (C(CH₃)₃), 25.0 (OCH₂CH₂), 20.7 (C(CH₃)₃) and -1.4 (SiCH₃). Anal. (%): Calcd. for C₃₆H₅₉N₂O₂FeYSi₂ 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%. ¹H NMR (with 15% **1c**) (500 MHz, C₆D₆, 25 °C) δ , ppm: 8.08 (d, 2H, *ortho-CH*), 7.52 (t, 2H, *meta-CH*), 7.35 (t, 1H, *para-CH*), 4.03 (t, 4H) and 3.30 (t, 4H), both belong to CH on Cp, 4.00 (br s, 8H, OCH₂CH₂), 1.35 (br s, 8H, OCH₂CH₂), 1.03 (s, 18H, C(CH₃)₃), and 0.27 (s, 12H, SiCH₃). ¹³C NMR (126 MHz, C₆D₆, 25 °C) δ , ppm: 193.6 (*ipso-C*), 139.6 (*ortho-CH*), 126.6 and 126.1 (*meta-* and *para-CH*), 104.3 (CN), 71.9 (OCH₂CH₂), 67.2 and 66.4 (CH on Cp), 28.2 (C(CH₃)₃), 25.1 (OCH₂CH₂), 21.0 (C(CH₃)₃) and -1.3 (SiCH₃). Anal. (%): Calcd. for C₃₆H₅₉N₂O₂FeLuSi₂ 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%. ¹H NMR (500 MHz, C₆D₆, 25 °C) δ , ppm: 7.81 (m, 1H, *ortho-CH*), 7.30 (m, 2H, *meta-CH*), 7.23 (m, 1H, *para-CH*), 4.12, 4.04, 3.60, and 2.97 (br s, 2H each, all belong to CH on Cp), 4.04 (br s, 4H, OCH₂CH₂), 2.65 (s, 3H, benzylic CH₃), 1.29 (m, 4H, OCH₂CH₂), 0.92 (s, 18H, C(CH₃)₃), and 0.12 and 0.06 (br s, 6H each, SiCH₃). ¹³C NMR (126 MHz, C₆D₆, 25 °C) δ , ppm: 184.3 (*ipso-C*), 143.0, 135.1, 127.5, 127.1, and 123.8 (aromatic-CH), 102.2 (CN), 73.1 (OCH₂CH₂), 69.1, 68.2, 67.7, and 67.2 (CH on Cp), 27.8 (C(CH₃)₃), 26.3 (benzylic CH₃), 25.0 (OCH₂CH₂), 20.3 (C(CH₃)₃) and -2.4 (SiCH₃). Anal. (%): Calcd. for C₃₃H₅₃N₂OFeScSi₂, 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%. ¹H NMR (500 MHz, C₆D₆, 25 °C) δ , ppm: 8.04 (s, 1H, *ortho-CH*), 7.98 (d, 1H, *ortho-CH*), 7.39 (t, 1H, *meta-CH*), 7.17 (1H, *para-CH*), 4.01, 3.99, and 3.56 (br, 8H total, all belong to CH on Cp), 3.90 (m, 4H, OCH₂CH₂), 2.46 (s, 3H, benzylic CH₃), 1.29 (m, 4H, OCH₂CH₂), 1.03 (s, 18H, C(CH₃)₃), and 0.24 (s, 12H, SiCH₃). ¹³C NMR (126 MHz, C₆D₆, 25 °C) δ , ppm: 182.2 (*ipso-C*), 138.0, 134.9, 134.0, 127.6, and 126.7 (aromatic-CH), 103.0 (CN), 68.4 (OCH₂CH₂), 71.7, 69.2, and 68.7 (CH on Cp), 27.8 (C(CH₃)₃), 22.1 (benzylic CH₃), 25.2 (OCH₂CH₂), 20.4 (C(CH₃)₃) and -2.3 (SiCH₃). Anal. (%): Calcd. for C₃₃H₅₃N₂OFeScSi₂, 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%. ¹H NMR (500 MHz, C₆D₆, 25 °C) δ , ppm: 8.09 (d, 2H, *ortho-CH*), 7.27 (t, 2H, *meta-CH*), 3.99 and 3.55 (br s, 4H each, both belong to CH on Cp), 3.91 (m, 4H, OCH₂CH₂), 2.31 (s, 3H, benzylic CH₃), 1.30 (m, 4H, OCH₂CH₂), 1.03 (s, 18H, C(CH₃)₃), and 0.24 (s, 12H, SiCH₃). ¹³C NMR (126 MHz, C₆D₆, 25 °C) δ , ppm: 178.6 (*ipso-C*), 137.2, 135.6, and 127.5 (aromatic-CH), 105.4 (CN), 68.3 (OCH₂CH₂), 71.6, and 68.3 (CH on Cp), 27.8 (C(CH₃)₃), 21.9 (benzylic CH₃), 25.2 (OCH₂CH₂), 20.4 (C(CH₃)₃) and -2.4 (SiCH₃). Anal. (%): Calcd. for C₃₃H₅₃N₂OFeScSi₂, 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)₂Li, **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)₂Li could be assigned based on integration (Figure S51); a relatively pure sample of (NN^{fc})Lu(α -naphthyl)₂Li could be obtained by fractional crystallization to confirm the assignment of its ¹H 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)₂Li, 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)₂Li(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)₂Li 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 = CH₂Ph): 0.2500 g of ScBr₃(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 ScBr₃(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 H₂(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 ScBn₃(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%. ¹H NMR (500 MHz, C₆D₆, 25 °C) δ , ppm: 7.33 (m, 2H, *ortho*-CH), 7.23 (m, 2H, *meta*-CH), 6.83 (m, 1H, *para*-CH), 3.97, and 3.23 (br, 8H total, CH on Cp), 3.74 (m, 4H, OCH₂CH₂), 2.52 (s, 2H, ScCH₂), 1.31 (m, 4H, OCH₂CH₂), 1.02 (s, 18H, C(CH₃)₃), and 0.25 (s, 12H, SiCH₃). ¹³C NMR (126 MHz, C₆D₆, 25 °C) δ , ppm: 150.1 (*ipso*-C), 129.0, 126.2, and 119.5 (aromatic-CH), 103.8 (CN), 70.9 (OCH₂CH₂), 69.4, and 68.1 (CH on Cp), 55.4 (ScCH₂), 27.8 (C(CH₃)₃), 25.2 (OCH₂CH₂), 20.4 (C(CH₃)₃) and -2.4 (SiCH₃). Anal. (%): Calcd. for C₃₃H₅₃N₂OFeScSi₂, 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/KC₈ system and product identification: 0.1500 g of **1a** (0.198 mmol) was dissolved in 3.0 mL of toluene. 0.0440 g of KC₈ (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 ^1H NMR spectroscopy. The reaction went to completion after 5 h. The ^1H 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 ^1H NMR spectra.

Determination of intermolecular 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 ^1H NMR spectroscopy. The reaction went to completion after 3 h. Integration of the *o*-CH of the phenyl group against SiCH_3 of **3a** (for both $-\text{H}_5$ and $-\text{D}_5$) 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 $k_{\text{H}}/k_{\text{D}}$ is a genuine kinetic isotope effect. The intermolecular KIE was calculated based on the following equation: $(2.28 \times 11.6/2.0)/[24.00 - (2.28 \times 11.6/2.0)] = 1.2(1)$. The factor 11.6/2.0 is derived from the relative integration of the ^1H NMR spectrum of pure **ScPh** (Figure S4).

Determination of intramolecular kinetic isotope effect: 0.0320 g of **1a** (0.042 mmol) was dissolved in 0.500 g of 1,3,5- $\text{C}_6\text{H}_3\text{D}_3$ (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 ^1H 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 ^1H 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 ^1H 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 ^1H 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 ^1H 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 ^1H 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 ^1H 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 ^1H 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 ^1H NMR spectrum of the second aliquot still showed no formation of **2a** and **3a** and intact **1a** (Figure S49).

C-H activation of $[(\text{NN}^{\text{f}})\text{M}(\text{THF})_2(\mu\text{-C}_{10}\text{H}_8)]_x$, **5 ($\text{M} = \text{Sc}$, $x = 0$, **6a**; $\text{M} = \text{Lu}$, $x = 1$, **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 ^1H 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 ^1H 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 functional²⁻³ was employed to optimize the equilibrium molecular structure of the model complexes. In the model structures, the Si^tBuMe₂ substituents on the nitrogen atoms were replaced by SiMe₃ 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 as part of the valence shell. ECP10MDF RECP⁶ 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 potential⁷ 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 Gaussian09⁸ suite of codes and NBO [ENREF_9](#)⁹ analysis was employed for charge determination.

Full citation for reference 8 in SI:

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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 KC₈. 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. ^1H NMR spectrum (C_6D_6 , 300 MHz, 298 K) of benzene activation by **1a**/KC₈ 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. ^1H NMR spectrum (C_6D_6 , 300 MHz, 298 K) of benzene activation by **1a**/KC₈ at 25 °C after 3.75 h (aliquot).

C-H activation of benzene by ScI/KC8 25 C 4.5 h aliquot

Figure S3. ^1H NMR spectrum (C_6D_6 , 300 MHz, 298 K) of benzene activation by **1a**/KC₈ 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. ^1H 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. ^1H 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. ^1H 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. ^1H 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. ^1H 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. ^1H 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. ^1H 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. ^1H 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. ¹H NMR spectrum of **4p** (C₆D₆, 500 MHz, 298 K).

Figure S26. ¹³C NMR spectrum of **4p** (C₆D₆, 126 MHz, 298 K).

Figure S27. HMBC spectrum of **4p** (C₆D₆, 500 MHz, 228 K).

Figure S28. ¹H NMR spectrum of **7** (C₆D₆, 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. ^1H 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. 1H NMR spectrum (C_6D_6 , 300 MHz, 298 K) of regioselectivity study on toluene activation at 25 °C after 1.00 h.

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

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

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

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

Figure S39. ¹H NMR spectrum (C₆D₆, 300 MHz, 298 K) of *intermolecular* KIE study at 25 °C after 1.00 h.

Figure S40. ¹H NMR spectrum (C₆D₆, 300 MHz, 298 K) of *intermolecular* KIE study at 25 °C after 2.00 h.

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

Figure S42. ^1H NMR spectrum ($\text{C}_6\text{H}_3\text{D}_3$, 300 MHz, 298 K) of **1a** in neat $\text{C}_6\text{H}_3\text{D}_3$.

Figure S43. ^1H NMR spectrum (C₆D₆, 300 MHz, 298 K) showing the aromatic region (8.5 to 6.5 ppm) of *intramolecular* KIE study at 25 °C after 3 h (crude product).

Figure S44. ^1H NMR spectrum (C₆D₆, 300 MHz, 298 K) of benzene activation by **1a**/KC₈ under H₂ at 25 °C after 0.5 h (crude product).

Figure S45. ^1H NMR spectrum (C_6D_6 , 300 MHz, 298 K) of benzene activation by **1a**/KC₈ under argon at 25 °C after 1.0 h (crude product).

Figure S46. ^1H NMR spectrum (C_6D_6 , 300 MHz, 298 K) of benzene activation by **1a**/KC₈ under vacuum at 25 °C after 2.2 h (crude product).

Figure S47. ^1H 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. ^1H 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. ^1H 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. ^2H 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**/KC₈ system (crude product).

Figure S51. ^1H NMR spectrum (C₆D₆, 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)₂Li; the peak at 0.50 ppm was assigned to **1c**. The assignment of **6c- α** and (NN^{fc})Lu(α -naphthyl)₂Li was based on the relative integration of peaks in the aromatic region and the peak of SiCH₃ (close to 0 ppm). See also Figure S52 for the ^1H NMR spectrum of a pure sample of (NN^{fc})Lu(α -naphthyl)₂Li.

Figure S52. ^1H NMR spectrum (C₆D₆, 300 MHz, 298 K) of the ate complex, (NN^{fc})Lu(α -naphthyl)₂Li. The integration confirmed the 1 : 2 ratio for the NN^{fc} vs. α -naphthyl ligand.

Figure S53. ^1H 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, $(\text{NN}^{\text{fc}})\text{Lu}(\beta\text{-naphthyl})_2\text{Li}$. 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 SiCH_3 . The ratio of **1c** : **6c- β** : $(\text{NN}^{\text{fc}})\text{Lu}(\beta\text{-naphthyl})_2\text{Li}$ was 0.6 : 1 : 0.7.

Figure S54. ^1H 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. ^1H 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. ^1H 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 ^1H NMR spectroscopy.

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

Figure S58. ^1H 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. ^1H 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. ^1H 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. ^1H 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. ^1H 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

$[(\text{NN}^{\text{fc}})\text{Sc}(\text{THF})](\mu\text{-H})_2[\text{Sc}(\text{NN}^{\text{fc}})]$ (**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 $\text{C}_{52}\text{H}_{96}\text{Fe}_2\text{N}_4\text{O}_2\text{Sc}_2\text{Si}_4$; $M_r = 1123.31$; Triclinic; space group P-1; $a = 12.729(6)$ Å; $b = 14.432(7)$ Å; $c = 17.929(8)$ Å; $\alpha = 89.220(5)^\circ$; $\beta = 72.659(6)^\circ$; $\gamma = 76.126(6)^\circ$; $V = 3046(2)$ Å³; $Z = 2$; $T = 100(2)$ K; $\lambda = 0.71073$ Å; $\mu = 0.797$ mm⁻¹; $d_{\text{calc}} = 1.225$ g·cm⁻³; 14943 reflections collected; 13856 unique ($R_{\text{int}} = 0.1091$); giving $R_1 = 0.0943$, $wR_2 =$

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

(NN^{fc})Sc(*p*-Me-C₆H₄)(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 C₇₁H₁₁₇Fe₂N₄O₂Sc₂Si₄; $M_r = 1372.67$; Orthorhombic; space group Pbcn; $a = 24.002(3) \text{ \AA}$; $b = 15.7124(16) \text{ \AA}$; $c = 20.586(2) \text{ \AA}$; $\alpha = 90^\circ$; $\beta = 90^\circ$; $\gamma = 90^\circ$; $V = 7763.5(14) \text{ \AA}^3$; $Z = 4$; $T = 100(2) \text{ K}$; $\lambda = 0.71073 \text{ \AA}$; $\mu = 0.637 \text{ mm}^{-1}$; $d_{\text{calc}} = 1.174 \text{ g} \cdot \text{cm}^{-3}$; 73849 reflections collected; 11376 unique ($R_{\text{int}} = 0.0331$); giving $R_1 = 0.0632$, $wR_2 = 0.1593$ for 9335 data with $[I > 2\sigma(I)]$ and $R_1 = 0.0760$, $wR_2 = 0.1656$ for all 11376 data. Residual electron density ($e^- \cdot \text{\AA}^{-3}$) max/min: 1.337/-1.137.

(NN^{fc})Sc(*o*-Me-C₆H₄)(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 C₃₃H₅₃FeN₂O₂ScSi₂; 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) Å³; 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 R₁ = 0.0584, wR₂ = 0.1634 for

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

$[(\text{NN}^{\text{fc}})\text{Y}(\text{THF})](\mu\text{-H})_2[\text{Y}(\text{NN}^{\text{fc}})]$ (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 $\text{C}_{26}\text{H}_{46}\text{FeN}_2\text{O}_2\text{Si}_2\text{Y}$; $M_r = 603.59$; Triclinic; space group P-1; $a = 11.618(6) \text{ \AA}$; $b = 15.479(6) \text{ \AA}$; $c = 16.953(7) \text{ \AA}$; $\alpha = 77.348(5)^\circ$; $\beta = 87.648(5)^\circ$; $\gamma = 88.981(3)^\circ$; $V = 2972(2) \text{ \AA}^3$; $Z = 4$; $T = 100(2) \text{ K}$; $\lambda = 0.71073 \text{ \AA}$; $\mu = 2.531 \text{ mm}^{-1}$; $d_{\text{calc}} = 1.349 \text{ g}\cdot\text{cm}^{-3}$; 20307 reflections collected; 10229 unique ($R_{\text{int}} = 0.0405$); giving $R_1 = 0.0957$, $wR_2 = 0.2607$ for 7885

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

(NN^{fc})Y(C₆H₅)(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 $P(2)1/n$; $a = 9.7595(10) \text{ \AA}$; $b = 29.761(3) \text{ \AA}$; $c = 12.8474(13) \text{ \AA}$; $\alpha = 90^\circ$; $\beta = 94.5390(10)^\circ$; $\gamma = 90^\circ$; $V = 3719.8(6) \text{ \AA}^3$; $Z = 4$; $T = 100(2) \text{ K}$; $\lambda = 0.71073 \text{ \AA}$; $\mu = 2.165 \text{ mm}^{-1}$; $d_{\text{calc}} = 1.358 \text{ g} \cdot \text{cm}^{-3}$; 25972 reflections collected; 6548 unique ($R_{\text{int}} = 0.0237$); giving $R_1 = 0.0346$, $wR_2 = 0.0721$ for 6104 data with $[I > 2\sigma(I)]$ and $R_1 = 0.0380$, $wR_2 = 0.0731$ for all 6548 data. Residual electron density ($e^- \cdot \text{\AA}^{-3}$) max/min: 0.721/-0.323.

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 $\text{C}_{52}\text{H}_{94}\text{Fe}_2\text{Lu}_2\text{N}_4\text{O}_2\text{Si}_4$; $M_r = 1381.31$; Triclinic; space group P-1; $a = 10.8150(10)$ Å; $b = 12.4852(11)$ Å; $c = 23.535(2)$ Å; $\alpha = 95.9360(10)^\circ$; $\beta = 100.1200(10)^\circ$; $\gamma = 104.3810(10)^\circ$; $V = 2994.2(5)$ Å³; $Z = 2$; $T = 100(2)$ K; $\lambda = 0.71073$ Å; $\mu = 3.862$ mm⁻¹; $d_{\text{calc}} = 1.532$ g·cm⁻³; 15326 reflections collected; 9671 unique ($R_{\text{int}} = 0.0196$); giving $R_1 = 0.0232$, $wR_2 = 0.0555$ for 8565 data with $[I > 2\sigma(I)]$ and $R_1 = 0.0286$, $wR_2 = 0.0574$ for all 9671 data. Residual electron density ($\text{e}^- \cdot \text{Å}^{-3}$) max/min: 1.331/-0.904.

(NN^{fc})Lu(C₆H₅)(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}LuN₂O₂Si₂; 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) Å³; Z = 4; T = 105(2) K; λ = 0.71073 Å; μ = 3.177 mm⁻¹; d_{calc} = 1.507 g·cm⁻³; 25908 reflections collected; 6525 unique (R_{int} = 0.0233); giving R₁ = 0.0193, wR₂ = 0.0404 for 6036 data with [I > 2σ(I)] and R₁ = 0.0222, wR₂ = 0.0413 for all 6525 data. Residual electron density (e⁻·Å⁻³) max/min: 0.956/-0.470.

(NN^{fc})Lu(α -C₁₀H₇)(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 C₄₀H₆₁FeLuN₂O₂Si₂; 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)

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

$(\text{NN}^{\text{fc}})\text{Lu}(\beta\text{-C}_{10}\text{H}_7)_2\text{Li}(\text{THF})$ (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 $\text{C}_{46}\text{H}_{60}\text{FeLiLuN}_2\text{OSi}_2$; $M_r = 950.90$; Triclinic; space group P-1; $a = 11.682(4) \text{ \AA}$; $b = 11.922(4) \text{ \AA}$; $c = 17.793(5) \text{ \AA}$; $\alpha = 80.603(3)^\circ$; $\beta = 86.689(3)^\circ$; $\gamma = 62.727(3)^\circ$; $V = 2172.6(11) \text{ \AA}^3$; $Z = 2$; $T = 100(2) \text{ K}$; $\lambda = 0.71073 \text{ \AA}$; $\mu = 2.683 \text{ mm}^{-1}$; $d_{\text{calc}} = 1.454 \text{ g}\cdot\text{cm}^{-3}$; 28597 reflections collected; 12297 unique ($R_{\text{int}} = 0.0274$); giving $R_1 = 0.0258$, $wR_2 = 0.0554$ for 11015 data with

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

5. Optimized coordinates

<i>Optimized structure and free energy for I</i>					
21	10.989817000	8.029043000	1	7.910950000	11.576514000
0.871543000			-1.258812000		
26	8.555996000	9.844835000	6	9.831702000	10.615769000
0.921587000			-0.609176000		
14	9.954743000	6.302219000	6	9.184239000	7.130197000
3.829902000			5.381550000		
14	13.278489000	10.742801000	1	9.620918000	8.119625000
1.376771000			5.558929000		
7	9.757402000	7.276322000	1	9.374067000	6.509448000
2.340788000			6.265958000		
7	11.739435000	9.931045000	1	8.099915000	7.245240000
0.945728000			5.276056000		
6	12.030166000	5.201944000	6	11.842948000	6.130582000
0.225500000			4.109438000		
6	8.569556000	7.931531000	1	12.295732000	7.111113000
1.965881000			4.300453000		
6	7.830716000	8.951173000	1	12.339008000	5.682551000
2.681643000			3.241031000		
1	8.069563000	9.308289000	1	12.044296000	5.490797000
3.670910000			4.976950000		
6	6.739362000	9.392876000	6	9.168597000	4.564043000
1.860816000			3.631824000		
1	6.007190000	10.139651000	6	13.096387000	11.923674000
2.128507000			2.879954000		
6	6.815194000	8.704986000	1	12.388738000	12.731764000
0.603850000			2.664299000		
1	6.142524000	8.830465000	1	14.065046000	12.377507000
-0.231146000			3.123211000		
6	7.936419000	7.812684000	1	12.740257000	11.381874000
0.659150000			3.763670000		
1	8.228195000	7.100837000	6	14.523467000	9.358374000
-0.100441000			1.827661000		
6	10.552234000	10.646645000	1	14.163139000	8.760088000
0.656857000			2.673171000		
6	9.755245000	11.454332000	1	15.486572000	9.797599000
1.556598000			2.114169000		
1	9.996230000	11.646724000	1	14.697967000	8.687755000
2.590561000			0.978737000		
6	8.607215000	11.939531000	6	13.957228000	11.761519000
0.846802000			-0.100384000		
1	7.830171000	12.569559000	6	12.375364000	6.564231000
1.252620000			-0.194601000		
6	8.648736000	11.411950000	1	13.419587000	6.883423000
-0.488201000			-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	1	4.768819000	-3.903041000
-5.224420000			-1.752979000		
1	9.299522000	3.967085000	6	2.626515000	-3.271651000
4.542666000			-1.539265000		
1	8.094573000	4.648726000	1	2.154412000	-3.715167000
3.429019000			-2.402380000		
1	9.628409000	4.027959000	6	1.977991000	-2.480920000
2.794148000			-0.534363000		
1	10.172013000	10.108222000	6	6.471846000	2.723045000
-1.499042000			0.039032000		
1	12.604090000	4.745038000	1	6.726959000	1.905651000
1.027567000			0.723267000		
1	10.837606000	3.455348000	1	7.008107000	3.622239000
-0.061231000			0.366401000		
Sum of electronic and thermal Free Energies=			1	6.831913000	2.461699000
-3199.439504			-0.962179000		
			6	4.026027000	3.528123000
<i>Optimized structure and free energy for TS_{1-II}</i>					
21	2.199333000	0.382100000	1.807173000		
0.376078000			1	4.310639000	2.752374000
26	3.525513000	-1.365321000	2.527787000		
-1.513052000			1	2.940566000	3.667256000
14	4.581021000	3.057648000	1.862783000		
0.039468000			1	4.503868000	4.465429000
14	3.012443000	-1.593594000	2.116580000		
3.266360000			6	4.229916000	4.506498000
7	3.625685000	1.608470000	-1.166129000		
-0.422699000			6	4.796054000	-2.238385000
7	2.703055000	-1.217125000	3.566453000		
1.538908000			1	4.972322000	-3.183078000
6	3.900258000	0.786862000	3.040143000		
-1.534364000			1	4.955529000	-2.413726000
6	5.088870000	0.012586000	4.637500000		
-1.826344000			1	5.539435000	-1.508641000
1	5.993720000	0.023722000	3.225455000		
-1.239214000			6	2.759122000	0.042935000
6	4.857318000	-0.758866000	4.220613000		
-3.013882000			1	3.520178000	0.781460000
1	5.564384000	-1.426608000	3.942561000		
-3.482390000			1	2.837553000	-0.129924000
6	3.508800000	-0.528331000	5.300586000		
-3.446245000			1	1.771912000	0.472297000
1	3.028927000	-0.977500000	4.015788000		
-4.302049000			6	1.781538000	-2.921144000
6	2.914285000	0.411339000	3.898452000		
-2.541340000			21	-1.946461000	0.276023000
1	1.932411000	0.854367000	0.147730000		
-2.635868000			26	-4.584093000	-0.871111000
6	2.965391000	-2.092323000	0.978010000		
0.465896000			14	-1.856311000	-2.249843000
6	4.232534000	-2.629804000	-2.385671000		
0.016922000			14	-3.403194000	3.021061000
1	5.178165000	-2.481917000	-1.629116000		
0.514739000			7	-2.014285000	-1.624500000
6	4.013723000	-3.378222000	-0.701030000		
-1.187406000			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	6	16.115997000	7.416447000
2.764129000			4.857899000		
1	16.467500000	8.617320000	6	15.288539000	6.249199000
0.354924000			4.793435000		
1	16.994678000	6.945231000	6	13.917993000	6.678364000
2.120595000			4.743254000		
Sum of electronic and thermal Free Energies=			6	13.899481000	8.111661000
-3199.473859			4.767476000		
<i>Optimized structure and free energy for ScPh</i>			6	16.807027000	12.334947000
26	14.960985000	7.430884000	-0.308468000		
3.085346000			6	17.051224000	9.488165000
21	16.452624000	10.512133000	-1.547838000		
3.123927000			6	14.259962000	10.808616000
14	15.990024000	10.601952000	-1.212487000		
-0.401367000			6	16.757480000	9.641833000
14	15.670833000	10.654496000	7.817041000		
6.602823000			6	16.336138000	12.452284000
7	15.860336000	9.902548000	6.541554000		
1.254803000			6	13.884564000	10.709595000
7	15.697596000	9.940652000	7.307248000		
4.947089000			1	22.630614000	10.862964000
8	15.964037000	12.621214000	3.324154000		
3.065641000			1	21.459729000	10.569116000
6	18.686070000	10.623069000	1.146036000		
3.204827000			1	19.004171000	10.407136000
6	19.485877000	10.549758000	1.067247000		
2.032947000			1	18.851852000	10.814467000
6	20.885838000	10.635004000	5.363753000		
2.067532000			1	21.305166000	10.979823000
6	21.546580000	10.797602000	5.429122000		
3.291238000			1	17.347687000	12.494783000
6	20.799004000	10.865352000	6.123657000		
4.473320000			1	15.681674000	13.101421000
6	19.399727000	10.776635000	5.949941000		
4.423426000			1	16.376058000	12.853249000
6	14.552434000	13.107213000	7.561645000		
2.963215000			1	13.885016000	11.115735000
6	14.645094000	14.608421000	8.326229000		
3.247626000			1	13.236365000	11.339317000
6	16.049551000	14.987382000	6.686256000		
2.722561000			1	13.449466000	9.704832000
6	16.914349000	13.782610000	7.340340000		
3.100066000			1	16.425974000	15.911482000
6	15.380298000	8.567674000	3.170239000		
1.326639000			1	16.028767000	15.120616000
6	16.194064000	7.367044000	1.635255000		
1.370353000			1	17.717422000	13.559106000
6	15.327499000	6.227320000	2.399565000		
1.400494000			1	17.308697000	13.841925000
6	13.970499000	6.700116000	4.116005000		
1.385673000			1	14.573736000	14.801552000
6	13.999277000	8.133072000	4.323758000		
1.350878000			1	13.847668000	15.166384000
6	15.263451000	8.590773000	2.748768000		
4.855478000			1	14.207909000	12.884978000
			1.949814000		

1	13.968695000	12.541119000	1	9.851401000	10.637559000
3.690771000			9.268680000		
1	16.983802000	12.701185000	1	10.109318000	9.043042000
-1.327154000			9.999261000		
1	16.160487000	13.058021000	6	8.661928000	9.071349000
0.199717000			8.323137000		
1	17.771276000	12.296820000	1	8.580709000	7.980373000
0.208948000			8.400045000		
1	18.087540000	9.436005000	1	7.742274000	9.508816000
-1.195600000			8.723504000		
1	16.653117000	8.468093000	6	8.932415000	9.489439000
-1.576012000			6.868673000		
1	17.054717000	9.884386000	1	8.590341000	10.514432000
-2.570557000			6.673532000		
1	17.194562000	7.443024000	1	8.481874000	8.820450000
4.905375000			6.130237000		
1	15.632993000	5.226399000	Sum of electronic and thermal Free Energies=		
4.764461000			-232.292901		
1	17.273757000	7.358029000	<i>Optimized structure and free energy for Sc₂H₂</i>		
1.377318000			21	14.453099000	9.384941000
1	15.636969000	5.194196000	4.616079000		
1.451345000			21	11.204652000	9.661725000
1	13.085630000	6.082239000	4.725689000		
1.421171000			26	16.228423000	9.529695000
1	13.145227000	8.793469000	2.215370000		
1.348400000			26	9.260389000	9.921391000
1	13.055851000	6.032256000	1.772822000		
4.671092000			14	16.336211000	11.906163000
1	13.025224000	8.743577000	6.331284000		
4.726706000			14	15.966726000	6.339708000
1	14.357417000	11.226896000	5.716198000		
-2.221845000			14	10.887163000	13.157560000
1	13.748057000	9.843209000	4.941791000		
-1.290145000			14	10.385741000	6.245040000
1	13.626452000	11.480749000	4.670013000		
-0.621380000			7	10.596853000	11.540489000
1	16.680742000	10.047886000	4.189828000		
8.833044000			7	10.284841000	7.952962000
1	16.437605000	8.594376000	4.081889000		
7.841183000			7	15.376532000	7.562726000
1	17.810222000	9.665702000	4.542843000		
7.514072000			7	15.618585000	11.031178000
Sum of electronic and thermal Free Energies=			4.938230000		
-1947.510711			8	10.394241000	9.678260000
<i>Optimized structure and free energy for THF</i>			6.772522000		
8	10.393713000	9.435182000	6	15.213934000	11.401572000
6.698734000			2.455356000		
6	11.036504000	9.304227000	1	14.148869000	11.573525000
8.017048000			2.510484000		
1	11.858945000	10.023438000	6	11.069010000	9.578841000
8.065976000			8.103904000		
1	11.447045000	8.290262000	1	11.903525000	10.277421000
8.110209000			8.092720000		
6	9.931390000	9.565018000	1	11.442007000	8.557578000
9.054115000			8.202912000		

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

1	8.729349000	4.388133000	1	14.247380000	4.551983000
5.060845000			5.262457000		
1	8.168902000	5.449242000	1	15.685619000	4.302932000
3.751412000			4.257668000		
6	9.969238000	9.912032000	1	16.500539000	14.175010000
9.115257000			5.242909000		
1	9.916338000	10.993839000	1	14.984693000	14.026481000
9.285181000			6.149558000		
1	10.142655000	9.425952000	1	16.511171000	14.327789000
10.079691000			7.012171000		
6	15.464492000	11.248780000	1	12.971166000	13.828693000
7.904539000			3.687433000		
1	15.660508000	10.180161000	1	11.521904000	14.376722000
8.050626000			2.823037000		
1	14.380941000	11.395591000	1	12.087734000	15.262586000
7.847707000			4.254676000		
1	15.836404000	11.782800000	1	12.825164000	9.601748000
8.787339000			3.571098000		
6	8.680043000	9.413487000	Sum of electronic and thermal Free Energies=		
8.423127000			-3200.864710		
1	8.574561000	8.329456000	<i>Optimized structure and free energy for IV</i>		
8.545981000			21	2.337533000	-0.390867000
1	7.779169000	9.889053000	1.281218000		
8.821568000			26	3.708479000	0.939901000
6	8.910854000	9.769407000	3.460403000		
6.952592000			14	0.568321000	-2.606196000
1	8.618401000	10.794595000	3.500415000		
6.709812000			14	5.133363000	-2.589630000
1	8.465502000	9.074326000	0.653947000		
6.239435000			7	1.383698000	-1.111011000
6	18.223393000	11.598489000	2.927492000		
6.529554000			7	4.250781000	-1.109503000
1	18.444242000	10.525278000	1.155187000		
6.561752000			6	0.004556000	3.190700000
1	18.576338000	12.048928000	0.116326000		
7.465717000			1	0.278690000	4.197297000
1	18.792893000	12.043937000	-0.186221000		
5.706663000			6	-1.022574000	2.999159000
6	11.782175000	12.915519000	1.053393000		
6.617546000			1	-1.528412000	3.859345000
1	12.686737000	12.309029000	1.480743000		
6.501792000			6	-1.401772000	1.704607000
1	11.127616000	12.437256000	1.420708000		
7.353645000			1	-2.206774000	1.546349000
1	12.079216000	13.894156000	2.130455000		
7.013488000			6	-0.721700000	0.602819000
1	12.915112000	9.406687000	0.879177000		
5.858799000			1	-0.993467000	-0.400267000
1	12.527580000	5.559636000	1.190551000		
3.528010000			6	0.307031000	0.768181000
1	11.508690000	4.138365000	-0.071119000		
3.854477000			6	1.826131000	-0.085838000
1	11.129031000	5.212757000	3.790580000		
2.492847000			6	2.711102000	-0.177988000
1	15.717404000	3.844568000	4.933972000		
5.973098000					

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	1	7.147755000	-3.040436000
-3.241295000			-0.793121000		
6	-1.999055000	-0.145294000	1	-1.665597000	-1.264557000
-3.644814000			-1.723267000		
6	-2.578218000	-0.606389000	1	-2.682385000	-0.008158000
-4.889868000			-5.780743000		
6	-2.962979000	-1.981384000	1	-4.365478000	1.839946000
-4.740590000			-2.062281000		
1	-3.422713000	-2.597422000	1	-3.192446000	2.739378000
-5.498691000			-1.081853000		
6	-2.596868000	-2.407677000	1	-4.324444000	3.614315000
-3.419579000			-2.142843000		
1	-2.741087000	-3.395286000	1	4.401863000	-0.666258000
-3.007979000			-6.098414000		
6	-2.006219000	-1.290297000	1	5.063281000	0.924495000
-2.747268000			-6.532289000		
6	2.041832000	1.083333000	1	4.822695000	0.493930000
-7.729735000			-4.824615000		
1	1.027315000	1.486471000	1	-1.423132000	-3.074660000
-7.826097000			4.970611000		
1	2.713760000	1.697443000	1	-0.640093000	-1.555191000
-8.342091000			5.449998000		
1	2.050127000	0.066035000	1	-1.685130000	-1.596629000
-8.135176000			4.019035000		
6	2.660312000	2.940514000	1	4.214930000	1.734998000
-5.316650000			0.658335000		
1	1.658684000	3.383866000	Sum of electronic and thermal Free Energies=		
-5.354602000			-3353.011006		
1	3.036414000	3.035001000	<i>Optimized structure and free energy for III</i>		
-4.292367000			21	-0.766314000	-0.067277000
1	3.315435000	3.526403000	2.783273000		
-5.972821000			26	1.072782000	0.729557000
6	4.403289000	0.397163000	5.073697000		
-5.832697000			14	-3.674875000	0.208955000
6	-3.405560000	2.726542000	4.833034000		
-5.134370000			14	0.358407000	-3.495495000
1	-4.159333000	1.936404000	3.022881000		
-5.216624000			7	-1.971970000	0.483064000
1	-3.921808000	3.693489000	4.341378000		
-5.185814000			7	0.408648000	-1.704527000
1	-2.731582000	2.654031000	3.165148000		
-5.995821000			6	-0.144532000	1.604138000
6	-1.249560000	4.118195000	0.978133000		
-3.410440000			1	0.472909000	2.465261000
1	-0.577357000	4.127443000	1.214002000		
-4.276235000			6	-1.575082000	1.701502000
1	-1.833010000	5.047116000	1.148367000		
-3.423873000			1	-2.014126000	2.615102000
1	-0.642801000	4.108130000	1.533870000		
-2.500817000			6	-2.354554000	0.584968000
6	-3.704212000	2.714259000	0.901585000		
-2.049451000			1	-3.425560000	0.601406000
1	6.214435000	-1.669227000	1.069116000		
-1.431958000			6	-1.714120000	-0.630958000
1	7.273429000	-1.443214000	0.450424000		
-0.027818000					

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

1	-1.065855000	-1.780875000	1	1.078684000	3.582586000
-7.715242000			-0.951157000		
6	-0.664083000	-2.702964000	6	-1.951425000	4.150753000
-5.708889000			-2.181222000		
1	-1.366811000	-3.521457000	1	2.061325000	-3.715098000
-5.671072000			1.182318000		
6	0.269029000	-2.342906000	1	2.838447000	-3.883015000
-4.684608000			2.766838000		
1	0.434331000	-2.872445000	1	1.921192000	-5.243081000
-3.757837000			2.086857000		
6	-1.423242000	1.052100000	1	-2.225064000	-0.404571000
-3.897394000			-2.375510000		
6	-1.793775000	1.224145000	1	-1.353741000	1.941273000
-5.288131000			-5.962562000		
6	-2.826513000	0.281280000	1	-2.838447000	3.883015000
-5.611027000			-2.766838000		
1	-3.307821000	0.173262000	1	-2.061325000	3.715098000
-6.571293000			-1.182318000		
6	-3.079293000	-0.523703000	1	-1.921192000	5.243081000
-4.450162000			-2.086857000		
1	-3.790554000	-1.332619000	1	4.363604000	-2.624924000
-4.380356000			-5.070138000		
6	-2.225842000	-0.058201000	1	5.786846000	-1.596534000
-3.398778000			-4.802189000		
6	3.843739000	0.246110000	1	4.731567000	-2.032659000
-6.689279000			-3.440110000		
1	3.301704000	1.169596000	1	-5.786846000	1.596534000
-6.921764000			4.802189000		
1	4.901136000	0.398928000	1	-4.363604000	2.624924000
-6.937958000			5.070138000		
1	3.456738000	-0.551709000	1	-4.731567000	2.032659000
-7.332372000			3.440110000		
6	4.335068000	1.248969000	1	2.225064000	0.404571000
-3.780397000			2.375510000		
1	3.767412000	2.163418000	Sum of electronic and thermal Free Energies=		
-3.987943000			-3353.020418		
1	4.271001000	1.039011000	<i>Optimized structure and free energy for TS_{IV-V}</i>		
-2.706778000			21	1.910609000	0.242373000
1	5.387691000	1.441076000	0.157722000		
-4.020589000			26	2.761882000	-2.371035000
6	4.745430000	-1.767707000	-1.120488000		
-4.503536000			14	4.705675000	1.941219000
6	-0.180206000	4.371612000	-1.373266000		
-4.725747000			14	3.246238000	-0.821871000
1	-1.074897000	4.241453000	3.325556000		
-5.344240000			7	3.400608000	0.713274000
1	-0.031229000	5.447967000	-1.170926000		
-4.573285000			7	2.443157000	-0.974077000
1	0.682243000	3.981569000	1.714511000		
-5.278627000			6	3.333696000	-0.455377000
6	1.170016000	3.964986000	-1.956603000		
-1.972006000			6	4.344020000	-1.475392000
1	2.094346000	3.572093000	-2.155020000		
-2.410748000			1	5.348224000	-1.437120000
1	1.258006000	5.057235000	-1.765935000		
-1.923087000					

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	1	4.164489000	2.580865000
4.745482000			-3.750730000		
1	-4.346645000	-1.406954000	1	3.352415000	3.669839000
4.553445000			-2.607348000		
6	-2.420187000	-3.708324000	1	0.320537000	-2.505102000
1.799386000			0.493242000		
1	-3.313386000	-3.859739000	1	-0.038364000	-0.005210000
1.182096000			-0.487174000		
1	-1.548525000	-3.661460000	6	-0.455400000	1.360683000
1.137313000			-0.234224000		
1	-2.295586000	-4.585867000	6	-0.281128000	2.078361000
2.445627000			-1.511867000		
6	-1.046016000	-1.910983000	6	0.338095000	3.290795000
3.958144000			-1.596129000		
6	-4.460705000	-2.578256000	1	-0.728067000	1.648653000
-3.683571000			-2.406071000		
1	-5.233858000	-1.859212000	6	0.950534000	3.927244000
-3.976348000			-0.448407000		
1	-4.305160000	-3.268489000	6	0.348644000	1.887816000
-4.521752000			0.865410000		
1	-4.834236000	-3.156505000	1	0.117319000	1.531788000
-2.830867000			1.874434000		
6	-1.533195000	-2.996425000	6	0.951057000	3.212537000
-2.675566000			0.792812000		
1	-1.931848000	-3.585437000	6	1.511495000	5.218118000
-1.840832000			-0.515712000		
1	-1.298477000	-3.687360000	1	1.501781000	5.744716000
-3.494484000			-1.466691000		
1	-0.596800000	-2.528039000	6	1.502486000	3.855385000
-2.350670000			1.929110000		
6	-2.177798000	-0.808802000	1	1.479487000	3.342416000
-4.828561000			2.886102000		
1	1.876578000	-2.542350000	6	2.053959000	5.825823000
4.560990000			0.615079000		
1	3.325426000	-3.286863000	1	2.475616000	6.823358000
3.859291000			0.552131000		
1	3.458740000	-2.312458000	6	2.037248000	5.139223000
5.337224000			1.842258000		
1	-3.114305000	2.370349000	1	2.439101000	5.613738000
-1.993812000			2.732543000		
1	-5.853750000	-0.975473000	1	0.356085000	3.824668000
-1.322832000			-2.543993000		
1	-2.873729000	-0.018959000	Sum of electronic and thermal Free Energies=		
-5.134568000			-3352.983933		
1	-1.199346000	-0.347526000	<i>Optimized structure and free energy for TS_{IV-VI}</i>		
-4.651948000			21	1.969280000	0.040387000
1	-2.078309000	-1.516919000	-0.529001000		
-5.660337000			26	3.010819000	0.296260000
1	-1.169848000	-1.053608000	2.274479000		
4.630023000			14	4.826168000	-1.996592000
1	-0.871992000	-2.805787000	-1.423558000		
4.568238000			14	3.363575000	3.197500000
1	-0.158758000	-1.732384000	-1.415207000		
3.341057000			7	3.527986000	-1.291602000
1	5.086108000	3.871871000	-0.392007000		
-2.948307000					

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

1	-5.827655000	-2.869868000	1	-0.970253000	4.443078000
-1.748463000			-2.028430000		
6	-4.161552000	-2.260260000	1	-0.579772000	5.393710000
-0.378956000			-0.577503000		
6	-3.859163000	4.805574000	1	0.056468000	3.741975000
-0.502211000			-0.760881000		
1	-4.730397000	4.579438000	1	5.357729000	-4.326376000
0.121912000			-2.233836000		
1	-3.582771000	5.852569000	1	4.734595000	-4.363298000
-0.327586000			-0.570513000		
1	-4.152033000	4.701985000	1	3.611741000	-4.146040000
-1.552395000			-1.922465000		
6	-2.092916000	3.731501000	1	0.525183000	1.732200000
1.822759000			1.700916000		
1	-2.969818000	3.333597000	1	0.041238000	-0.406468000
2.346343000			0.107147000		
1	-1.215492000	3.150125000	6	-0.432478000	-0.887346000
2.126457000			-1.172233000		
1	-1.933127000	4.764780000	6	-0.188837000	-2.360865000
2.154669000			-1.236875000		
6	-0.810102000	4.386306000	6	0.518892000	-2.946679000
-0.945378000			-2.338840000		
6	-4.338899000	-0.762521000	6	1.066629000	-2.107123000
4.248316000			-3.377279000		
1	-5.228330000	-1.321135000	6	0.277449000	-0.106258000
3.936515000			-2.188831000		
1	-4.177712000	-0.951931000	1	0.010584000	0.946432000
5.316701000			-2.306960000		
1	-4.540493000	0.306958000	6	0.944073000	-0.742951000
4.118703000			-3.290052000		
6	-1.286036000	-0.272906000	6	0.663130000	-4.355682000
3.840325000			-2.391315000		
1	-1.494674000	0.800572000	6	0.154634000	-5.174776000
3.759482000			-1.391299000		
1	-1.068331000	-0.494720000	6	-0.696205000	-3.222545000
4.892285000			-0.235862000		
1	-0.386409000	-0.494178000	1	-1.230374000	-2.787839000
3.255086000			0.605525000		
6	-2.483158000	-3.161433000	6	-0.524037000	-4.603761000
3.594243000			-0.298943000		
1	2.061555000	5.262159000	1	1.571236000	-2.574663000
-0.772442000			-4.216639000		
1	3.475065000	5.058911000	1	1.346888000	-0.110558000
0.279906000			-4.078309000		
1	3.681691000	5.690066000	1	-0.914387000	-5.236051000
-1.366343000			0.492383000		
1	-3.325200000	-2.850667000	1	0.285509000	-6.250829000
-0.722853000			-1.449603000		
1	-5.759054000	-0.048724000	1	1.196286000	-4.790677000
1.599163000			-3.232595000		
1	-3.305883000	-3.767209000	Sum of electronic and thermal Free Energies=		
3.196795000			-3352.979979		
1	-1.553190000	-3.501932000	<i>Optimized structure and free energy for V</i>		
3.125056000			21	11.140280000	7.755538000
1	-2.411750000	-3.349095000	0.388636000		
4.672542000					

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

6	14.625739000	2.521667000	1	13.908338000	2.189825000
-2.831284000			-3.565638000		
6	16.040651000	2.288986000	1	13.751742000	1.308163000
-2.854063000			0.805955000		
1	16.582369000	1.748071000	1	12.836184000	2.427054000
-3.615362000			1.834215000		
6	16.618746000	2.934924000	1	12.142917000	0.849980000
-1.708810000			1.404905000		
1	17.668929000	2.962584000	1	13.586604000	9.957177000
-1.459882000			-3.515968000		
6	15.561246000	3.555984000	1	11.983758000	10.239836000
-0.969993000			-4.225961000		
6	13.528032000	7.967706000	1	12.125747000	9.565330000
-6.053603000			-2.590807000		
1	13.511806000	7.030177000	1	11.102802000	4.608721000
-6.618006000			5.072096000		
1	13.034338000	8.739200000	1	9.955317000	4.241111000
-6.657291000			3.766099000		
1	14.573909000	8.260353000	1	11.675477000	4.447045000
-5.912801000			3.398651000		
6	10.845150000	7.156538000	1	9.853911000	8.485222000
-4.704481000			-2.325188000		
1	10.894438000	6.266478000	1	11.099654000	6.491575000
-5.343239000			-1.186133000		
1	10.334928000	6.872808000	6	13.410098000	7.013198000
-3.777471000			0.411746000		
1	10.237380000	7.912734000	6	13.753818000	6.054136000
-5.215948000			1.380078000		
6	12.567147000	9.559339000	6	14.429738000	7.992132000
-3.593004000			0.109580000		
6	11.613248000	1.038568000	6	15.013038000	6.029530000
-1.785258000			2.051852000		
1	12.541721000	0.530603000	1	13.038996000	5.279460000
-2.065906000			1.652410000		
1	10.939408000	0.296478000	6	15.658315000	8.008696000
-1.339390000			0.743208000		
1	11.142809000	1.425295000	1	14.221310000	8.745950000
-2.696526000			-0.643072000		
6	10.273437000	3.252585000	6	15.334287000	5.044192000
-0.067893000			3.030345000		
1	9.773811000	3.656511000	6	15.987352000	7.034711000
-0.955626000			1.729343000		
1	9.613030000	2.498011000	1	16.394744000	8.769910000
0.376276000			0.496648000		
1	10.396672000	4.060776000	6	16.561821000	5.052131000
0.660103000			3.662662000		
6	12.748196000	1.685183000	1	14.595210000	4.284850000
1.032319000			3.269493000		
1	11.533288000	12.554279000	6	17.243121000	7.015996000
-1.625828000			2.399824000		
1	10.061660000	12.844616000	6	17.523292000	6.047938000
-0.682443000			3.344363000		
1	11.557025000	13.713753000	1	16.798020000	4.297903000
-0.278695000			4.406114000		
1	15.661494000	4.108768000	1	17.978604000	7.777069000
-0.048460000			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
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 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	1	16.745364000	8.219725000
-0.678289000			-2.681532000		
1	15.339918000	10.759550000	6	14.775535000	7.286552000
-2.182586000			-3.231734000		
1	17.846945000	9.086966000	6	14.120579000	0.819366000
0.893363000			-4.216699000		
1	17.007562000	7.255421000	1	13.769710000	1.472090000
2.306535000			-5.024238000		
1	17.500284000	10.721620000	1	13.752129000	-0.195576000
-0.938168000			-4.411464000		
Sum of electronic and thermal Free Energies=			1	15.215352000	0.790381000
-3353.035689			-4.250623000		
			6	11.572153000	1.274577000
<i>Optimized structure and free energy for VII</i>			-2.500556000		
71	12.864794000	5.085326000	1	11.107251000	1.949345000
-2.388415000			-3.229217000		
26	15.895426000	5.497053000	1	11.165852000	1.506204000
-2.895700000			-1.510086000		
14	13.479374000	1.438906000	1	11.280070000	0.249475000
-2.512368000			-2.757101000		
14	12.337308000	5.608964000	6	14.231443000	0.322753000
-6.035746000			-1.145946000		
7	13.851812000	3.165813000	6	13.327683000	4.490885000
-2.196726000			-7.247977000		
7	13.112599000	5.796462000	1	14.264212000	4.963972000
-4.429159000			-7.562953000		
6	15.172930000	3.628977000	1	12.729798000	4.299450000
-2.031382000			-8.147777000		
6	16.325145000	3.436147000	1	13.566665000	3.526569000
-2.886885000			-6.785126000		
1	16.337045000	2.834750000	6	10.627379000	4.795134000
-3.782250000			-5.758233000		
6	17.432471000	4.179263000	1	10.727170000	3.804199000
-2.354830000			-5.300720000		
1	18.427457000	4.218553000	1	10.115352000	4.673651000
-2.771851000			-6.720295000		
6	16.979183000	4.890537000	1	9.993210000	5.407738000
-1.194715000			-5.109183000		
1	17.573662000	5.544579000	6	12.100164000	7.319984000
-0.575291000			-6.873434000		
6	15.597178000	4.564886000	71	10.858090000	8.044608000
-0.997558000			0.915908000		
1	14.988070000	4.872374000	26	8.369279000	9.738241000
-0.158726000			1.151052000		
6	14.403849000	6.334713000	14	13.033324000	10.950681000
-4.272091000			1.574301000		
6	15.640608000	5.968916000	14	10.097836000	6.536696000
-4.931257000			4.224900000		
1	15.729026000	5.237659000	7	11.542340000	10.064628000
-5.718851000			1.114330000		
6	16.716432000	6.735999000	7	9.760013000	7.265088000
-4.368673000			2.623386000		
1	17.751000000	6.692811000	6	10.303381000	10.708254000
-4.673843000			0.875822000		
6	16.187448000	7.537184000	6	9.462433000	11.420555000
-3.304102000			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	-3.744383000	-1.352937000
-1.078753000			-4.605833000		
6	1.438282000	-1.883451000	6	-2.210737000	-0.048559000
-1.043392000			-3.610572000		
1	1.803069000	-2.858055000	6	3.706359000	0.836004000
-1.349715000			-6.706189000		
6	2.307339000	-0.828383000	1	3.073076000	1.727461000
-0.837404000			-6.633895000		
1	3.376460000	-0.946983000	1	4.725429000	1.158865000
-0.972543000			-6.952678000		
6	1.766044000	0.467535000	1	3.340866000	0.218510000
-0.473871000			-7.534040000		
1	2.449087000	1.299245000	6	4.482276000	0.981257000
-0.331501000			-3.698478000		
6	0.458586000	0.556440000	1	3.887898000	1.891530000
0.109091000			-3.553067000		
71	0.739065000	-0.032603000	1	4.554898000	0.457120000
-2.849011000			-2.739112000		
26	-1.005979000	-0.791248000	1	5.493582000	1.286802000
-5.216053000			-3.991350000		
14	3.712491000	-0.137227000	6	4.794063000	-1.704577000
-5.049154000			-5.281821000		
14	-0.334974000	3.515496000	6	-0.115479000	4.353664000
-3.259658000			-4.976340000		
7	2.074073000	-0.569728000	1	-1.001287000	4.219031000
-4.466819000			-5.606851000		
7	-0.413142000	1.724966000	1	0.043317000	5.431544000
-3.354614000			-4.847116000		
6	1.131039000	-1.277338000	1	0.751348000	3.941668000
-5.235051000			-5.505649000		
6	0.612876000	-0.980688000	6	1.186722000	3.951729000
-6.553864000			-2.184963000		
1	0.953011000	-0.174617000	1	2.110272000	3.554486000
-7.184370000			-2.622264000		
6	-0.417877000	-1.927147000	1	1.292866000	5.040405000
-6.874668000			-2.109082000		
1	-0.976352000	-1.965242000	1	1.078350000	3.547884000
-7.797728000			-1.173286000		
6	-0.608233000	-2.786366000	6	-1.924570000	4.221957000
-5.742699000			-2.451600000		
1	-1.317588000	-3.596307000	1	2.060223000	-3.804686000
-5.668906000			1.446425000		
6	0.326998000	-2.386167000	1	2.813940000	-3.955355000
-4.730977000			3.043873000		
1	0.501092000	-2.900009000	1	1.881443000	-5.311939000
-3.795561000			2.378032000		
6	-1.398634000	1.055477000	1	-2.271417000	-0.345670000
-4.110651000			-2.572509000		
6	-1.706937000	1.169219000	1	-1.238573000	1.861332000
-5.520877000			-6.202505000		
6	-2.727149000	0.215190000	1	-2.809420000	3.959658000
-5.852964000			-3.043125000		
1	-3.170512000	0.076180000	1	-2.055460000	3.808362000
-6.827425000			-1.445836000		
6	-3.026224000	-0.550491000	1	-1.874791000	5.315126000
-4.677486000			-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	6	14.340353000	6.724155000
-5.784116000			-4.264623000		
1	-3.543340000	3.777467000	6	15.743354000	6.439936000
-2.382339000			-4.486783000		
1	-2.025465000	4.177846000	1	16.125905000	5.675521000
-1.556301000			-5.143967000		
1	-2.724680000	5.313938000	6	16.536727000	7.341203000
-2.734959000			-3.697003000		
1	2.560119000	-3.469928000	1	17.615470000	7.379471000
-6.081377000			-3.674641000		
1	3.956358000	-2.587630000	6	15.651274000	8.144147000
-6.734246000			-2.910010000		
1	3.694449000	-2.671350000	1	15.939182000	8.916381000
-4.977510000			-2.213650000		
1	-0.387788000	-5.250621000	6	14.303136000	7.765357000
2.909355000			-3.247080000		
1	-0.317009000	-3.864053000	6	13.676794000	1.129525000
4.015378000			-2.792025000		
1	-1.039614000	-3.675478000	1	13.539100000	1.452704000
2.407099000			-3.830370000		
1	2.509215000	2.516995000	1	13.321450000	0.095332000
2.027369000			-2.704435000		
Sum of electronic and thermal Free Energies=			1	14.748957000	1.138319000
-5732.099480			-2.569202000		
			6	10.833340000	1.967258000
<i>Optimized structure and free energy for TS_{IX-XI}</i>			-1.900266000		
71	12.206935000	5.747774000	1	10.543237000	2.224679000
-2.788493000			-2.925241000		
26	15.395516000	6.117802000	1	10.217407000	2.547108000
-2.439865000			-1.205440000		
14	12.699107000	2.267276000	1	10.609319000	0.905016000
-1.589917000			-1.745936000		
14	13.176864000	5.353953000	6	13.117701000	1.746608000
-6.385853000			0.207344000		
7	13.065068000	4.015856000	6	14.351611000	3.838124000
-1.846456000			-6.584975000		
7	13.202131000	6.055106000	1	15.403177000	4.135871000
-4.729474000			-6.660685000		
6	14.387851000	4.453281000	1	14.093795000	3.283958000
-1.536611000			-7.496124000		
6	15.628499000	4.048124000	1	14.250046000	3.159200000
-2.161857000			-5.730369000		
1	15.709734000	3.354991000	6	11.414595000	4.724171000
-2.984467000			-6.783320000		
6	16.714738000	4.752476000	1	11.079467000	3.971803000
-1.542200000			-6.061009000		
1	17.758592000	4.664039000	1	11.415525000	4.261115000
-1.803557000			-7.777511000		
6	16.167238000	5.618116000	1	10.690398000	5.543862000
-0.535858000			-6.789586000		
1	16.725239000	6.294942000	6	13.671133000	6.684458000
0.093081000			-7.676374000		
6	14.749791000	5.443087000	71	11.047162000	8.011128000
-0.532049000			0.850259000		
1	14.047064000	5.933938000	26	9.045015000	9.494028000
0.121461000			2.411444000		

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

1	9.841123000	5.323385000	6	4.215444000	0.222585000
-0.430244000			-3.531525000		
6	10.024168000	7.335383000	1	4.153297000	-0.270201000
-3.809547000			-4.489904000		
6	9.749572000	5.911115000	6	3.109597000	0.687229000
-3.795955000			-2.750097000		
6	9.575445000	5.271893000	1	2.069876000	0.655752000
-2.553237000			-3.037411000		
1	9.179456000	4.261327000	6	3.738484000	-1.926165000
-2.529806000			0.111489000		
1	9.420214000	5.433981000	6	5.163701000	-1.866335000
-4.709298000			-0.138022000		
6	10.369538000	8.007900000	1	5.895761000	-1.442864000
-2.586621000			0.531990000		
6	10.647844000	9.394928000	6	5.438399000	-2.469160000
-2.635800000			-1.411364000		
6	9.949986000	8.093941000	1	6.413514000	-2.583654000
-5.008771000			-1.860227000		
6	10.572272000	10.113720000	6	4.190088000	-2.853323000
-3.823037000			-2.002899000		
1	10.946508000	9.897582000	1	4.058601000	-3.320119000
-1.719490000			-2.966972000		
6	10.211850000	9.454474000	6	3.146083000	-2.515961000
-5.016607000			-1.079934000		
1	9.683112000	7.584374000	6	4.806127000	4.202648000
-5.929570000			-0.199488000		
1	10.792894000	11.176108000	1	5.553779000	3.658522000
-3.832907000			0.387760000		
1	10.146871000	10.013374000	1	4.839834000	5.256406000
-5.944827000			0.103307000		
Sum of electronic and thermal Free Energies=			1	5.088774000	4.142192000
-5732.06976			-1.255569000		
			6	2.706819000	3.552541000
			1.991442000		
<i>Optimized structure and free energy for X</i>			1	3.415754000	2.898662000
71	1.822317000	0.020169000	2.513219000		
0.118398000			1	1.691116000	3.229380000
26	4.235986000	-0.777921000	2.240896000		
-1.679121000			1	2.837796000	4.570163000
14	3.038159000	3.521498000	2.378971000		
0.105413000			6	1.811442000	4.703264000
14	3.629303000	-1.772746000	-0.782826000		
2.881612000			6	4.994625000	-0.528140000
7	2.822502000	1.830216000	3.417433000		
-0.481828000			1	5.879791000	-0.594181000
7	3.006745000	-1.429970000	2.775477000		
1.218481000			1	5.308730000	-0.730283000
6	3.617141000	1.301514000	4.448960000		
-1.531316000			1	4.619286000	0.500935000
6	5.056441000	1.152202000	3.370197000		
-1.574265000			6	2.194657000	-1.622801000
1	5.733012000	1.468786000	4.136015000		
-0.796766000			1	1.738311000	-0.627949000
6	5.420204000	0.523272000	4.124167000		
-2.811325000			1	2.577356000	-1.807631000
1	6.423986000	0.288646000	5.147106000		
-3.131894000					

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	6	7.802907000	7.962583000
-1.199138000			2.100131000		
1	0.405683000	-0.707172000	1	7.867680000	8.631513000
-1.282209000			2.943634000		
6	-0.300655000	0.622500000	6	6.657404000	7.766622000
1.312025000			1.259536000		
6	-0.668740000	1.980633000	1	5.702465000	8.258999000
1.296006000			1.364457000		
6	-0.600634000	-0.088434000	6	7.013904000	6.831835000
2.537742000			0.229538000		
6	-1.286191000	2.645618000	1	6.373676000	6.494463000
2.398033000			-0.571384000		
1	-0.477602000	2.583891000	6	8.371038000	6.435578000
0.408948000			0.445787000		
6	-1.187339000	0.521118000	1	8.923690000	5.713386000
3.631069000			-0.134271000		
1	-0.352851000	-1.143909000	6	9.759371000	10.075202000
2.606143000			-0.273435000		
6	-1.649056000	4.022779000	6	8.515590000	10.629774000
2.349187000			0.219617000		
6	-1.546618000	1.898730000	1	8.405686000	11.197984000
3.597238000			1.128511000		
1	-1.383461000	-0.046641000	6	7.463246000	10.303675000
4.537375000			-0.701645000		
6	-2.240636000	4.634747000	1	6.428611000	10.597561000
3.436267000			-0.608562000		
1	-1.450968000	4.583769000	6	8.012360000	9.481775000
1.440283000			-1.739065000		
6	-2.156608000	2.559262000	1	7.474015000	9.062612000
4.700750000			-2.575070000		
6	-2.495337000	3.895854000	6	9.414933000	9.328176000
4.622128000			-1.475744000		
1	-2.513631000	5.683924000	6	8.985751000	6.686122000
3.390228000			4.978200000		
1	-2.351996000	1.993457000	1	8.763493000	7.746726000
5.607065000			5.136911000		
1	-2.960110000	4.389844000	1	9.195542000	6.233959000
5.469372000			5.955222000		
Sum of electronic and thermal Free Energies=			1	8.091380000	6.207892000
-5732.124235			4.565472000		
			6	11.970966000	7.447649000
			4.550922000		
<i>Optimized structure and free energy for XI</i>					
71	11.237277000	7.906686000	1	11.707611000	8.509664000
0.490856000			4.617353000		
26	8.236849000	8.545963000	1	12.873361000	7.357213000
0.128190000			3.937014000		
14	10.504466000	6.446319000	1	12.213429000	7.093171000
3.831806000			5.560122000		
14	11.799567000	11.546564000	6	10.943877000	4.575974000
1.004102000			3.849459000		
7	10.198301000	7.010796000	6	10.599894000	12.637147000
2.147070000			2.038739000		
7	11.034729000	10.062994000	1	9.819662000	13.089138000
0.327019000			1.417536000		
6	8.877576000	7.112271000	1	11.169766000	13.450151000
1.632772000			2.505871000		

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

1	11.957559000	9.550587000	6	-0.091466000	2.417068000
-3.688772000			-0.000022000		
1	11.138735000	4.233488000	6	-0.791678000	3.629937000
4.873169000			-0.001050000		
1	10.113998000	3.986563000	6	-2.192062000	3.630005000
3.443173000			-0.001514000		
1	11.833061000	4.364324000	6	-2.892390000	2.417213000
3.244616000			-0.000923000		
1	10.126422000	8.843309000	1	-2.735087000	0.264140000
-2.129092000			0.000493000		
1	11.202083000	6.578188000	1	-0.248985000	0.264012000
-1.145573000			0.001258000		
6	13.660004000	7.248206000	1	0.994271000	2.417090000
0.384836000			0.000326000		
6	14.733731000	8.180470000	1	-0.248691000	4.570148000
0.077353000			-0.001477000		
6	13.902096000	6.356747000	1	-2.734944000	4.570279000
1.446367000			-0.002286000		
6	14.607828000	9.136331000	1	-3.978126000	2.417332000
-0.975649000			-0.001258000		
6	15.966838000	8.168893000	Sum of electronic and thermal Free Energies=		
0.825180000			-232.124315		
6	15.108732000	6.347431000	<i>Optimized structure and free energy for benzene</i>		
2.200112000			6	-4.637994000	-0.740251000
1	13.142571000	5.624896000	0.000332000		
1.719075000			6	-3.257556000	-0.738616000
6	15.629855000	10.018780000	0.000150000		
-1.276838000			6	-2.528130000	0.484713000
1	13.681852000	9.169695000	0.000236000		
-1.541727000			6	-3.254742000	1.725593000
6	17.001537000	9.088323000	0.000515000		
0.492253000			6	-4.678520000	1.688129000
6	16.117910000	7.234318000	0.000695000		
1.889866000			6	-5.355516000	0.485091000
1	15.231255000	5.638140000	0.000608000		
3.012928000			1	-0.557610000	-0.416780000
6	16.839622000	9.994157000	-0.000163000		
-0.537637000			1	-5.182334000	-1.679326000
1	15.507298000	10.735441000	0.000265000		
-2.082370000			1	-2.706144000	-1.674832000
1	17.923881000	9.066341000	-0.000060000		
1.066209000			6	-1.104347000	0.522178000
1	17.046382000	7.233050000	0.000056000		
2.454577000			6	-2.525321000	2.948932000
1	17.634037000	10.691464000	0.000603000		
-0.782685000			1	-5.225265000	2.627084000
Sum of electronic and thermal Free Energies=			0.000910000		
-5732.119893			1	-6.440838000	0.469904000
			0.000749000		
<i>Optimized structure and free energy for benzene</i>			6	-1.144886000	2.950560000
6	-2.192223000	1.204422000	0.000424000		
0.000059000			6	-0.427363000	1.725219000
6	-0.791749000	1.204354000	0.000150000		
0.000481000			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	6	6.614836000	-1.609907000
0.538497000			-1.070181000		
1	10.665567000	2.350778000	1	6.770795000	-0.564203000
-0.585973000			-0.781634000		
1	11.256948000	2.826190000	1	7.345009000	-1.859173000
1.016749000			-1.850310000		
Sum of electronic and thermal Free Energies=			1	6.821266000	-2.245646000
-3238.718524			-0.202672000		
<i>Optimized structure and free energy for TS_{xii-xvi}</i>					
21	1.977316000	-0.013990000	6	4.690770000	-0.869934000
-0.605903000			-3.373002000		
26	3.047887000	-0.124747000	1	4.785834000	0.204137000
2.224130000			-3.175338000		
14	4.841641000	-1.888555000	1	3.733614000	-1.049925000
-1.759497000			-3.869615000		
14	3.309357000	3.237633000	1	5.494547000	-1.156931000
-1.078189000			-4.061907000		
7	3.542908000	-1.357588000	6	4.664187000	-3.754838000
-0.636262000			-2.161721000		
7	2.542332000	1.896843000	6	5.211268000	3.012200000
-0.150739000			-1.254374000		
6	3.547501000	-1.641624000	1	5.720323000	3.144952000
0.739800000			-0.293106000		
6	4.597274000	-1.444081000	1	5.616170000	3.753327000
1.719452000			-1.954818000		
1	5.598212000	-1.111184000	1	5.452978000	2.012537000
1.498162000			-1.632280000		
6	4.082299000	-1.760270000	6	2.533916000	3.198315000
3.022074000			-2.827741000		
1	4.637105000	-1.722844000	1	2.709768000	2.238295000
3.947556000			-3.327239000		
6	2.693963000	-2.090751000	1	2.972868000	3.984546000
2.889407000			-3.453370000		
1	2.024411000	-2.363614000	1	1.452838000	3.365606000
3.690635000			-2.772950000		
6	2.358120000	-2.016554000	6	2.992401000	4.933762000
1.495052000			-0.249317000		
1	1.414851000	-2.308042000	21	-2.155844000	-0.041347000
1.052373000			-0.023347000		
6	2.691464000	1.767711000	26	-4.759872000	-0.297969000
1.248964000			-1.137876000		
6	3.907372000	1.783998000	14	-2.467855000	3.534593000
2.035898000			0.622498000		
1	4.899601000	1.944115000	14	-2.736897000	-2.195586000
1.643624000			2.829838000		
6	3.574740000	1.524439000	7	-2.708821000	1.942991000
3.407868000			-0.176399000		
1	4.272519000	1.475428000	7	-2.959807000	-1.461735000
4.230137000			1.209082000		
6	2.157860000	1.310727000	6	-3.746914000	1.649776000
3.493863000			-1.078451000		
1	1.601650000	1.075858000	6	-5.181001000	1.749783000
4.388645000			-0.886075000		
6	1.615265000	1.452091000	1	-5.658823000	2.161785000
2.178063000			-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	1	-1.980952000	-3.168350000
3.180172000			2.960201000		
1	-2.142406000	4.192831000	6	-2.286213000	-2.318095000
2.433761000			0.902799000		
1	-1.853749000	4.010634000	6	-4.212232000	4.299610000
4.171110000			1.244090000		
1	-0.514995000	4.406801000	1	-5.199174000	3.827416000
3.082350000			1.281843000		
1	-1.444065000	-0.676338000	1	-4.353430000	5.369644000
4.566545000			1.047665000		
Sum of electronic and thermal Free Energies=			1	-3.746809000	4.189455000
-3238.760159			2.229031000		
			6	-4.091503000	3.687995000
<i>Optimized structure and free energy for TS_{XII-XV}</i>			-1.787751000		
21	-2.081250000	0.227010000	1	-5.019811000	3.108757000
-0.938843000			-1.722519000		
26	-3.183520000	-0.740262000	1	-3.522194000	3.315498000
2.021523000			-2.645012000		
14	-3.116908000	3.549493000	1	-4.353005000	4.735770000
-0.139802000			-1.981421000		
14	-4.927170000	-1.654459000	6	-1.540969000	4.646440000
-2.134208000			-0.245600000		
7	-2.705642000	1.818214000	6	-6.376046000	-0.436791000
0.193863000			-1.787368000		
7	-3.497023000	-1.297079000	1	-6.730204000	-0.511297000
-1.084721000			-0.753431000		
6	-2.915480000	1.311316000	1	-7.220927000	-0.645623000
1.506329000			-2.455326000		
6	-4.178602000	1.091492000	1	-6.050043000	0.596645000
2.177986000			-1.955819000		
1	-5.149266000	1.274980000	6	-4.526627000	-1.500273000
1.744167000			-4.002225000		
6	-3.920436000	0.564586000	1	-4.192126000	-0.498460000
3.487810000			-4.285668000		
1	-4.664890000	0.290585000	1	-5.444929000	-1.716653000
4.220150000			-4.562639000		
6	-2.498373000	0.431019000	1	-3.767944000	-2.227549000
3.642684000			-4.309995000		
1	-1.988181000	0.038183000	6	-5.526653000	-3.456757000
4.509129000			-1.862242000		
6	-1.881740000	0.882597000	21	2.189585000	-0.083841000
2.433987000			-0.210830000		
1	-0.824642000	0.921787000	26	4.855968000	-0.386320000
2.228341000			-1.192274000		
6	-3.478039000	-1.866662000	14	2.319178000	-2.857627000
0.205888000			2.101454000		
6	-4.572903000	-2.023435000	14	3.058809000	2.988180000
1.143709000			1.554297000		
1	-5.597464000	-1.740595000	7	2.746038000	-1.829934000
0.959866000			0.687748000		
6	-4.069814000	-2.608870000	7	3.020138000	1.743145000
2.354314000			0.254626000		
1	-4.652364000	-2.852065000	6	3.931341000	-1.992321000
3.230177000			-0.066144000		
6	-2.652423000	-2.769621000	6	5.298194000	-1.747147000
2.215703000			0.352291000		

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

1	-1.756470000	-1.265856000	6	8.451618000	9.626260000
-3.914905000			-1.988909000		
1	-2.574967000	1.095035000	1	7.969828000	9.251769000
-4.051023000			-2.878796000		
6	0.230847000	-2.312820000	6	9.812478000	9.383039000
-2.443710000			-1.601559000		
1	1.210574000	-2.430178000	6	9.015152000	6.669455000
-2.926293000			4.667158000		
1	0.342267000	-2.668322000	1	8.783760000	7.725761000
-1.409662000			4.839397000		
1	-0.473616000	-2.976037000	1	9.197016000	6.199372000
-2.956050000			5.641376000		
Sum of electronic and thermal Free Energies=			1	8.136230000	6.196013000
-3238.695405			4.217548000		
<i>Optimized structure and free energy for XV</i>			6	12.006844000	7.454096000
21	11.346799000	7.873758000	4.347315000		
0.357946000			1	11.736214000	8.513020000
26	8.459145000	8.661034000	4.427346000		
-0.117301000			1	12.927514000	7.378129000
14	10.572609000	6.449271000	3.759367000		
3.571408000			1	12.218906000	7.079114000
14	11.873248000	11.267707000	5.356299000		
1.450438000			6	11.031340000	4.586702000
7	10.301367000	7.019068000	3.600018000		
1.876599000			6	10.684882000	11.654919000
7	11.283912000	9.946274000	2.915176000		
0.369988000			1	9.805555000	12.226159000
6	8.989028000	7.185176000	2.599305000		
1.353365000			1	11.218605000	12.251372000
6	7.955480000	8.083132000	3.665726000		
1.828958000			1	10.343016000	10.729946000
1	8.048370000	8.738150000	3.393590000		
2.680544000			6	13.536523000	10.725633000
6	6.810326000	7.963670000	2.216944000		
0.974015000			1	13.431278000	9.816519000
1	5.883326000	8.507253000	2.818783000		
1.076649000			1	13.901467000	11.522409000
6	7.123286000	7.020872000	2.876925000		
-0.063193000			1	14.296334000	10.539804000
1	6.474535000	6.734432000	1.453575000		
-0.877034000			6	12.122280000	12.870778000
6	8.451780000	6.544936000	0.429607000		
0.158937000			21	12.990872000	5.798060000
1	8.979005000	5.818208000	-1.638660000		
-0.436234000			26	15.649924000	4.447913000
6	10.085030000	10.081832000	-2.969670000		
-0.352929000			14	12.106877000	7.107228000
6	8.840052000	10.718697000	-4.812955000		
0.026813000			14	11.972997000	2.516550000
1	8.674842000	11.280408000	-0.641562000		
0.931383000			7	13.221197000	6.401779000
6	7.860448000	10.469559000	-3.573338000		
-0.993613000			7	13.111089000	3.820238000
1	6.842753000	10.829694000	-1.161946000		
-0.992471000			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	1	4.191280000	2.340188000
2.777188000			3.934916000		
1	16.611672000	9.031954000	6	2.095113000	2.009744000
0.104318000			3.201969000		
1	17.145895000	7.536929000	1	1.519810000	1.959722000
2.000880000			4.113664000		
6	14.329731000	9.222677000	6	1.582887000	1.877388000
-1.328736000			1.872556000		
1	15.228716000	9.767843000	6	6.538106000	-2.088147000
-1.636755000			-0.562951000		
1	13.911760000	8.729456000	1	6.810426000	-1.027789000
-2.213094000			-0.510511000		
1	13.583312000	9.952394000	1	7.241812000	-2.585902000
-0.990515000			-1.241929000		
Sum of electronic and thermal Free Energies=			1	6.660754000	-2.529636000
-3238.749739			0.431621000		
			6	4.693983000	-1.578896000
<i>Optimized structure and free energy for TS_{XII-XIV}</i>			-2.994330000		
21	1.986272000	-0.115353000	1	4.946909000	-0.512200000
-0.533627000			-2.974277000		
26	3.022075000	0.353647000	1	3.704912000	-1.694454000
2.277194000			-3.446648000		
14	4.750804000	-2.317909000	1	5.424519000	-2.087236000
-1.230116000			-3.635145000		
14	3.346101000	2.969227000	6	4.391178000	-4.200742000
-1.644732000			-1.288471000		
7	3.508673000	-1.469662000	6	5.255749000	2.746697000
-0.247263000			-1.706937000		
7	2.554095000	1.852102000	1	5.732677000	3.095781000
-0.475388000			-0.784217000		
6	3.522393000	-1.441377000	1	5.674042000	3.324020000
1.159875000			-2.541053000		
6	4.582526000	-1.027101000	1	5.520974000	1.693021000
2.056520000			-1.850614000		
1	5.576462000	-0.742082000	6	2.644013000	2.529771000
1.752081000			-3.370237000		
6	4.086529000	-1.053803000	1	2.859166000	1.488107000
3.403714000			-3.636816000		
1	4.650062000	-0.805604000	1	3.097340000	3.170456000
4.290541000			-4.135993000		
6	2.701441000	-1.423518000	1	1.558804000	2.675365000
3.366405000			-3.398851000		
1	2.043607000	-1.517185000	6	2.973974000	4.798008000
4.216733000			-1.218896000		
6	2.349176000	-1.660740000	21	-2.170249000	-0.091763000
1.995921000			-0.021199000		
1	1.403892000	-2.042902000	26	-4.758244000	-0.510640000
1.636416000			-1.076691000		
6	2.679234000	2.007026000	14	-2.498706000	3.525587000
0.922376000			0.142555000		
6	3.876862000	2.189778000	14	-2.753352000	-1.729111000
1.716468000			3.158512000		
1	4.877695000	2.276336000	7	-2.711673000	1.850868000
1.323179000			-0.474801000		
6	3.512340000	2.215143000	7	-2.975225000	-1.276287000
3.104943000			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	6	7.462112000	10.215589000
-2.428158000			-0.711004000		
6	0.895489000	-1.208585000	1	6.463143000	10.585454000
-3.204122000			-0.536103000		
1	0.223660000	-4.285924000	6	7.866075000	9.362788000
-1.955521000			-1.791796000		
1	1.335492000	-0.707664000	1	7.228631000	8.983125000
-4.065927000			-2.575597000		
6	1.457270000	-3.451914000	6	9.266212000	9.100263000
-4.255660000			-1.645287000		
1	1.812282000	-2.843438000	6	9.207812000	7.074855000
-5.094786000			4.939521000		
1	2.305401000	-4.057654000	1	9.054974000	8.159041000
-3.905649000			4.973184000		
1	0.707942000	-4.153513000	1	9.481481000	6.741401000
-4.648595000			5.948295000		
Sum of electronic and thermal Free Energies=			1	8.258782000	6.600810000
-3238.690453			4.669597000		
			6	12.172255000	7.594475000
			4.232299000		
<i>Optimized structure and free energy for XIV</i>			1	11.972848000	8.669416000
21	11.202903000	7.700892000	4.149355000		
0.371116000			1	13.041561000	7.355046000
26	8.187236000	8.408906000	3.612814000		
0.060947000			1	12.430036000	7.377088000
14	10.618396000	6.594134000	5.276334000		
3.730783000			6	10.939611000	4.716925000
14	11.822583000	11.285258000	3.969488000		
0.601015000			6	11.287215000	11.734293000
7	10.225883000	6.961912000	2.393782000		
2.004288000			1	10.209259000	11.912906000
7	11.083414000	9.727387000	2.468939000		
0.035461000			1	11.804905000	12.645313000
6	8.881917000	7.026933000	2.719411000		
1.552360000			1	11.546380000	10.927174000
6	7.816853000	7.877195000	3.088963000		
2.046158000			6	13.730741000	11.174354000
1	7.904922000	8.566404000	0.604310000		
2.869922000			1	14.104003000	10.380856000
6	6.641801000	7.651012000	1.258166000		
1.255200000			1	14.134007000	12.129064000
1	5.687640000	8.139042000	0.964573000		
1.384951000			1	14.116320000	11.002326000
6	6.966670000	6.696642000	-0.405975000		
0.233494000			6	11.311678000	12.705051000
1	6.299955000	6.337471000	-0.579523000		
-0.535753000			21	12.883067000	5.693427000
6	8.334306000	6.313693000	-1.628061000		
0.407379000			26	15.605830000	4.283305000
1	8.874799000	5.594428000	-3.071730000		
-0.185008000			14	12.591907000	7.791632000
6	9.754697000	9.789771000	-4.428147000		
-0.462143000			14	11.939475000	2.418325000
6	8.606327000	10.455111000	-0.583743000		
0.121008000			7	13.446616000	6.602382000
1	8.616215000	11.030000000	-3.354854000		
1.033334000					

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	1	-5.434568000	0.047548000
0.641823000			-2.115794000		
1	14.268100000	8.600646000	6	-3.869097000	-0.627999000
-0.751779000			-3.581010000		
6	16.045183000	6.941958000	1	-4.432217000	-1.214701000
1.639802000			-4.291175000		
1	15.297877000	5.256754000	6	-2.448186000	-0.421581000
2.763730000			-3.598620000		
1	16.455551000	8.630495000	1	-1.758234000	-0.816923000
0.360538000			-4.328588000		
6	17.406367000	6.943757000	6	-2.110521000	0.394901000
2.297441000			-2.469992000		
1	17.358709000	6.550694000	6	-4.030347000	-4.171977000
3.318218000			2.530258000		
1	18.113971000	6.316076000	1	-4.997900000	-4.076796000
1.738629000			2.026976000		
1	17.829543000	7.952786000	1	-4.185992000	-4.704872000
2.338601000			3.476135000		
Sum of electronic and thermal Free Energies=			1	-3.378497000	-4.781425000
-3238.758932			1.895301000		
<i>Optimized structure and free energy for TS_{XII-XIII}</i>					
21	-2.472732000	0.392126000	6	-4.482816000	-1.428671000
0.916362000			3.936428000		
26	-3.024529000	-1.424334000	1	-5.447498000	-1.349912000
-1.838825000			3.421741000		
14	-3.251805000	-2.457390000	1	-4.113822000	-0.413182000
2.884985000			4.116045000		
14	-4.270267000	3.075206000	1	-4.649291000	-1.909257000
-0.598311000			4.908401000		
7	-2.871559000	-1.577569000	6	-1.659627000	-2.759166000
1.351649000			3.923568000		
7	-3.403826000	1.487284000	6	-5.671661000	3.088543000
-0.553855000			-1.909862000		
6	-2.912387000	-2.286190000	1	-5.291017000	2.871362000
0.122528000			-2.913256000		
6	-4.085782000	-2.737674000	1	-6.136708000	4.082142000
-0.593142000			-1.926507000		
1	-5.103720000	-2.571940000	1	-6.448925000	2.354039000
-0.274506000			-1.672519000		
6	-3.666015000	-3.420938000	6	-5.064787000	3.392907000
-1.782180000			1.113052000		
1	-4.314354000	-3.863230000	1	-5.791177000	2.605682000
-2.523540000			1.348053000		
6	-2.231575000	-3.378874000	1	-5.594785000	4.353574000
-1.837692000			1.103037000		
1	-1.615677000	-3.787697000	1	-4.316667000	3.428555000
-2.624360000			1.911185000		
6	-1.766478000	-2.681941000	6	-3.056133000	4.497190000
-0.675806000			-1.030106000		
1	-0.737159000	-2.489853000	21	2.154998000	0.020231000
-0.411457000			-0.078219000		
6	-3.322662000	0.710539000	26	4.672155000	-0.049487000
-1.735182000			1.266748000		
6	-4.401993000	0.038057000	14	2.894372000	2.948575000
-2.427743000			-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	6	9.486993000	10.728147000
3.219339000			1.520726000		
1	-2.350574000	4.554470000	1	10.076303000	11.024398000
3.664204000			2.375404000		
6	-0.271226000	2.683462000	6	8.089569000	10.974089000
1.693353000			1.317130000		
6	-0.884371000	3.793381000	1	7.427779000	11.488174000
2.226240000			1.997990000		
1	-1.911650000	0.290415000	6	7.712148000	10.387469000
3.577146000			0.060682000		
1	-3.090612000	2.300071000	1	6.718229000	10.382564000
4.370045000			-0.361293000		
1	0.547242000	2.806096000	6	8.874006000	9.775706000
0.984656000			-0.510434000		
1	-0.561004000	4.784247000	6	10.648042000	5.564389000
1.919830000			4.998148000		
1	-0.107643000	-0.747036000	1	11.442820000	6.270137000
2.108002000			5.267780000		
1	1.275908000	0.347971000	1	10.768147000	4.666137000
1.828542000			5.616477000		
Sum of electronic and thermal Free Energies=			1	9.684989000	6.022558000
-3238.638309			5.245396000		
<i>Optimized structure and free energy for XIII</i>					
21	11.709362000	7.728271000	6	12.417886000	4.231608000
0.867936000			2.847455000		
26	8.451634000	8.905030000	1	13.256501000	4.820380000
1.356572000			3.235418000		
14	10.729869000	5.090246000	1	12.596244000	4.009561000
3.135889000			1.790153000		
14	12.306281000	10.874683000	1	12.410587000	3.279495000
-0.718066000			3.393231000		
7	10.531297000	6.565188000	6	9.333372000	3.822429000
2.084017000			2.798474000		
7	11.343346000	9.595654000	6	12.754645000	12.307256000
0.151305000			0.477232000		
6	9.197594000	7.070529000	1	11.847013000	12.751611000
2.120063000			0.900812000		
6	8.596289000	7.865282000	1	13.301941000	13.092847000
3.173276000			-0.058505000		
1	9.116692000	8.230813000	1	13.378859000	11.948808000
4.045405000			1.302656000		
6	7.218692000	8.087479000	6	13.910142000	10.140296000
2.847505000			-1.454510000		
1	6.512067000	8.659005000	1	14.610275000	9.838842000
3.430543000			-0.671751000		
6	6.950905000	7.451795000	1	14.400862000	10.909978000
1.587265000			-2.063991000		
1	6.008774000	7.465546000	1	13.705863000	9.277612000
1.060189000			-2.096866000		
6	8.160022000	6.828232000	6	11.286177000	11.621976000
1.137759000			-2.161444000		
1	8.297901000	6.271759000	21	13.317197000	5.903017000
0.223375000			-1.283284000		
6	9.994299000	9.987479000	26	15.918087000	4.670404000
0.384002000			-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	6	8.087333000	8.397754000
1.884300000			-0.000741000		
6	15.247817000	8.946739000	1	8.420435000	7.821083000
1.693663000			-0.850953000		
6	13.421858000	8.105822000	6	11.016942000	10.581520000
3.037934000			1.121245000		
6	15.421709000	9.998111000	6	10.186946000	11.332356000
2.590927000			2.039932000		
1	15.917750000	8.850874000	1	10.216745000	11.241672000
0.844395000			3.114413000		
6	13.593672000	9.174977000	6	9.317109000	12.184077000
3.933211000			1.281295000		
1	12.688893000	7.342011000	1	8.579705000	12.860005000
3.282450000			1.687079000		
6	14.588110000	10.127748000	6	9.568700000	11.955625000
3.714803000			-0.114098000		
1	16.215936000	10.719097000	1	9.058688000	12.433041000
2.421745000			-0.937172000		
1	12.954808000	9.241279000	6	10.606675000	10.977279000
4.808744000			-0.218846000		
1	14.728083000	10.949103000	6	8.163037000	6.589309000
4.409285000			4.528537000		
Sum of electronic and thermal Free Energies=			1	8.639369000	7.447603000
-3238.748954			5.015813000		
			1	8.069186000	5.786825000
<i>Optimized structure and free energy for I (triplet state)</i>			5.270694000		
21	11.072094000	7.924890000	1	7.154438000	6.882689000
0.724632000			4.218685000		
26	8.928905000	10.172772000	6	10.938141000	5.471780000
0.832267000			3.708913000		
14	9.209139000	5.962315000	1	11.415259000	6.322751000
3.044762000			4.209430000		
14	13.495078000	10.041904000	1	11.599617000	5.128302000
2.30709600			2.906560000		
7	9.457794000	7.209880000	1	10.842855000	4.659040000
1.779034000			4.439201000		
7	11.988453000	9.595197000	6	8.335316000	4.413574000
1.428296000			2.324245000		
6	12.716698000	6.206227000	6	13.135018000	10.781821000
0.121718000			4.040832000		
6	8.468781000	8.129292000	1	12.581810000	11.723966000
1.380093000			3.962500000		
6	7.749569000	9.091681000	1	14.076279000	10.984227000
2.189365000			4.566434000		
1	7.837157000	9.188530000	1	12.545167000	10.085918000
3.259720000			4.648236000		
6	6.913461000	9.884067000	6	14.534602000	8.449358000
1.333291000			2.526501000		
1	6.254759000	10.678337000	1	13.981001000	7.678565000
1.650964000			3.075030000		
6	7.135704000	9.469345000	1	15.443220000	8.678583000
-0.021811000			3.096095000		
1	6.667989000	9.888254000	1	14.841948000	8.035054000
-0.899791000			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	6	2.981800000	-2.227675000
0.969334000			0.630786000		
1	11.043533000	7.590389000	6	4.221186000	-2.837306000
-6.482509000			0.130099000		
1	9.592530000	6.609172000	1	5.175733000	-2.781868000
-6.779335000			0.632235000		
1	9.902246000	7.278068000	6	3.920504000	-3.601043000
-5.162181000			-1.035211000		
1	8.206488000	3.644768000	1	4.604343000	-4.226536000
3.095779000			-1.589406000		
1	7.345557000	4.676009000	6	2.555997000	-3.332027000
1.933100000			-1.382387000		
1	8.921023000	3.986292000	1	2.019716000	-3.768196000
1.502950000			-2.212387000		
1	11.053730000	10.611985000	6	1.959779000	-2.541539000
-1.13140300			-0.327995000		
1	13.558157000	6.031506000	6	6.347514000	2.675221000
0.781693000			0.456312000		
1	11.788105000	4.268740000	1	6.619309000	1.779723000
0.552577000			1.026661000		
Sum of electronic and thermal Free Energies=			1	6.840700000	3.537690000
-3199.429070			0.921590000		
			1	6.740478000	2.571050000
Optimized structure and free energy for TS_{II}			-0.560783000		
(triplet state)			6	3.849668000	3.202739000
21	2.126155000	0.196178000	2.249912000		
0.434589000			1	4.163017000	2.370304000
26	3.678155000	-1.463122000	2.890099000		
-1.506698000			1	2.758525000	3.289536000
14	4.446886000	2.947581000	2.301535000		
0.452385000			1	4.282272000	4.122893000
14	3.553359000	-1.461820000	2.660906000		
3.303534000			6	4.067375000	4.507525000
7	3.534530000	1.540234000	-0.594183000		
-0.202750000			6	5.424727000	-1.022770000
7	2.804861000	-1.314718000	3.306235000		
1.670954000			1	6.008016000	-1.736180000
6	3.846734000	0.880439000	2.713306000		
-1.404171000			1	5.814197000	-1.037485000
6	5.091900000	0.191749000	4.331727000		
-1.769125000			1	5.588778000	-0.021975000
1	6.008677000	0.250531000	2.890590000		
-1.202150000			6	2.625258000	-0.230204000
6	4.910158000	-0.445738000	4.430735000		
-3.031897000			1	2.719801000	0.800762000
1	5.660819000	-0.975976000	4.072184000		
-3.598804000			1	3.026115000	-0.270183000
6	3.525586000	-0.315471000	5.450660000		
-3.381812000			1	1.558179000	-0.473237000
1	3.064434000	-0.689371000	4.467660000		
-4.284427000			6	3.334094000	-3.248503000
6	2.891501000	0.554726000	3.956497000		
-2.420617000			21	-2.035201000	0.121716000
1	1.886228000	0.950122000	0.172610000		
-2.486646000			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	6	8.630727000	10.580045000
2.058160000			-0.176586000		
6	-0.642075000	3.268524000	1	8.569324000	11.243952000
2.030812000			0.671596000		
1	0.745003000	3.175107000	6	7.598435000	10.334151000
0.421481000			-1.127962000		
6	-1.403666000	1.191995000	1	6.607283000	10.762416000
3.014695000			-1.127555000		
1	-0.384254000	-0.588119000	6	8.096653000	9.357837000
2.337135000			-2.052799000		
6	-1.438454000	2.570941000	1	7.556987000	8.955406000
3.002261000			-2.897770000		
1	-0.621647000	4.355889000	6	9.494698000	9.142019000
2.052491000			-1.782651000		
1	-1.957736000	0.642185000	6	9.342627000	7.373288000
3.773840000			4.939234000		
1	-2.025213000	3.126037000	1	9.197819000	8.458045000
3.725757000			4.889509000		
Sum of electronic and thermal Free Energies=			1	9.668738000	7.122764000
-3199.397569			5.956461000		
			1	8.378005000	6.887581000
<i>Optimized structure and free energy for II</i>			4.761723000		
<i>(triplet state)</i>			6	12.287116000	7.754820000
21	11.143805000	7.699836000	4.078689000		
0.272916000			1	12.123808000	8.831437000
26	8.074784000	8.487511000	3.958134000		
-0.027252000			1	13.119015000	7.456544000
14	10.683616000	6.779075000	3.434400000		
3.702722000			1	12.584305000	7.573365000
14	11.710965000	11.202374000	5.119229000		
0.98245700			6	10.970607000	4.910782000
7	10.221525000	7.039844000	4.030278000		
1.970357000			6	10.762513000	11.504969000
7	11.076686000	9.765183000	2.629717000		
0.070556000			1	9.761975000	11.917308000
6	8.861071000	7.017481000	2.462059000		
1.566521000			1	11.320087000	12.216036000
6	7.781353000	7.899211000	3.251888000		
2.034869000			1	10.652745000	10.569954000
1	7.877330000	8.605158000	3.189975000		
2.844861000			6	13.547168000	10.918562000
6	6.582807000	7.566330000	1.425291000		
1.337059000			1	13.704935000	10.000950000
1	5.605536000	7.997902000	2.000204000		
1.494372000			1	13.898945000	11.762545000
6	6.930500000	6.608221000	2.031626000		
0.331105000			1	14.165410000	10.865908000
1	6.249329000	6.163143000	0.523943000		
-0.379986000			6	11.575773000	12.763628000
6	8.303048000	6.221953000	-0.11789500		
0.518416000			21	12.837752000	5.660424000
1	8.831736000	5.469131000	-1.70848200		
-0.043119000			26	15.591204000	4.243181000
6	9.849016000	9.875441000	-3.15047100		
-0.605838000			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	15.356442000	5.309240000
1.808563000			2.566344000		
1	13.112973000	5.254888000	1	16.387172000	8.707662000
1.555251000			0.128534000		
6	15.669917000	7.951146000	1	17.007652000	7.033141000
0.434065000			1.859903000		
1	14.144324000	8.667345000	Sum of electronic and thermal Free Energies=		
-0.891477000			-3199.473859		
6	16.018999000	7.010694000			
1.411322000					

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