- Electronic Supplementary Information -

The Role of 5f-Orbital Participation in Unexpected Inversion of the σ-Bond Metathesis Reactivity Trend of Triamidoamine Thorium(IV) and Uranium(IV) Alkyls

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General Experimental Considerations

All manipulations were carried out under an inert atmosphere of dry nitrogen utilising standard Schlenk techniques, or an MBraun UniLab glovebox operating under an atmosphere of dry nitrogen with H_2O and O_2 < 0.1 ppm. All glassware was dried either by overnight storage in an oven at 150 °C or by flame-drying with subsequent cooling under 10^{-3} mm Hg vacuum followed by repeated alternate evacuation and purging with nitrogen or argon. Oxygen-free nitrogen gas was supplied by BOC Gases UK. Me_3SiI was purchased from Sigma-Aldrich, filtered from activated magnesium to remove acid traces, degassed by three freeze-pump-thaw cycles and stored under nitrogen at 5 °C. $Th(NO_3)_4(H_2O)_5$ was purchased from Strem.

$[ThCl_4(THF)_{3.5}]$ was prepared from $[ThCl_4(DME)_2]$ by an adapted method based on the reported procedure[1] where $[ThCl_4(DME)_2]$ (2.78 g, 5 mmol) was refluxed in 40 ml THF before the solvent was removed and replaced with 40 ml fresh THF. This was repeated two more times until the white precipitate obtained was isolated by filtration, washed with hexane (10 ml) and dried *in vacuo* to give $[ThCl_4(THF)_{3.5}]$ in 90% yield. $Li_3(Tren^{TIPS})$,[2] **2a**,[2] benzyl potassium,[3] and $[Ph_3C][BAr^f_4]$ [Ar^f = 3,5-$(CF_3)_2$-C_6H_3][4] were prepared according to published procedures. THF, hexane, pentane and toluene were dried by passage through activated alumina, degassed prior to use, and stored over activated 4Å molecular sieves (THF) or a potassium mirror (hexane, pentane, toluene). Methylcyclohexane was distilled from potassium and stored over a potassium mirror. Deuterated NMR solvents were purchased from Goss Scientific Ltd. C_6D_6 and C_7D_8 were distilled from a potassium mirror, degassed by three freeze-pump-thaw cycles and stored under nitrogen. Nujol® was purchased from Sigma-Aldrich and used as received.

^1H, ^{13}C and ^{29}Si NMR spectra were recorded on a Bruker AV400 or AV(III)400 spectrometer [operating at 400.2 (^1H), 100.6 (^{13}C) and 79.5 (^{29}Si) MHz, respectively]. Chemical shifts (δ) are quoted in ppm and are relative to external TMS. Samples were prepared in the glovebox and placed in J. Young PTFE 5mm screw-topped borosilicate NMR tubes. Crystals were examined on an Oxford Diffraction Ltd. SuperNova Atlas CCD diffractometer. FTIR spectra were recorded on a Bruker Tensor™ 27 spectrometer and samples were prepared in the glovebox as Nujol® mulls between KBr discs. Elemental analyses were carried out by Tong Liu (University of Nottingham).

Preparation of [Th(Tren^{TIPS})(Cl)] (1b)

THF (15 ml) was added to a cold (−78 °C) mixture of [$ThCl_4(THF)_{3.5}$] (3.13 g, 5.0 mmol) and $Tren^{TIPS}Li_3$ (3.17 g, 5.0 mmol). The resulting suspension was allowed to warm to ambient temperature whilst being stirred (1 hour) and stirred at ambient temperature for a further 16 hours to afford a pale yellow suspension. The solvent was removed *in vacuo* to afford an off-white solid. Toluene (10 ml) was added and the suspension was warmed to 60 °C, allowed to settle and filtered whilst warm to give a pale yellow solution. The residual white solid was washed with toluene (3 × 2 ml) and the combined extracts reduced to dryness *in vacuo* to afford an essentially pure off-white solid. Crystalline material was obtained by dissolution in warm (60 °C) toluene (4 ml) and storage −30 °C for 24 hours. The colourless crystals were isolated by filtration at −30 °C, washed with hexane (3 × 2 ml) and dried *in vacuo* for 30 minutes. A second crop of crystals was obtained by reduction of the supernatant solution to 1 ml and storage at −30 °C for 24 hours. Yield: solid 4.31 g (98%) or crystalline 2.11 g (48%). ^{1}H NMR (C_6D_6, 298 K): δ 1.38 (d, $^3J_{HH}$ = 7.4 Hz, 54H, 3×Si^i*Pr*$_3$), 1.56 (sept, $^3J_{HH}$ = 7.2 Hz, 9H, 3×C*H*), 2.71 (t, $^2J_{HH}$ = 5.2 Hz, 6H, CH_2), 3.71 (t, $^2J_{HH}$ = 4.8 Hz, 6H, CH_2) ppm. ^{13}C{^{1}H} NMR (C_6D_6, 298 K): δ 12.97 (s, *C*H), 19.60 (s, *C*H_3), 46.30 (s, *C*H_2), 63.55 (s, *C*H_2) ppm. ^{29}Si{^{1}H} NMR (C_6D_6, 298 K): δ 4.63 ppm. FTIR (Nujol®): $\tilde{\nu}$ 1305.19 (w), 1261.51 (s), 1095.27 (s), 1075.02 (s), 1046.38 (s), 1019.64 (s), 925.93 (m), 882.38 (m), 800.47 (s), 741.93 (s), 723.15 (m), 692.13 (m), 588.28 (w), 516.96 (w) cm^{-1}. Anal. calc'd for $C_{33}H_{75}ClN_4Si_3Th$: C 45.05; H 8.59; N 6.37%. Found: C 45.15; H 8.60; N 6.25%.

Preparation of [Th(Tren^{TIPS})(I)] (2b)

Me_3SiI (0.76 ml, 5.4 mmol) was added *via* syringe to a cold (0 °C) stirring suspension of [Th(Tren^{TIPS})(Cl)] (4.29 g, 4.9 mmol) in toluene (10 ml). The mixture was allowed to warm to room temperature over 1 hour before being heated to 65 °C and maintained at this

temperature for 16 hours to afford a white suspension. Volatiles were removed *in vacuo* and the off-white solid obtained was washed with hexane (2 × 3 ml) and dried *in vacuo* for 30 minutes to afford essentially pure material as a white solid. Crystalline material was obtained by dissolution of the solid in 3 ml warm (60 °C) toluene and storage at −30 °C for 24 hours to afford colourless crystals that were isolated by filtration, washed with hexane (3 × 2 ml) and dried *in vacuo* for 30 minutes. Yield: solid 4.20 g (89%) or crystalline 1.42 g (30%). ^{1}H NMR (C_6D_6, 298 K): δ 1.36 (d, $^{3}J_{HH}$ = 7.6 Hz, 54H, 3×Si^{i}*Pr*$_3$), 1.62 (sept, $^{3}J_{HH}$ = 7.6 Hz, 9H, 3×C*H*), 2.65 (t, $^{2}J_{HH}$ = 4.4 Hz, 6H, C*H*$_2$), 3.70 (t, $^{2}J_{HH}$ = 4.4 Hz, 6H, C*H*$_2$) ppm. ^{13}C{^{1}H} NMR (C_6D_6, 298 K): δ 13.31 (s, *C*H), 19.73 (s, *C*H$_3$), 46.20 (s, *C*H$_2$), 64.40 (s, *C*H$_2$) ppm. ^{29}Si{^{1}H} NMR (C_6D_6, 298 K): δ 5.32 ppm. FTIR (Nujol®): $\tilde{\nu}$ 1297.87 (w), 1260.40 (m), 1133.79 (m), 1042.22 (s), 1012.46 (s), 926.42 (s), 882.35 (s), 813.39 (m), 801.58 (m), 734.22 (s), 675.31 (m), 633.72 (m), 566.34 (w), 548.50 (w), 516.48 (w) cm^{-1}. Anal. calc'd for $C_{33}H_{75}IN_4Si_3Th$: C 45.05; H 8.60; N 6.37%. Found: C 45.18; H 8.44; N 6.29%.

Preparation of [U{N(CH$_2$CH$_2$NSiPr$^{i}_3$)$_2$(CH$_2$CH$_2$*N* SiPr$^{i}_2$C[H]Me*C*H$_2$)}] (3a)

Toluene (30 ml) was added to [U(I)(Tren^{TIPS})] (0.98 g, 1.0 mmol) and benzylpotassium (0.13 g, 1.0 mmol) at –78 °C. The mixture was allowed to warm to room temperature and then stirred at room temperature for a further 16 hours to afford a turbid orange-brown mixture. Volatiles were removed *in vacuo* and the product extracted into hexanes. The mixture was filtered, concentrated to 2 ml and stored at 4 °C for 72 hours to yield orange crystals, which were isolated by filtration at 0 °C and washed with cold pentane. Yield: 0.55 g, 65%. ^{1}H NMR (C_6D_6, 298 K): δ 46.75 (1H, s, C*H*$_2$), 32.65 (1H, s, C*H*$_2$), 28.89 (1H, s, C*H*$_2$), 23.20 (1H, s, C*H*$_2$), 15.93 (1H, s, UCH$_2$C*H*), 15.76 (3H, s, UCH$_2$CH*Me*), 11.73 (1H, s, C*H*$_2$), 11.30 (1H, m, C*H*Me$_2$), 9.54 (1H, m, C*H*Me$_2$), 8.38 (3H, d, $^{3}J_{HH}$ = 7.3 Hz, Si*Me*), 6.82 (1H, s, C*H*$_2$), 6.02 (3H, d, $^{3}J_{HH}$ = 7.3 Hz, Si*Me*), 5.65 (3H, d, $^{3}J_{HH}$ = 6.4 Hz, Si*Me*), 4.01 (9H, s,

3×Si*Me*), 3.72 (3H, d, $^{3}J_{HH}$ = 6.4 Hz, Si*Me*), 2.77 (1H, s, CH_2), 1.52 (3H, s, 3×C*H*Me$_2$), –0.53 (1H, s, CH_2), –1.33 (2H, s, UCH_2), –2.61 (9H, 3×Si*Me*), –2.89 (9H, s, 3×Si*Me*), –4.70 (9H, s, 3×Si*Me*), –20.84 (3H, s, 3×C*H*Me$_2$), –23.09 (1H, s, CH_2), –24.14 (1H, s, CH_2), –31.64 (1H, s, CH_2), –35.20 (1H, s, CH_2) ppm. ^{29}Si{^{1}H} NMR (C_6D_6, 298 K): δ −112.25 (s, *Si*^{i}Pr$_3$), −118.04 (s, *Si*^{i}Pr$_3$), −125.66 (s, *Si*^{i}Pr$_2$C[H]MeCH$_2$U) ppm. μ_{eff} (Evans method, C_6D_6, 298 K): 2.90 μ_B. FTIR: (Nujol®): $\tilde{\nu}$ 1281 (w), 1135 (w), 1103 (s), 1064 (m), 1040 (m), 1011 (m), 990 (m), 922 (s), 904 (m), 881 (s) cm^{-1}. Anal. Calcd for $C_{33}H_{74}N_4Si_3U$: C, 46.67; H, 8.78; N, 6.60%. Found: C, 46.67; H, 8.81; N, 6.37%.

Preparation of [Th{N(CH$_2$CH$_2$NSiPr$^{i}_3$)$_2$(CH$_2$CH$_2$*N* SiPr$^{i}_2$C[H]Me*C*H$_2$)}] (3b)

A solution of [Th(Tren^{TIPS})(CH$_2$Ph)] (1.48 g, 1.6 mmol) in toluene (15 ml) was heated at 80 °C for 2 hours. The solvent was removed *in vacuo* to afford an off-white solid that was dissolved in warm (50 °C) hexane (10 ml), filtered and the volume of the solution reduced to 1.5 ml. The white solid that precipitated was essentially pure but crystalline material could be obtained by dissolution in hexane (1.5 ml) and storage at 5 °C for 24 hours to afford colourless crystals that were isolated by filtration at 0 °C, washed with cold hexane (3 × 2 ml) and dried *in vacuo* for 30 minutes. A second crop of crystals was obtained by the reduction of the supernatant solution to 0.5 ml and storage at −30 °C for 24 hours. Yield: solid 1.31g (90%) or crystalline 0.65 g (45%). ^{1}H NMR (C_6D_6, 298 K): δ 0.68 (s, 1H, ThCH_2), 0.70 (d, $^{3}J_{HH}$ = 3.2 Hz, 1H, ThCH_2), 1.25 (s, 1H, C*H*), 1.27 (d, $^{3}J_{HH}$ = 6.0 Hz, 1H, C*H*), 1.31 (d, $^{3}J_{HH}$ = 4.0 Hz, 18H, 6×Si*Me*), 1.33 (d, $^{3}J_{HH}$ = 4.2 Hz, 18H, 6×Si*Me*), 1.36 (d, $^{3}J_{HH}$ = 7.5 Hz, 3H, 3×C*H*), 1.42 (m, 12H, 4×Si*Me*), 1.53 (d, $^{3}J_{HH}$ = 7.5 Hz, 3H, 3×C*H*), 1.69 (d, $^{3}J_{HH}$ = 7.0 Hz, 3H, ThCH$_2$CH*Me*), 1.87 (m, 1H, ThCH$_2$C*H*Me), 2.55 (m, 3H, CH_2), 2.70 (m, 3H, CH_2), 3.52 (m, 2H, CH_2), 3.69 (m, 3H, CH_2), 3.90 (m, 1H, CH_2) ppm. ^{13}C{^{1}H} NMR (C_6D_6, 298 K): δ 11.73 (s, *C*H), 11.92 (s, *C*H), 12.30 (s, *C*H), 18.64 (s, *C*H$_3$), 18.81 (s, ThCH$_2$*C*HMe), 18.92

(s, CH_3), 19.05 (s, CH_3), 19.20 (s, CH_3), 19.48 (s, CH_3), 19.55 (s, CH_3), 19.72 (s, CH_3), 19.81 (s, CH_3), 26.69 (s, $ThCH_2CHMe$), 46.56 (s, CH_2), 46.92 (s, CH_2), 49.03 (s, CH_2), 58.69 (s, CH_2), 58.98 (s, CH_2), 59.24 (s, CH_2), 105.65 (s, $ThCH_2$) ppm. Assignments of the ^1H and ^{13}C resonances for the $ThCH_2CHMe$ group observed in the ^1H and $^{13}C\{^1H\}$ NMR spectra were confirmed using additional DEPT45, DEPT90, DEPT135 and ^1H,^{13}C-HMBC NMR spectra. $^{29}Si\{^1H\}$ NMR (C_6D_6, 298 K): δ 1.84 (s, Si^iPr_3), 2.33 (s, Si^iPr_3), 4.31 (s, $Si^iPr_2C[H]MeCH_2Th$) ppm. FTIR (Nujol®): $\tilde{\nu}$ 1261.56 (s), 1179.03 (w), 1091.65 (s), 1074.97 (s), 1022.67 (s), 920.34 (m), 882.16 (m), 846.66 (w), 800.39 (m), 770.44 (s), 748.31 (m), 723.54 (m), 672.01 (m), 633.39 (w), 588.82 (w), 571.11 (w), 551.05 (w), 513.60 (w) cm^{-1}. Anal. calc'd for $C_{33}H_{74}N_4Si_3Th$: C 47.00; H 8.85; N 6.65%. Found: C 46.36; H 8.86; N 6.41%.

Preparation of [Th(Tren^{TIPS})(CH_2Ph)] (4)

Toluene (15 ml) was added to a cold (−78 °C) mixture of [Th(Tren^{TIPS})(I)] (2.00 g, 2.1 mmol) and benzylpotassium (0.27 g, 2.1 mmol). The resulting mixture was allowed to warm to ambient temperature whilst being stirred (1 hour) and stirred at ambient temperature for a further 16 hours to afford a yellow suspension, which was filtered. The solvent was removed *in vacuo* to afford a virtually pure yellow solid. Crystalline material was obtained *via* extraction into warm (50 °C) methylcyclohexane (5 ml), filtration and reduction in volume to 2 ml. Storage at −30 °C for 18 hours afforded colourless crystals that were isolated by filtration at −10 °C, washed with pentane (2 × 2 ml) and dried *in vacuo* for 30 minutes. Yield: solid 1.48 g (77%) or crystalline 0.58 g (30%). ^1H NMR (C_6D_6, 298 K): δ 1.35 (d, $^3J_{HH}$ = 5.3 Hz, 54H, 3×Si$^iPr_3$), 1.39 (sept, $^3J_{HH}$ = 4.7 Hz, 9H, C*H*), 1.75 (s, 2H, CH_2Ph), 2.63 (t, $^2J_{HH}$ = 4.6 Hz, 6H, CH_2), 3.67 (t, $^2J_{HH}$ = 4.5 Hz, 6H, CH_2), 6.83 (t, $^2J_{HH}$ = 7.3 Hz, 1H, *p*-Ar*H*), 7.06 (d, $^2J_{HH}$ = 7.2 Hz, 2H, *m*-Ar*H*), 7.39 (t, $^2J_{HH}$ = 7.9 Hz, 2H, *o*-Ar*H*) ppm. $^{13}C\{^1H\}$ NMR

(C_6D_6, 298 K): δ 13.31 (s, *C*H), 19.80 (s, *C*H_3), 45.87 (s, *C*H_2), 64.40 (s, *C*H_2), 113.65 (s, *C*H_2Ph), 119.19 (s, *p*-Ar*C*), 124.42 (s, *m*-Ar*C*), 127.69 (s, *o*-Ar*C*), 154.10 (s, *i*-Ar*C*) ppm. $^{29}Si\{^1H\}$ NMR (C_6D_6, 298 K): δ 4.36 ppm. FTIR (Nujol®): $\tilde{\nu}$ 1302.66 (w), 1260.86 (s), 1201.73 (w), 1095.91 (s), 1046.65 (s), 1020.19 (s), 925.88 (w), 882.29 (m), 800.41 (s), 722.87 (m), 677.53 (w), 652.96 (w), 634.29 (w), 609.40 (w) cm^{-1}. Anal. calc'd for $C_{40}H_{82}N_4Si_3Th$: C 51.36; H 8.84; N 5.99%. Found: C 51.09; H 8.96; N 5.94%.

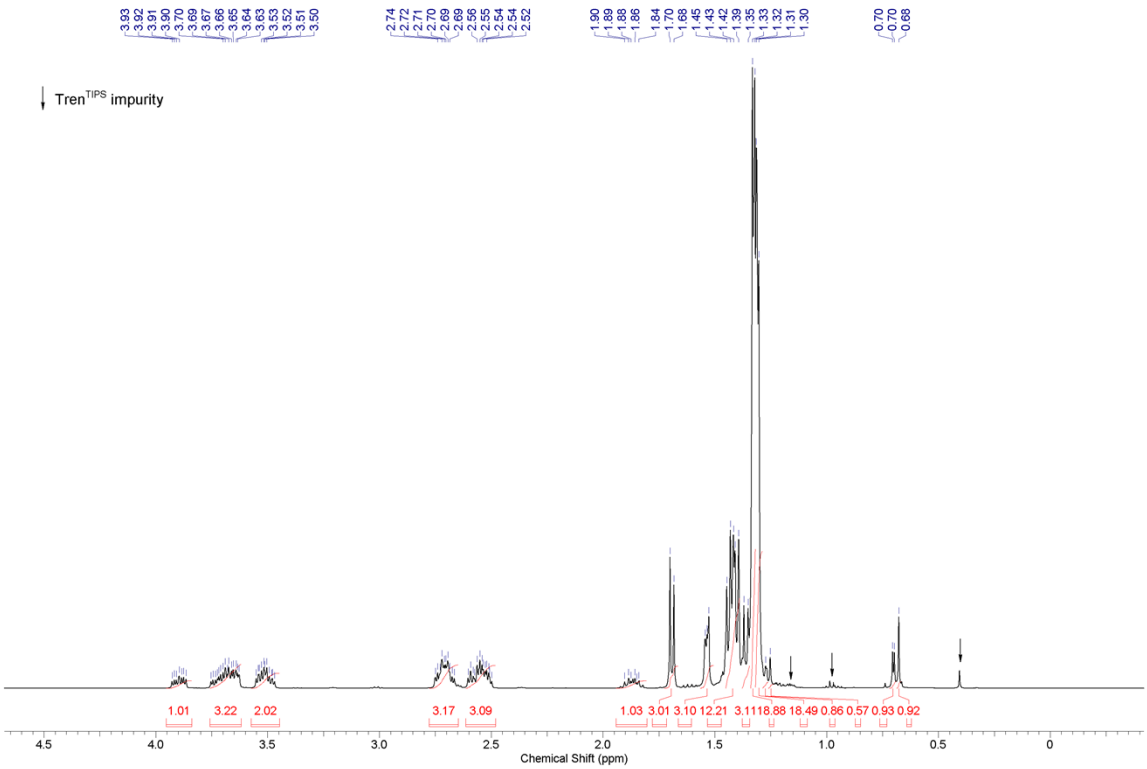
NMR Kinetics

All rate constants were determined by monitoring the benzyl-CH_2 ^1H NMR resonance (C_7D_8) of **4** for reactions performed in NMR tubes and sealed under nitrogen. In a typical experiment, a J. Young PTFE 5mm screw-topped borosilicate NMR tube was charged with ca. 10 mg of **4**, ca. 5 mg 1,3,5-$Bu^t_3C_6H_3$ (Mes*H) and ca. 0.5 ml C_7D_8. After the sample was dissolved, an initial spectrum (t = 0 min) was recorded at room temperature, and the sample was then immersed in a pre-heated thermostated paraffin oil bath. At appropriate time intervals, the sample was removed from the oil bath, rinsed free of oil and cooled to −78 °C. The sample was then briefly warmed to record a room-temperature ^1H NMR spectrum (typically requiring less than 5 minutes) and then returned to the oil bath. Offline processing software was used to determine the extent of reaction by integration and was standardised *vs* the (unchanged) Bu^t singlet resonance for Mes*H. Each experiment was monitored for *ca.* 3 half-lives. Plots of $\ln(A_0/A)$ *vs* t were fit to Eq. 1 by least squares analysis.

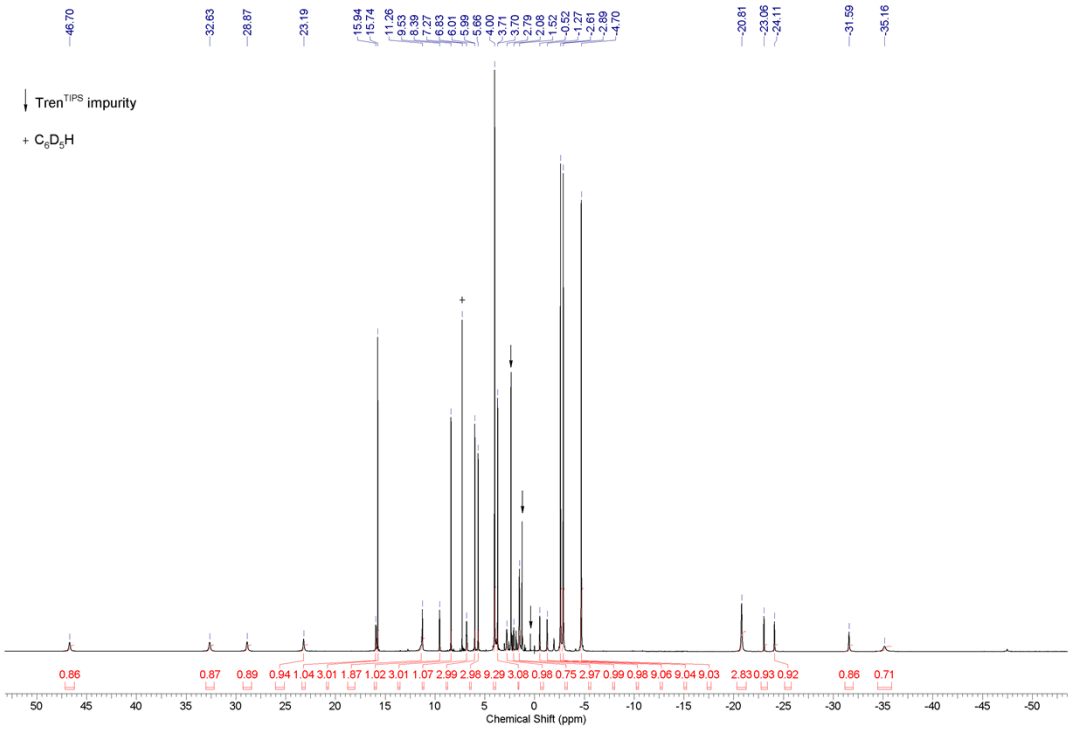
$$\ln(A_0/A) = kt + A \qquad \text{Eq. 1}$$

Experimental uncertainties for the regression parameters were estimated using standard regression analysis.

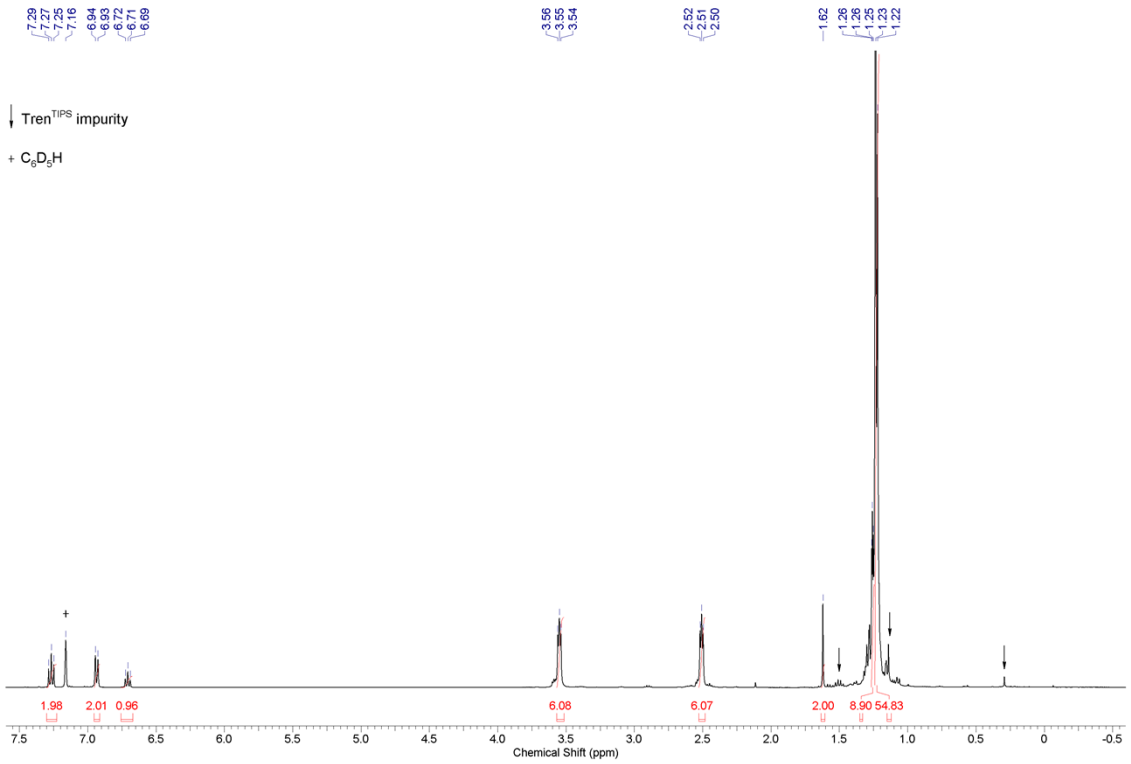
^1H NMR spectrum of 3a



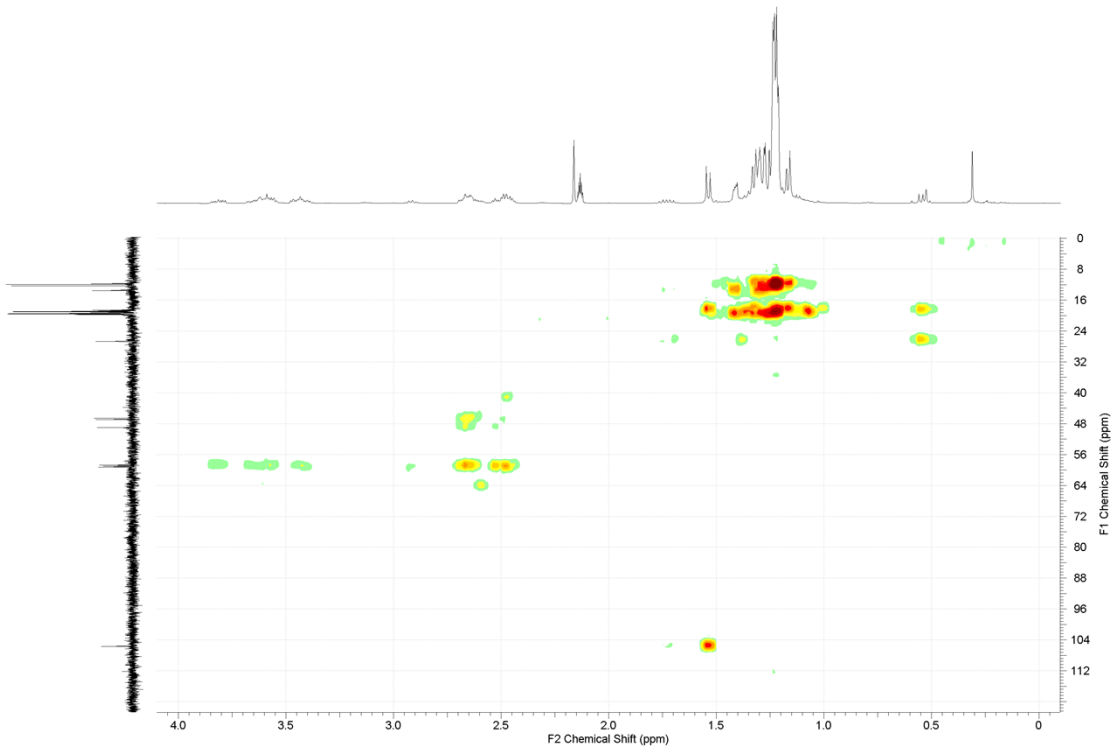
^{1}H NMR spectrum of 3b



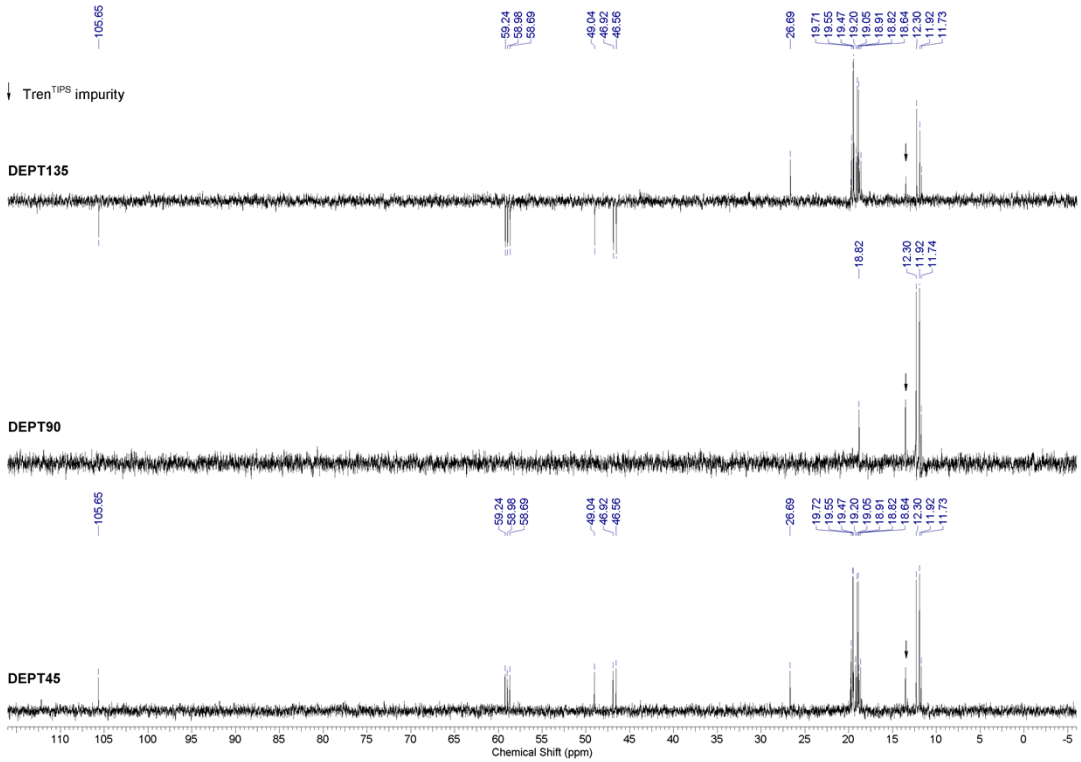
^{1}H NMR spectrum of 4



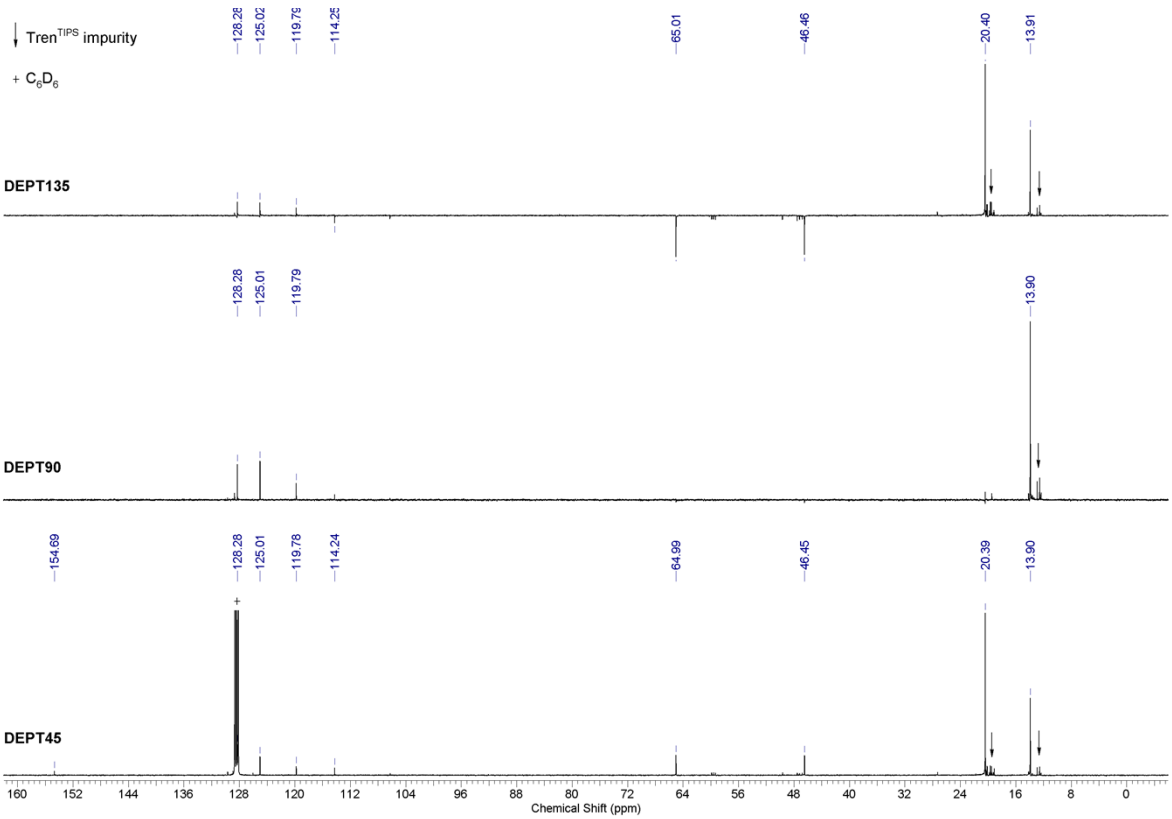
^{1}H-^{13}C HMBC Correlation spectrum of 3b



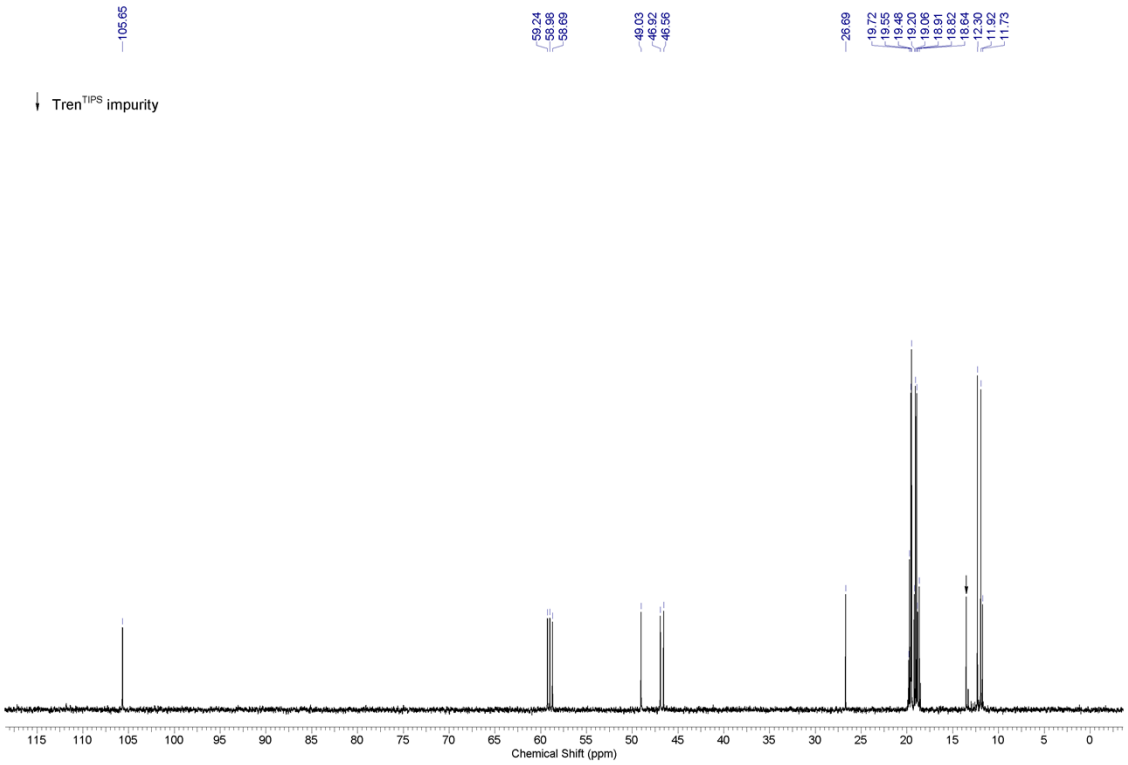
^{13}C DEPT NMR spectrum of 3b



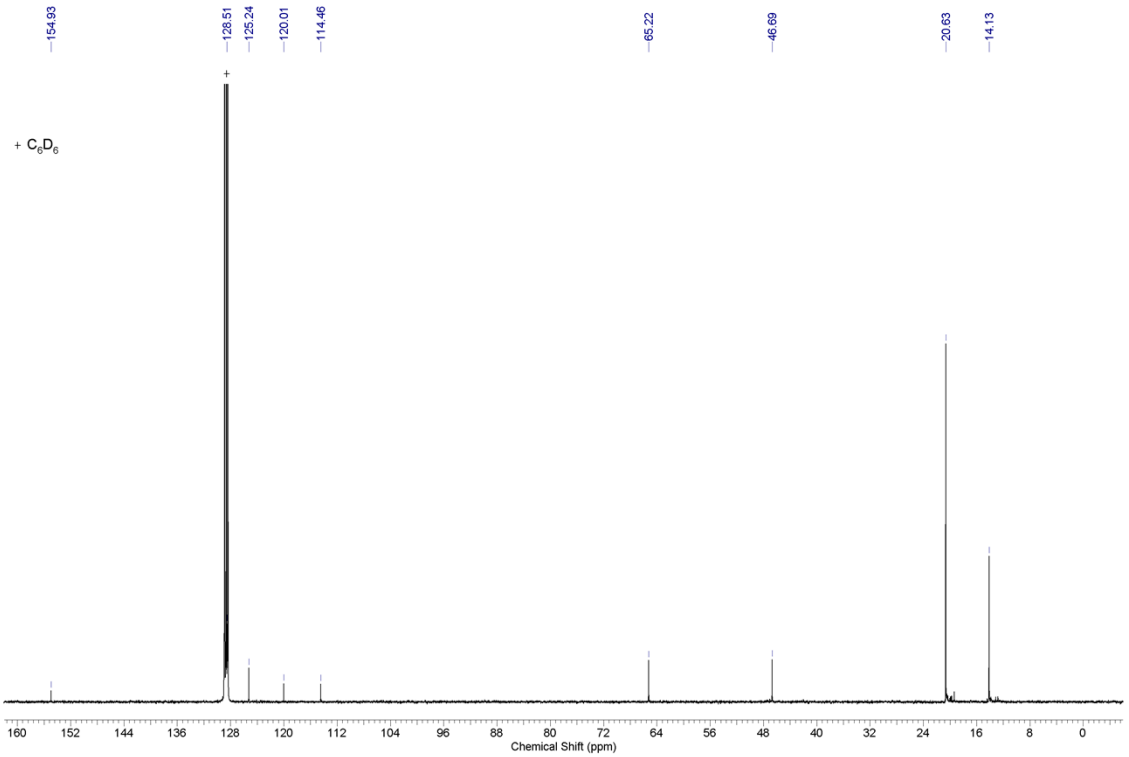
^{13}C DEPT NMR spectrum of 4



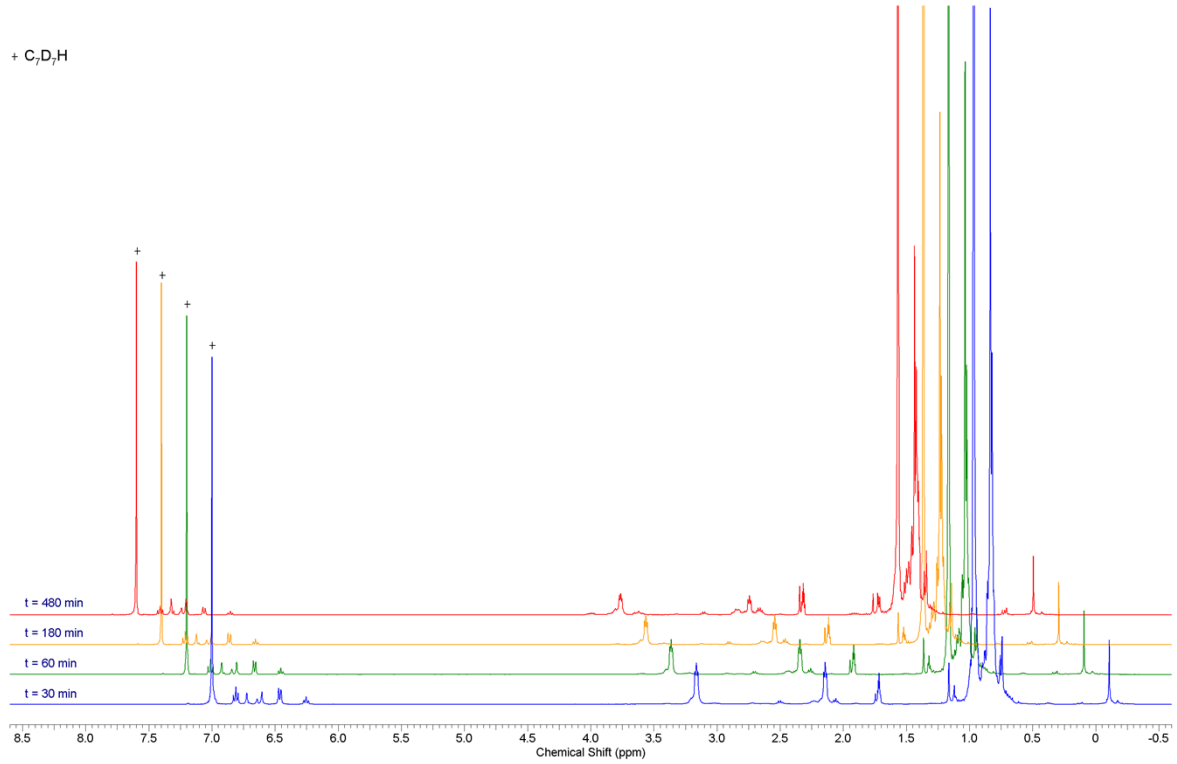
^{13}C{^{1}H} NMR spectrum of 3b



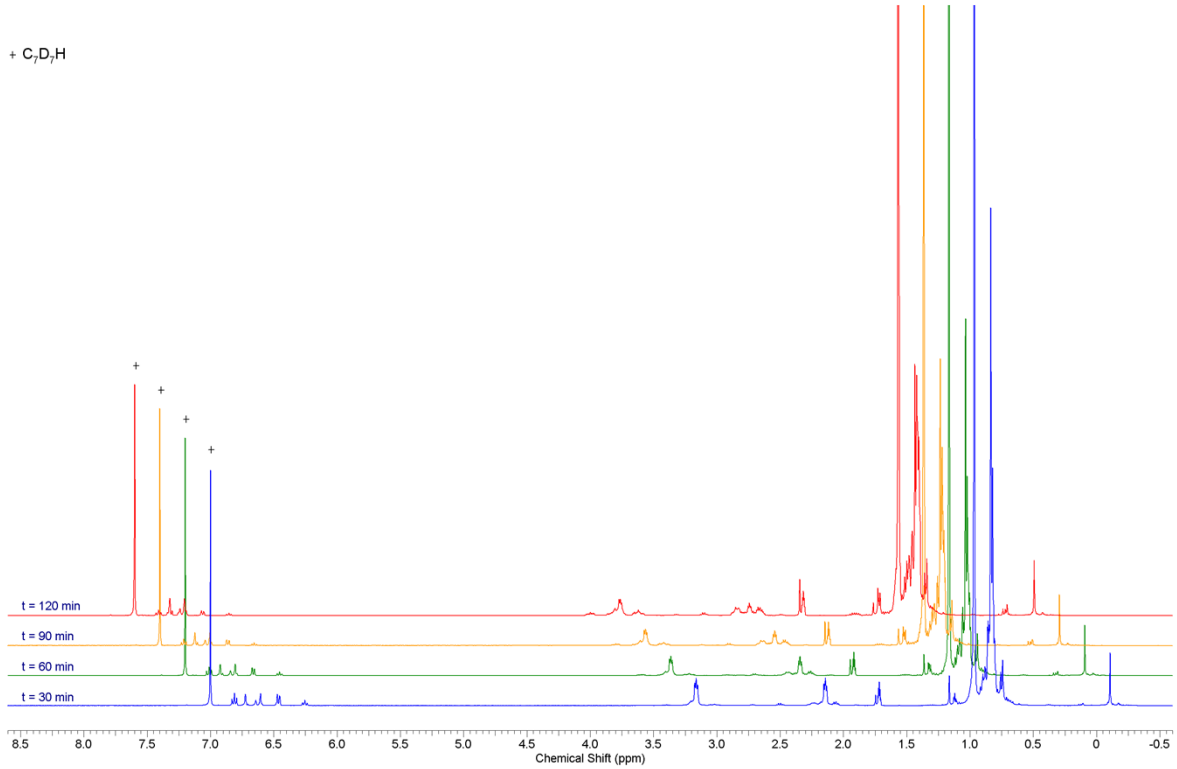
$^{13}C\{^{1}H\}$ NMR spectrum of 4



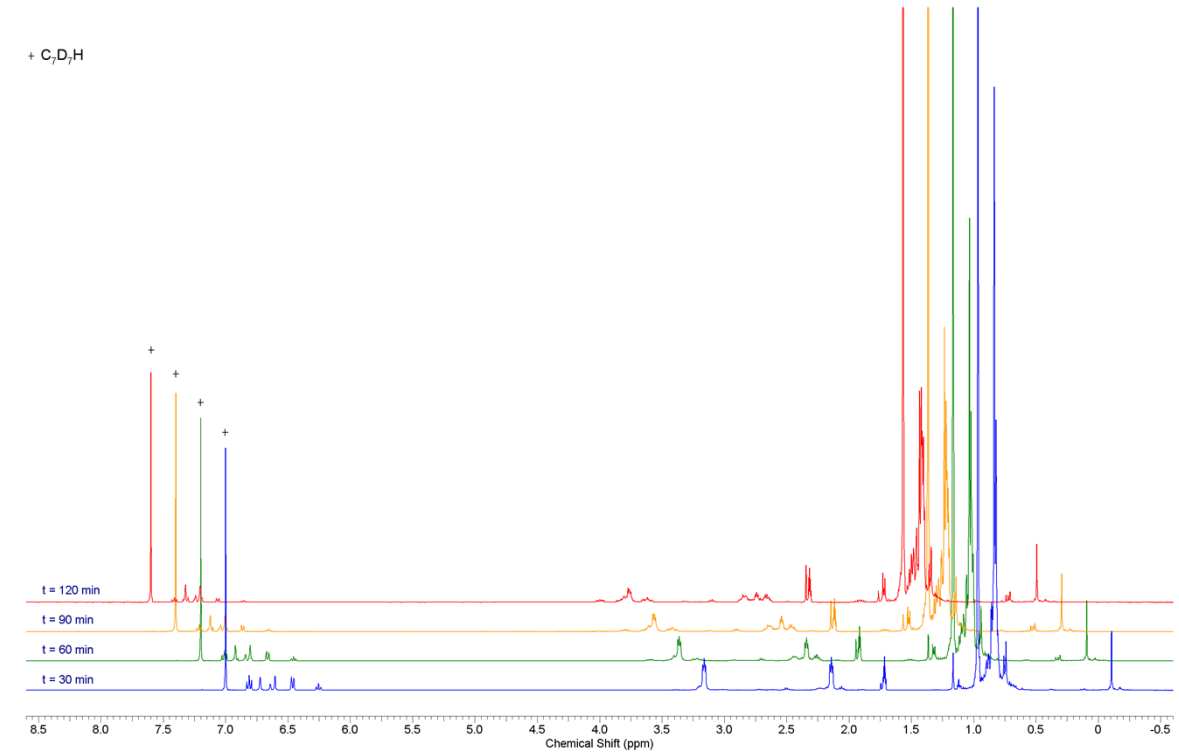
^{1}H NMR spectra monitoring the conversion of 4 to 3b at 40 °C



^{1}H NMR spectra monitoring the conversion of 4 to 3b at 50 °C



^{1}H NMR spectra monitoring the conversion of 4 to 3b at 60 °C



^{1}H NMR spectra monitoring the conversion of 4 to 3b at 70 °C

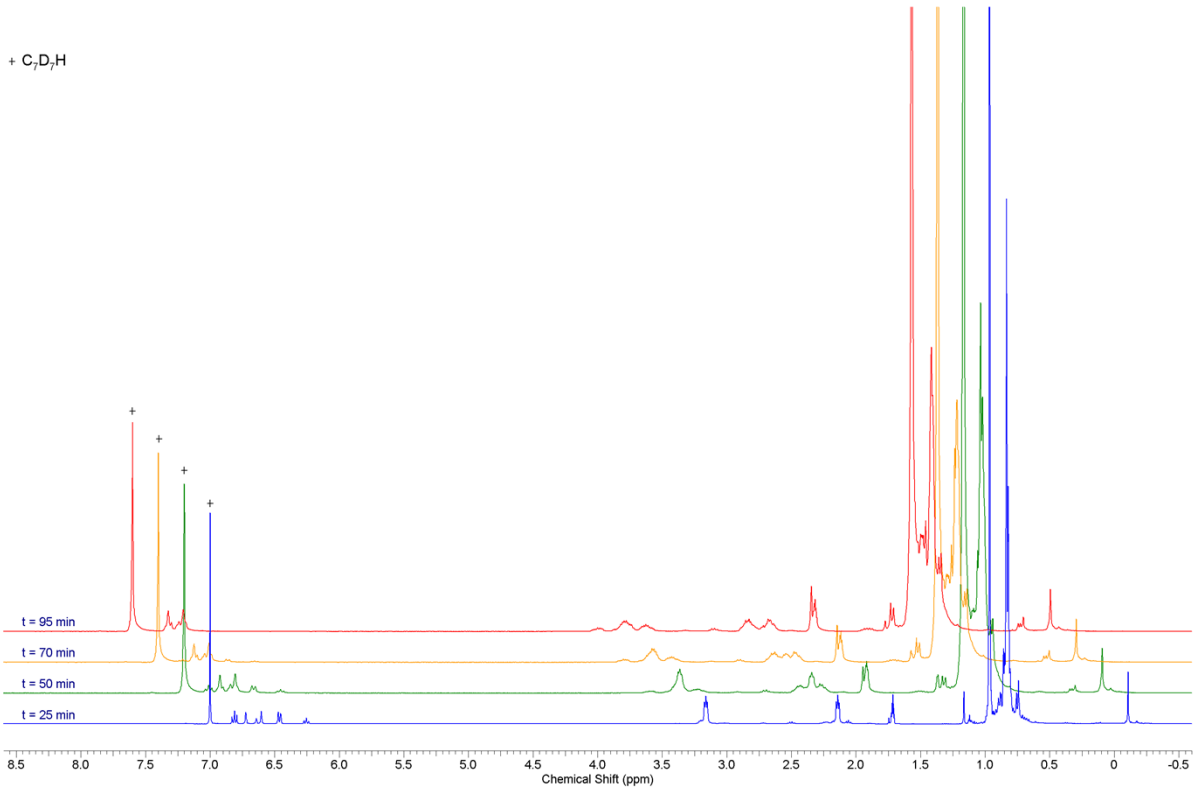
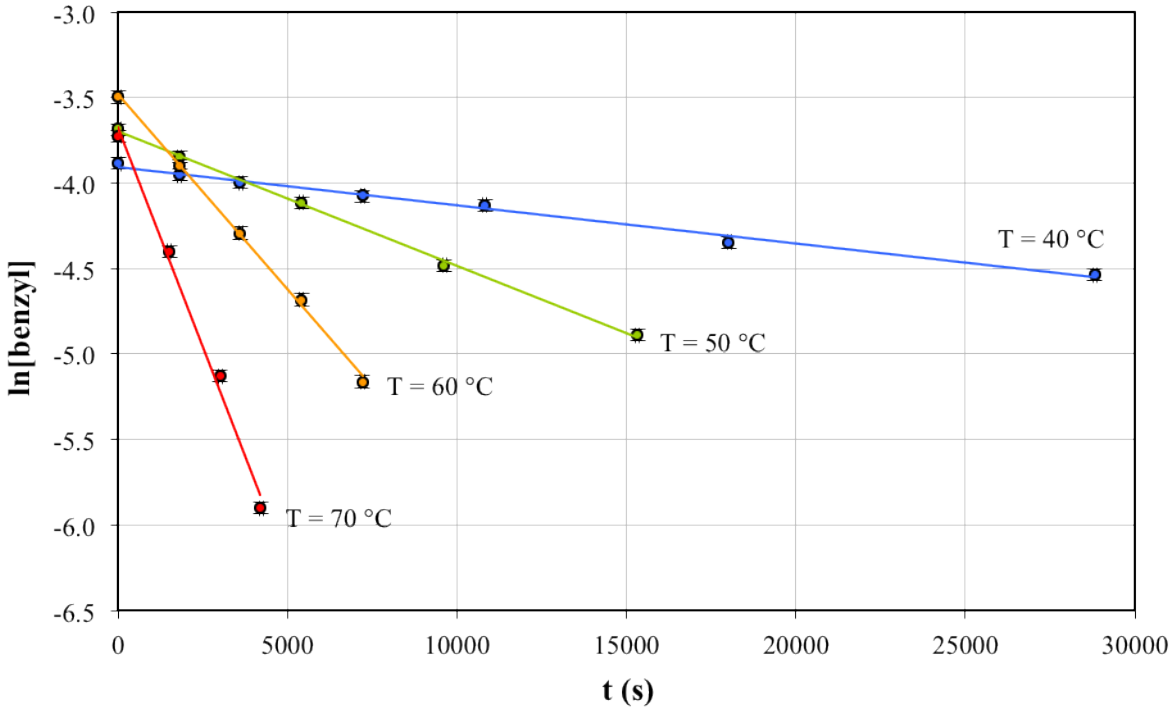


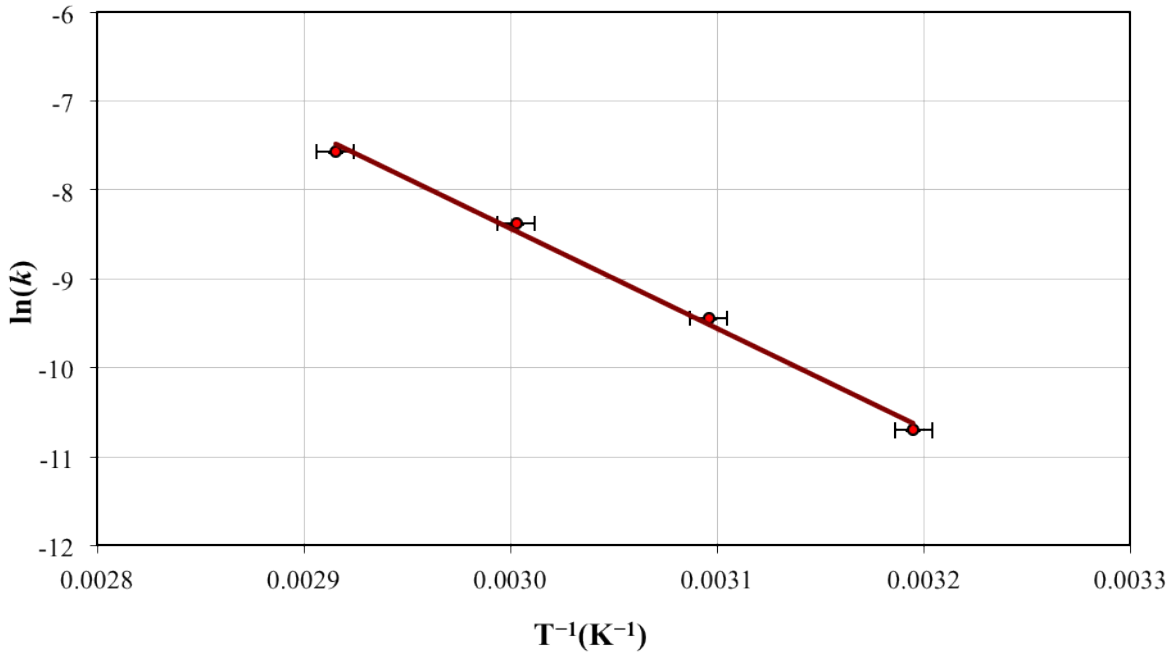
Table 1. Summary of First-Order Rate Constants (s^{-1})

Temperature, T (°C)	First-Order Rate Constant, k (s^{-1})
40	$2.25 \pm 0.1 \times 10^{-5}$
50	$7.89 \pm 0.1 \times 10^{-5}$
60	$2.29 \pm 0.1 \times 10^{-4}$
70	$5.13 \pm 0.3 \times 10^{-4}$

Graph 1: ln[4] *vs.* t (T = 40-70 °C)



Graph 2: Arrhenius Plot



Graph 3: Eyring Plot

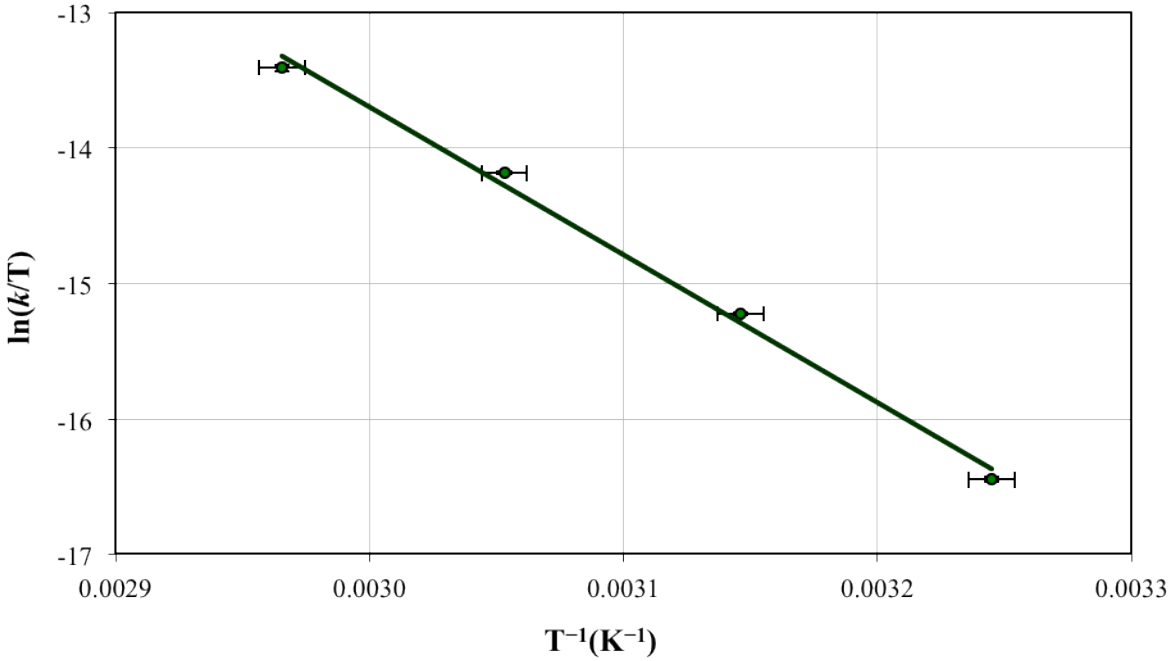


Table 2. Summary of Thermodynamic Activation Parameters

Activation Energy E_a	22.3 ± 0.1 kJ mol^{-1}
Enthalpy of Transition $\Delta H^{\ddagger}$	21.7 ± 3.6 kJ mol^{-1}
Entropy of Transition $\Delta S^{\ddagger}$	−10.5 ± 3.1 cal K^{-1} mol^{-1}

Computational Details

All the structures reported in this study were fully optimised with the Becke's 3-parameter hybrid functional combined with the non-local correlation functional provided by Perdew/Wang (denoted as B3PW91).[5,6] The basis set used for uranium and thorium atoms is the Stuttgart-Dresden small core RECP (relativistic effective core potential) in combination with its adapted basis set.[7-9] However, in order to study the effect of the f orbitals involvement on the cyclometallation step, the 5f-in-large-core ECPs (augmented by a f polarization function, α = 1.0) were used for fixed oxidation states IV.[10] In addition for the calculations involving the hypothetical Hf and Zr complexes the corresponding small core RECP SDD basis sets were used for describing these metals.[11,12] Also Si, and I atoms were treated as well with the corresponding Stuttgart-Dresden RECP in combination with their adapted basis sets,[13] each one augmented by an extra set of polarisation functions.[14] For the rest of the atoms the 6-31G(d,p) basis set was used.[15-17] In all computations no constrains were imposed on the geometry. All stationary points have been identified for minimum (number of imaginary frequencies Nimag=0) or transition states (Nimag=1). Intrinsic Reaction Paths (IRPs) were traced from the various transition structures to verify the reactant to product linkage.[18,19] Enthalpy energies were obtained at T=298.15K within the harmonic approximation. The natural population analysis (NPA) was performed using Weinhold's methodology.[20,21] GAUSSIAN09 program suite was used in all calculations.[22]

Enthalpy energies in a.u., along with cartesian coordinates of the optimised structures.

2a (small core triplet)
H= -2020.585979 au

U	0.06258500	-0.19181800	-0.27610400
N	-0.48888000	-1.55321600	1.42124900
Si	-1.43208300	-1.28786800	2.92875700
C	-0.31936200	-1.35072300	4.50538300
C	0.51533400	-0.08135200	4.71387700
C	0.57023700	-2.59847500	4.57766700
C	-0.03735500	-2.94163000	1.21207300
C	-0.71674000	-3.51187800	-0.02538800
N	-0.40007500	-2.66007600	-1.19043000
C	0.84532800	-3.07332100	-1.87202600
C	1.60864200	-1.83437300	-2.32542000

N	1.95360500	-0.99595200	-1.15803100
Si	3.71098300	-0.80731800	-0.84181200
C	3.92772200	0.04491800	0.85861100
C	3.20906800	-0.61665000	2.03735100
C	5.40483800	0.28022000	1.21164100
C	-1.54384200	-2.52189600	-2.11884700
C	-2.38252600	-1.31539400	-1.71115000
N	-1.57273900	-0.08261600	-1.79590800
Si	-2.10006900	1.10846700	-3.03668800
C	-3.68002700	2.06592600	-2.48549800
C	-3.39808400	3.15813300	-1.44575800
C	-4.81395700	1.14485000	-2.01594900
C	-2.55075700	0.14514600	-4.66364200
C	-1.32766800	-0.32196900	-5.46377700
C	-3.52442600	0.89397700	-5.58672500
C	-0.71339200	2.40901600	-3.29283100
C	0.68885400	1.85880400	-3.56601300
C	-1.09829400	3.43709400	-4.36803100
C	4.57040500	0.32701400	-2.14339400
C	4.24320900	1.81423300	-1.95633200
C	4.33080400	-0.10172800	-3.59702100
C	4.55613300	-2.55115700	-0.95837100
C	4.29145500	-3.45159000	0.25526000
C	6.06268800	-2.49723500	-1.25363300
C	-2.21113100	0.46476100	2.87706800
C	-3.01307800	0.76752900	4.15320200
C	-3.05588500	0.80224700	1.64545000
C	-2.74138400	-2.71344500	3.10048900
C	-3.19649800	-2.98551300	4.54253000
C	-3.96610900	-2.55000400	2.19048600
H	-3.75169900	0.29224600	-6.47711300
H	-1.62220900	-1.00893800	-6.26847500
H	-3.10642800	1.84293800	-5.94038200
H	-0.81760400	0.52353200	-5.93786300
H	-4.47585200	1.11677600	-5.09516600
H	-1.11047400	2.98832200	-5.36782400
H	-0.58905300	-0.83990200	-4.84268300
H	-0.37213200	4.25960600	-4.39487700
H	4.93261500	0.50406500	-4.28747100
H	-3.07861500	-0.75864400	-4.32468400
H	0.74992800	1.33738600	-4.52657400
H	-2.08454900	3.87956900	-4.19361100
H	4.59187800	-1.15150100	-3.77637900
H	3.28277000	0.03451000	-3.88482200
H	-4.02573500	2.56901200	-3.40088500
H	1.42283200	2.67354200	-3.59107900
H	-5.08380700	0.39400000	-2.76810400
H	-1.15577800	-2.34450600	-3.12578600
H	4.72741300	2.42025200	-2.73410800
H	0.99056000	-1.27624000	-3.04785400
H	2.49007200	-2.15069900	-2.89775400
H	1.03160800	1.15614600	-2.79608500
H	6.28581600	-1.99112500	-2.19751200
H	0.62547300	-3.75646700	-2.70767200
H	-0.66395800	2.94283600	-2.33247300
H	-3.28380300	-1.27965600	-2.33636100
H	5.64476400	0.20007400	-1.93976600
H	-5.72124800	1.72208600	-1.79387600
H	-2.13556300	-3.45049900	-2.14880800
H	3.16765600	2.00687000	-2.01525700

H	6.48047200	-3.51085400	-1.32171000
H	-2.72722900	3.93211300	-1.83071400
H	4.08411100	-3.03620100	-1.82635000
H	-4.32930600	3.65572600	-1.14282200
H	-4.53981600	0.61204000	-1.09899600
H	4.58388300	2.19575900	-0.98916000
H	1.46833100	-3.61547700	-1.15489300
H	6.61438300	-1.97644400	-0.46331500
H	-2.75535300	-1.46965500	-0.68621900
H	-2.93589000	2.75444700	-0.53963100
H	4.61730900	-4.48214700	0.05994000
H	-0.43112600	-4.55855700	-0.21729900
H	5.95685800	0.78393300	0.41157700
H	-1.79855400	-3.48888100	0.13529800
H	3.23203800	-3.48679900	0.53066100
H	3.46408000	1.03197700	0.71108000
H	4.84454700	-3.10527400	1.13501200
H	-2.52943600	0.64972000	0.69359200
H	5.92254100	-0.66171000	1.42838200
H	1.05415500	-2.98184700	1.08020500
H	-3.69405900	-2.32201100	1.15456900
H	-3.97112000	0.20438500	1.59815700
H	-3.35488800	1.85728800	1.66345400
H	5.49138600	0.90537500	2.10964900
H	2.14077300	-0.78767400	1.85364000
H	-0.24749600	-3.60224500	2.06390000
H	-4.57194900	-3.46615700	2.17805900
H	3.64638900	-1.58727200	2.29283900
H	-4.61958700	-1.74314000	2.54042100
H	3.27997500	0.01501500	2.93123200
H	-2.21324300	-3.61863600	2.76482200
H	-1.34419900	1.14257700	2.86647500
H	-3.91848700	0.15274500	4.21337700
H	1.31966100	-2.59823700	3.77895600
H	-3.33598200	1.81635700	4.16661900
H	1.18717300	0.10697400	3.87150100
H	-3.91042900	-3.81977600	4.57011800
H	-0.00215900	-3.53007300	4.49644200
H	-0.10565100	0.81081200	4.83813300
H	-3.70202100	-2.11880900	4.98284700
H	-2.43564900	0.59351800	5.06670700
H	-2.36353300	-3.24935500	5.20056400
H	-1.03645100	-1.41151000	5.33808300
H	1.11533000	-2.63574200	5.53026500
H	1.13982100	-0.17044700	5.61315400
I	0.63060200	2.66835100	0.64658900

4a (small core triplet)

H= -2279.783357 au

N	-0.37269200	-2.52360500	-0.72832200
U	0.13240000	0.03936300	-0.06858800
N	-0.67458900	-1.02703500	1.75892000
Si	-1.67856200	-0.71906100	3.20338500
C	-0.59443900	-0.46616100	4.78087200
C	0.19619200	0.84687300	4.76191700
C	-1.48693600	-2.51397800	-1.69722800
C	-2.32506000	-1.25624200	-1.50259400
N	-1.47843700	-0.05958800	-1.66237400
Si	-1.89084000	0.98554600	-3.04762700
C	-3.50992800	2.00035300	-2.75776800

C	-3.36123400	3.13300500	-1.73544300
C	0.87520500	-3.05505900	-1.31073500
C	1.64772100	-1.92876300	-1.98475600
N	1.99423500	-0.87803100	-1.00611200
Si	3.74145600	-0.80365400	-0.64891300
C	4.31564700	-2.51276800	0.09819800
C	4.64076300	-3.60759100	-0.92977500
C	-0.71890500	-3.17776100	0.55008800
C	-0.09594700	-2.38523300	1.69562000
C	-4.71812500	1.12189400	-2.40400100
C	5.47926500	-2.40040700	1.09641800
C	0.34851700	-1.64119600	5.07574000
C	-2.20651200	-0.10052700	-4.62728400
C	-0.92546200	-0.64456700	-5.27315400
C	-3.07729200	0.57858100	-5.69635800
C	-0.47871400	2.27015000	-3.28948100
C	0.94536200	1.71793300	-3.42181100
C	-0.77294800	3.23933300	-4.44494300
C	4.08310100	0.53260400	0.68770200
C	3.10373900	0.45269500	1.86443800
C	4.18848600	1.96785000	0.15700900
C	4.78281100	-0.27950700	-2.19125800
C	4.51018200	-0.97198200	-3.53227400
C	6.28880500	-0.29838900	-1.88322300
C	-2.69517200	0.89301500	2.95728000
C	-3.61717300	1.18308700	4.15157100
C	-3.47886800	0.98478100	1.64444100
C	-2.80905300	-2.26066900	3.54432500
C	-3.28169400	-2.39392500	5.00076400
C	-4.01131600	-2.37960700	2.59671000
C	0.01807900	2.39362500	0.68600300
C	0.95844000	3.52495400	0.82399100
C	1.56161300	3.82846200	2.06096400
C	2.46776000	4.87623100	2.19612900
C	2.80668500	5.66732800	1.09803000
C	2.21441500	5.39208200	-0.13476300
C	1.30764100	4.34446300	-0.26787800
H	-3.23669400	-0.09579100	-6.54869500
H	-1.15993100	-1.38572200	-6.04911900
H	-2.60550500	1.48525700	-6.09134000
H	-0.35666800	0.15562600	-5.75885200
H	-4.06429900	0.86129800	-5.31842600
H	-0.71085800	2.73292100	-5.41483300
H	-0.25830500	-1.12416100	-4.54955600
H	-0.04025700	4.05671000	-4.46552900
H	4.35110900	2.67778300	0.97637600
H	-2.77751800	-0.96819900	-4.26312600
H	1.08267100	1.18174900	-4.36605900
H	-1.76645500	3.69320200	-4.37325600
H	5.01982100	2.08199300	-0.54526500
H	3.27623000	2.29235700	-0.35304700
H	-3.71760600	2.46546300	-3.73359500
H	1.67996100	2.53369300	-3.40421500
H	-4.89115200	0.32565600	-3.13733000
H	-1.06437600	-2.49005200	-2.70590900
H	3.45438200	1.04407100	2.71955000
H	1.03734500	-1.51336400	-2.80091400
H	2.52611700	-2.36330000	-2.47867900
H	1.23079500	1.02074000	-2.62363200
H	6.54045800	0.23422000	-0.95970800

H	0.65867200	-3.88458000	-2.00425300
H	-0.51471500	2.86022700	-2.36133000
H	-3.16829600	-1.29024500	-2.20662400
H	5.07345900	0.26020000	1.07928400
H	-5.63766300	1.72036100	-2.35252600
H	-2.08779800	-3.43388200	-1.61034200
H	2.13142200	0.89951400	1.60374000
H	6.85778300	0.17388300	-2.69526300
H	-2.58183500	3.84935900	-2.01376800
H	4.48911000	0.77301700	-2.31926800
H	-4.29882200	3.69708800	-1.63757500
H	-4.58998300	0.64751400	-1.42481700
H	2.93430300	-0.57105700	2.21727300
H	1.49000100	-3.45808400	-0.50033100
H	6.66766900	-1.32222200	-1.78410200
H	-2.78710500	-1.28266400	-0.50337600
H	-3.11607700	2.74767900	-0.74035700
H	-0.46905200	2.18354000	1.65227500
H	5.14562100	-0.54174700	-4.31866700
H	-0.40022500	-4.23248100	0.54758000
H	5.24068500	-1.76076200	1.95150000
H	-1.80519000	-3.15960400	0.67179300
H	3.47273400	-0.84986500	-3.85561100
H	-0.79390100	2.64284900	-0.02149100
H	3.43814600	-2.85128100	0.67156200
H	1.29998600	3.23357800	2.93324700
H	4.73062500	-2.04509000	-3.49982100
H	-2.84787600	0.82784100	0.76250500
H	6.38438500	-1.99882000	0.62690000
H	0.99803800	-2.34813300	1.53896700
H	-3.73388500	-2.25485300	1.54470700
H	-4.28440600	0.24529200	1.59882700
H	-3.94211700	1.97426800	1.53862000
H	5.73935700	-3.39012800	1.49618500
H	3.81179600	-3.82121400	-1.61130000
H	-0.21309200	-2.94641200	2.63164400
H	-4.49564900	-3.36019400	2.69780700
H	5.50538600	-3.33616400	-1.54551200
H	-4.77366600	-1.62553300	2.82250100
H	2.90623200	5.08165500	3.17018500
H	4.89324600	-4.55053300	-0.42549000
H	-2.16232000	-3.12918700	3.34787300
H	0.85123100	4.15764600	-1.23721900
H	-1.94284400	1.69442400	2.93892300
H	-4.42692300	0.44817100	4.22311900
H	1.12343700	-1.73063800	4.30574600
H	-4.08825800	2.16899800	4.04656000
H	0.88694300	0.88085500	3.91179500
H	-3.86973600	-3.31240300	5.13197900
H	-0.17564200	-2.60221900	5.13095800
H	3.51065500	6.48810800	1.20269100
H	2.45532200	6.00356800	-1.00145400
H	-0.45403300	1.72525200	4.69702000
H	-3.92487500	-1.55932600	5.30047500
H	-3.08185500	1.17841800	5.10691200
H	-2.45027000	-2.43748900	5.71048400
H	-1.31565700	-0.40667900	5.61013100
H	0.86602300	-1.49839700	6.03382600
H	0.79984500	0.95661800	5.67296000

TS_{4a-3a} (small core triplet)

H= -2279.753131 au

N	-0.42095800	-2.63763300	-0.75855800
U	0.28467000	-0.14547100	-0.06489300
N	-0.58229100	-1.19395900	1.76855800
Si	-1.51440500	-0.81479600	3.23590100
C	-0.37930600	-0.74558000	4.79917600
C	0.54381600	0.47773900	4.81703200
C	-1.53240700	-2.50010500	-1.72154900
C	-2.24770400	-1.17523900	-1.47839000
N	-1.32486700	-0.04232300	-1.69093600
Si	-1.72527100	0.98228200	-3.09339400
C	-3.25766700	2.10786800	-2.75058200
C	-2.97053100	3.23831900	-1.75541800
C	0.76259500	-3.29611600	-1.34228700
C	1.61333800	-2.27726400	-2.08810400
N	1.94475300	-1.16032600	-1.20061300
Si	3.65760600	-0.87321900	-0.81937700
C	4.33192000	-2.37646200	0.21634500
C	4.74686300	-3.59860800	-0.61626200
C	-0.83801800	-3.28845400	0.50180600
C	-0.14427600	-2.60022300	1.67240700
C	-4.50759600	1.33087800	-2.31586600
C	5.45165600	-2.01549600	1.20368400
C	0.44092500	-2.02402900	5.01706400
C	-2.19131000	-0.12447700	-4.62146000
C	-0.98551500	-0.77033000	-5.31733900
C	-3.07864700	0.57204500	-5.66504400
C	-0.25445900	2.16906700	-3.46963100
C	1.11559500	1.50735400	-3.66120400
C	-0.55561000	3.10696300	-4.64891400
C	3.65829300	0.68052000	0.30288500
C	2.43264400	0.66529300	1.23645700
C	3.75819800	2.01370600	-0.45397300
C	4.73827300	-0.49808500	-2.37389200
C	4.58680600	-1.41887000	-3.59059200
C	6.22071200	-0.34188600	-1.99994300
C	-2.30096400	0.92980300	3.04478300
C	-3.08490500	1.36361500	4.29297900
C	-3.15416200	1.14472100	1.78875700
C	-2.83592400	-2.20259900	3.55684600
C	-3.29111300	-2.31570500	5.01942600
C	-4.05879600	-2.12013000	2.63297400
C	0.27403600	2.43370500	0.49008400
C	0.83779200	3.69980100	1.03834100
C	0.89678300	3.92229100	2.42416300
C	1.44515700	5.09150000	2.94417200
C	1.95627300	6.07038100	2.09216400
C	1.90923700	5.86394700	0.71405400
C	1.35641400	4.69540200	0.19539100
H	-3.32401000	-0.11753800	-6.48420000
H	-1.30877300	-1.53849700	-6.03285300
H	-2.57745400	1.43588400	-6.11548300
H	-0.41003900	-0.03095900	-5.88532300
H	-4.02513200	0.92593500	-5.24542200
H	-0.61575900	2.55411200	-5.59315800
H	-0.29599400	-1.24469600	-4.61149400
H	0.24220500	3.85218000	-4.76700700
H	3.70542500	2.86129200	0.23933000
H	-2.79220800	-0.94428800	-4.19919200

H	1.16222900	0.95244100	-4.60338400
H	-1.49609700	3.65367400	-4.52546400
H	4.69929200	2.10009700	-1.00682200
H	2.94479400	2.14285400	-1.17760300
H	-3.48088700	2.57122600	-3.72339100
H	1.91038600	2.26454300	-3.69845500
H	-4.77448700	0.53063500	-3.01586100
H	-1.11634500	-2.48804100	-2.73265700
H	2.59503300	1.35976500	2.07462100
H	1.06815100	-1.92152500	-2.97649200
H	2.49649100	-2.80082500	-2.47916900
H	1.37136000	0.79773600	-2.86549900
H	6.37284700	0.33129600	-1.14882900
H	0.46465500	-4.14255300	-1.98371700
H	-0.19094600	2.80531200	-2.57380800
H	-3.13927200	-1.13450500	-2.11878500
H	4.57024900	0.60397100	0.91588100
H	-5.37679300	1.99814500	-2.23986200
H	-2.21678700	-3.36125400	-1.65167500
H	1.32973000	1.55013700	0.81055700
H	6.79602800	0.06315100	-2.84335900
H	-2.18366700	3.91544600	-2.10360500
H	4.37430400	0.49338700	-2.68192200
H	-3.86790400	3.84817600	-1.58359500
H	-4.36889100	0.87547200	-1.32902700
H	2.29355100	-0.32112400	1.72026700
H	1.36182600	-3.70011600	-0.51972100
H	6.67389700	-1.30510000	-1.73933100
H	-2.64388600	-1.17577800	-0.44924800
H	-2.65808100	2.84397800	-0.78236500
H	-0.66914300	2.18989900	1.00488200
H	5.23462000	-1.07954600	-4.41077600
H	-0.63116400	-4.37021100	0.46641600
H	5.13940200	-1.25348300	1.92410500
H	-1.91730400	-3.16119300	0.62316400
H	3.56222700	-1.42879200	-3.97289100
H	0.04328500	2.55720200	-0.57827100
H	3.45823700	-2.67305300	0.81809400
H	0.50538400	3.16684700	3.10104000
H	4.87275600	-2.45288400	-3.36713400
H	-2.65066900	0.82890700	0.86782800
H	6.34543000	-1.64103900	0.69240000
H	0.94936100	-2.67352900	1.52485300
H	-3.78586200	-1.99039800	1.58023900
H	-4.09508900	0.58853700	1.84176500
H	-3.41430100	2.20471800	1.67047800
H	5.75956200	-2.89927100	1.77952100
H	3.95208000	-3.95140000	-1.28162500
H	-0.33158000	-3.17778500	2.58759600
H	-4.67045200	-3.02939800	2.70716800
H	5.62043100	-3.38035400	-1.24028800
H	-4.70616900	-1.27969500	2.90663000
H	1.47301000	5.23851600	4.02098400
H	5.02206200	-4.44010000	0.03433700
H	-2.31622800	-3.14263100	3.31655700
H	1.31943200	4.55155500	-0.88195800
H	-1.42997200	1.59866100	2.96961700
H	-3.98796000	0.75776000	4.42804000
H	1.18786600	-2.15407900	4.22592400
H	-3.41151200	2.40795400	4.20402200

H	1.20444500	0.49374400	3.94320800
H	-4.01862800	-3.13030500	5.13711800
H	-0.17903300	-2.92774900	5.03970000
H	2.38263700	6.98381600	2.49727900
H	2.29950300	6.61939900	0.03667500
H	-0.01625700	1.41855200	4.82936800
H	-3.77991200	-1.39861900	5.36651700
H	-2.49406300	1.28397700	5.21136800
H	-2.46067800	-2.52208200	5.70108100
H	-1.07257100	-0.65046500	5.64851600
H	0.98765300	-1.98196400	5.96867000
H	1.18630300	0.47360500	5.70802800

3a (small core triplet)

H= -2008.452948 au

N	-0.69618800	-3.12653700	-0.92572900
U	-0.19658500	-0.64313100	-0.16154100
N	-0.99685600	-1.82900600	1.62427500
Si	-1.51665400	-1.24277000	3.21993100
C	-0.29708800	-1.74915500	4.63373000
C	1.15067600	-1.36609100	4.30649500
C	-1.53403300	-3.04635200	-2.13929500
C	-2.45324500	-1.83024400	-2.07323500
N	-1.66528300	-0.59631600	-1.94255800
Si	-2.02118100	0.71087800	-3.09419700
C	-3.37634300	1.89489600	-2.39872300
C	-2.89740900	2.62269700	-1.13893500
C	0.60724800	-3.76744200	-1.18165700
C	1.58171800	-2.78118400	-1.81939800
N	1.63144500	-1.54451700	-1.04430600
Si	3.18816100	-0.79754500	-0.57503100
C	3.95267500	-1.85357500	0.86046500
C	4.56409500	-3.18896700	0.41404800
C	-1.42500900	-3.78282500	0.17753200
C	-0.93339700	-3.29460900	1.53236600
C	-4.69803100	1.16626900	-2.12567600
C	4.93362800	-1.10486400	1.77377200
C	-0.36881400	-3.22153200	5.06403700
C	-2.71519200	0.01410100	-4.76435400
C	-1.84324000	-1.03789700	-5.46121900
C	-3.10932900	1.11422100	-5.76151800
C	-0.40527400	1.73790500	-3.29089700
C	0.72280200	0.97541200	-3.99794100
C	-0.59901600	3.11748500	-3.93587000
C	2.73539900	0.94222000	0.12633500
C	1.38626300	0.89467800	0.88197400
C	2.72739700	2.05855300	-0.92476400
C	4.38973400	-0.56054700	-2.06922900
C	4.59450500	-1.74531600	-3.02150600
C	5.74885300	-0.01841800	-1.59946000
C	-1.57722200	0.68278200	3.12007000
C	-1.36530100	1.39539700	4.46383400
C	-2.85164700	1.21226700	2.44794000
C	-3.22242300	-2.02959900	3.68002400
C	-3.78326400	-1.50712700	5.01086500
C	-4.28701500	-1.97553700	2.57806700
H	-3.62281800	0.68305000	-6.63145400
H	-2.38795600	-1.51164200	-6.28902300
H	-2.23073200	1.64545900	-6.14359700
H	-0.93998700	-0.59102700	-5.88804500

H	-3.78180000	1.85933900	-5.32486000
H	-0.87690200	3.02772400	-4.99159500
H	-1.51884300	-1.83166000	-4.78255100
H	0.33184800	3.69823300	-3.89882500
H	2.45351500	3.01468000	-0.45833000
H	-3.65208200	-0.48502600	-4.47107300
H	0.48770000	0.82064700	-5.05621800
H	-1.37550700	3.71086400	-3.44401100
H	3.70359600	2.19672300	-1.40167100
H	1.99914000	1.87169400	-1.72043000
H	-3.56106100	2.65337500	-3.17394600
H	1.66383500	1.53992500	-3.96305000
H	-5.11960100	0.71355300	-3.02974700
H	-0.87132700	-2.92818000	-3.00095200
H	1.09215500	1.91462700	1.18483800
H	1.27776500	-2.58141600	-2.85981800
H	2.55354800	-3.28741900	-1.89326600
H	0.90753300	-0.00432800	-3.54561500
H	5.65348300	0.84464400	-0.93101500
H	0.48153100	-4.67278400	-1.79940400
H	-0.08071000	1.91944100	-2.24988100
H	-3.08474300	-1.85057000	-2.97233100
H	3.54903000	1.19145500	0.82791200
H	-5.45499300	1.85284500	-1.72321800
H	-2.10067600	-3.98284300	-2.27741400
H	6.36127900	0.29730500	-2.45485300
H	-2.02052600	3.25285800	-1.32169300
H	3.90203800	0.23461500	-2.65169100
H	-3.68306100	3.26848600	-0.72402600
H	-4.56302300	0.36628500	-1.38792000
H	1.52107600	0.33797800	1.83045600
H	1.01847400	-4.07934600	-0.21645300
H	6.31973000	-0.78538700	-1.06380500
H	-3.15882600	-1.95339000	-1.23435800
H	-2.63237100	1.90808200	-0.35058100
H	5.29390100	-1.47429800	-3.82459300
H	-1.35177900	-4.88011400	0.08948100
H	4.48936100	-0.20491600	2.20931400
H	-2.48158100	-3.51570600	0.08407700
H	3.66236500	-2.05792100	-3.50010800
H	3.06484900	-2.08795100	1.46831100
H	5.01878800	-2.61822700	-2.51286100
H	-3.07250800	0.71178700	1.49870100
H	5.84239400	-0.80155900	1.24268800
H	0.08922800	-3.66831000	1.71164500
H	-3.89353500	-2.30950000	1.61281800
H	-3.72658000	1.07035000	3.09167900
H	-2.77393500	2.28823300	2.24531900
H	5.25017800	-1.74668600	2.60747200
H	3.87159400	-3.79324400	-0.18131200
H	-1.55541300	-3.79661200	2.28940300
H	-5.14561300	-2.61298500	2.82919300
H	5.46763900	-3.03661900	-0.18773500
H	-4.67324700	-0.96120800	2.43603400
H	4.85873500	-3.79542000	1.28162800
H	-2.98206500	-3.09262000	3.83720400
H	-0.72139300	0.96121200	2.48370800
H	-2.15316000	1.14546100	5.18359700
H	-0.05373400	-3.89632800	4.26026900
H	-1.38633300	2.48492300	4.33002400

H	1.51503200	-1.91805300	3.43245200
H	-4.68287200	-2.06416300	5.30540500
H	-1.37491200	-3.52319800	5.37361100
H	1.26281400	-0.29962200	4.08433400
H	-4.07223600	-0.45205400	4.94054900
H	-0.40605200	1.14224400	4.92369100
H	-3.06324800	-1.59566700	5.83158000
H	-0.61449700	-1.14654400	5.49871300
H	0.30069200	-3.40842700	5.91458200
H	1.82279400	-1.59843300	5.14364500

2b (small core singlet)

H= -1951.363055 au

Th	0.01939600	-0.23111900	-0.29969700
N	-0.60695400	-1.66837000	1.39747800
Si	-1.36154600	-1.41541200	3.00683600
C	-0.21875400	-1.98812400	4.45769800
C	1.15167400	-1.30374800	4.42689400
C	-0.05058300	-3.50252900	4.64208700
C	-0.31819100	-3.09621900	1.15310600
C	-0.92052700	-3.55586100	-0.16556000
N	-0.42111500	-2.72649500	-1.28028600
C	0.86707000	-3.22948500	-1.79779000
C	1.71100500	-2.07730600	-2.32328100
N	1.93453300	-1.07053300	-1.26799000
Si	3.67270800	-0.75109700	-0.96701400
C	3.76378800	0.61164200	0.37807800
C	3.18886000	0.19996000	1.73853800
C	5.15792700	1.22695800	0.57242900
C	-1.43521400	-2.59980300	-2.34685700
C	-2.38353800	-1.45623000	-2.01466800
N	-1.63437600	-0.18961600	-1.90118600
Si	-2.19411800	1.06603600	-3.05542700
C	-3.96030000	1.71129700	-2.62482400
C	-4.01081600	2.45987000	-1.28832900
C	-5.06600300	0.64812900	-2.67832000
C	-2.29270800	0.29923400	-4.83425800
C	-0.92724800	-0.04305700	-5.44406600
C	-3.11722300	1.13249100	-5.82773400
C	-1.00051000	2.55734800	-2.92100000
C	0.47508900	2.23768300	-3.18217400
C	-1.42782000	3.77285800	-3.75748700
C	4.61503900	-0.07869000	-2.51100400
C	4.07630700	1.26278400	-3.02061000
C	4.78294600	-1.05587700	-3.68276700
C	4.54263200	-2.41573500	-0.49513500
C	4.00004300	-3.08573700	0.77296100
C	6.07505500	-2.32914900	-0.43006900
C	-1.65502300	0.46777900	3.21831100
C	-1.85418600	0.92943400	4.66946300
C	-2.77577400	1.02706400	2.33293000
C	-2.97087000	-2.48178100	3.14086000
C	-3.64837400	-2.36657300	4.51507300
C	-4.00166000	-2.26621200	2.02644700
H	-3.18289600	0.62370900	-6.79882900
H	-1.03956300	-0.66848100	-6.33963900
H	-2.66231300	2.11182000	-6.01220000
H	-0.39522900	0.86244800	-5.75373500
H	-4.14128700	1.30665000	-5.48374200
H	-1.33928700	3.57761500	-4.83234900

H	-0.27663900	-0.57780500	-4.74400900
H	5.48755000	-0.65621300	-4.42413600
H	-2.83283100	-0.65048900	-4.69959300
H	0.67127400	2.06749600	-4.24601800
H	-2.46057400	4.07713900	-3.56006700
H	5.16266000	-2.03510700	-3.37139000
H	3.83492800	-1.21785600	-4.20755500
H	-4.17129900	2.44108500	-3.42217900
H	1.11787400	3.06238400	-2.85310000
H	-5.07249100	0.08813000	-3.62046900
H	-0.92414700	-2.36141800	-3.28406100
H	4.73101600	1.67985900	-3.79733900
H	1.22069700	-1.62869000	-3.20184600
H	2.64653300	-2.50649300	-2.70797200
H	0.83145400	1.33778900	-2.66110200
H	6.51654000	-1.93287200	-1.34962700
H	0.69942400	-4.00158700	-2.56663700
H	-1.07786100	2.85505700	-1.86492500
H	-3.16201300	-1.42476600	-2.78798000
H	5.62043100	0.10573000	-2.10054200
H	-6.05667100	1.10876300	-2.56825800
H	-1.96727800	-3.55493900	-2.48767000
H	3.08333700	1.14417000	-3.46574200
H	6.51348500	-3.32153300	-0.25986900
H	-3.30488100	3.29501400	-1.24598100
H	4.29896300	-3.08313600	-1.33734200
H	-5.01333200	2.86834400	-1.10338100
H	-4.96284800	-0.07639600	-1.86260100
H	3.99093600	2.01286300	-2.22786400
H	1.40728700	-3.69883800	-0.97032400
H	6.40733200	-1.69055100	0.39597700
H	-2.92320500	-1.68499100	-1.08225000
H	-3.77543800	1.79296600	-0.45202100
H	4.35252300	-4.12262500	0.85413500
H	-0.71965100	-4.62238800	-0.35862800
H	5.57573100	1.62924600	-0.35564100
H	-2.00507300	-3.43103900	-0.10680200
H	2.90586900	-3.10343100	0.79657300
H	3.11657600	1.41146400	-0.01496400
H	4.33548200	-2.56570500	1.67617300
H	-2.71018300	0.69146800	1.28976100
H	5.87276800	0.49662400	0.96779000
H	0.76583300	-3.29043900	1.15346500
H	-3.54870800	-2.30076000	1.03092200
H	-3.76231500	0.72420400	2.70102700
H	-2.74920200	2.12281400	2.31522600
H	5.11255200	2.05386400	1.29239700
H	2.22669300	-0.32856400	1.67424900
H	-0.72355800	-3.75173600	1.93648400
H	-4.78604200	-3.03387700	2.06259600
H	3.86651000	-0.47507300	2.27165800
H	-4.49928500	-1.29601700	2.12030000
H	3.02172200	1.07616700	2.37501300
H	-2.61251600	-3.51911400	3.04943700
H	-0.71432300	0.92407800	2.87310000
H	-2.76595400	0.51352500	5.11299400
H	0.54211200	-3.94552000	3.83384700
H	-1.94612300	2.02219600	4.71091100
H	1.74343600	-1.65652000	3.57584800
H	-4.48139000	-3.07687200	4.60139800

H	-1.00774400	-4.03360000	4.68224400
H	1.07722000	-0.21435100	4.34293500
H	-4.06752000	-1.36604700	4.67038700
H	-1.01624800	0.65110900	5.31550100
H	-2.96246700	-2.56811500	5.34425600
H	-0.75356500	-1.61798400	5.34650500
H	0.48050200	-3.72242500	5.57774600
H	1.72678800	-1.52430300	5.33608100
H	-0.78734000	4.63586100	-3.53529300
I	0.41923400	2.72768300	0.73984400

4b (small core singlet)

H= -2210.558728 au

N	-0.59828600	-2.62633200	-0.68553500
Th	-0.12156500	0.01055700	-0.00852400
N	-0.85662500	-1.19210000	1.83398300
Si	-1.85623800	-0.87454500	3.27696600
C	-0.76457000	-0.62858300	4.84968900
C	0.03650300	0.67826600	4.82286200
C	-1.69402200	-2.61411700	-1.67437600
C	-2.56208600	-1.37208800	-1.49013900
N	-1.75674500	-0.14577500	-1.64385100
Si	-2.17312000	0.89970800	-3.02332800
C	-3.81140900	1.88244400	-2.73823800
C	-3.68997100	2.98872700	-1.68439100
C	0.66835200	-3.12708800	-1.25209200
C	1.44619300	-1.98384500	-1.89414900
N	1.80354900	-0.94781000	-0.90061700
Si	3.54660100	-0.88727000	-0.53998900
C	4.10245300	-2.60344300	0.20419200
C	4.42873000	-3.69309700	-0.82893500
C	-0.95597700	-3.30744100	0.57292700
C	-0.32350300	-2.56631400	1.74831100
C	-5.00428700	0.97147800	-2.41571000
C	5.25541400	-2.50737700	1.21600600
C	0.17078700	-1.81307400	5.13035600
C	-2.44608700	-0.17457500	-4.61586700
C	-1.15055800	-0.71705800	-5.23408200
C	-3.29548200	0.50788500	-5.69963600
C	-0.77273200	2.20686700	-3.20850300
C	0.65830000	1.67022700	-3.33501500
C	-1.05408800	3.20550800	-4.34198000
C	3.87951400	0.44540700	0.80439100
C	2.85711900	0.39511200	1.94616700
C	4.03840900	1.87821600	0.28028200
C	4.60695200	-0.36620200	-2.07093800
C	4.33584400	-1.04759300	-3.41801800
C	6.11043700	-0.40398100	-1.75311500
C	-2.84239100	0.75705800	3.02312500
C	-3.74563700	1.08030900	4.22307700
C	-3.64097700	0.85642700	1.71940000
C	-3.01699600	-2.39128700	3.62576700
C	-3.48159600	-2.51100100	5.08587300
C	-4.22828200	-2.48647400	2.68677100
C	-0.21996300	2.46441600	0.73776300
C	0.78028100	3.55100500	0.83196900
C	1.42840200	3.85144700	2.04701000
C	2.39025400	4.85375000	2.13692700
C	2.74334000	5.60229600	1.01397500
C	2.10713500	5.33126700	-0.19767900

C	1.14501600	4.32912300	-0.28545300
H	-3.43789400	-0.16229100	-6.55799900
H	-1.36645800	-1.46617700	-6.00750800
H	-2.81678800	1.41678800	-6.08109800
H	-0.57700100	0.08118500	-5.71795300
H	-4.28968300	0.78825600	-5.33922900
H	-0.97779500	2.72462700	-5.32376100
H	-0.49449300	-1.18645000	-4.49360400
H	-0.32477600	4.02583500	-4.33140000
H	4.21263300	2.57962000	1.10436800
H	-3.02397900	-1.04361100	-4.26536100
H	0.81339200	1.16049400	-4.29088600
H	-2.05021500	3.65370600	-4.27129200
H	4.88178600	1.96971400	-0.41051700
H	3.14298800	2.23459600	-0.23948200
H	-4.01995900	2.36833500	-3.70372700
H	1.38766900	2.48866300	-3.28181300
H	-5.15550100	0.18898300	-3.16854200
H	-1.25351800	-2.57506900	-2.67514200
H	3.20522900	0.95266700	2.82458600
H	0.83944100	-1.55433100	-2.70764500
H	2.32308900	-2.40974500	-2.39749000
H	0.94356300	0.94921900	-2.55721000
H	6.36167000	0.11782000	-0.82329300
H	0.47868300	-3.94521700	-1.96708800
H	-0.82868900	2.77173000	-2.26544100
H	-3.39604100	-1.43096100	-2.20336500
H	4.84807200	0.14923400	1.23128200
H	-5.93655200	1.54894400	-2.35725600
H	-2.28736200	-3.54109400	-1.61112300
H	1.92204600	0.90333000	1.66082700
H	6.69068900	0.06842300	-2.55689200
H	-2.93509700	3.73658100	-1.94698300
H	4.32602700	0.69036200	-2.19526700
H	-4.64311800	3.52071800	-1.56209000
H	-4.87364200	0.47676200	-1.44672100
H	2.62008700	-0.62331100	2.27498800
H	1.27204500	-3.53877500	-0.43785000
H	6.47726500	-1.43265400	-1.65978900
H	-3.03882300	-1.41261800	-0.49709200
H	-3.42347200	2.58124800	-0.70346800
H	-0.68279100	2.30106200	1.72576700
H	4.98286100	-0.62218600	-4.19743500
H	-0.65894900	-4.36867600	0.54155000
H	5.00903000	-1.87565700	2.07486900
H	-2.04235000	-3.27090800	0.69347300
H	3.30258900	-0.90988200	-3.74893400
H	-1.04735500	2.76295200	0.06909000
H	3.21558600	-2.93846400	0.76499900
H	1.15639900	3.29155000	2.93969600
H	4.54149600	-2.12376400	-3.38999100
H	-3.03351600	0.67567800	0.82395500
H	6.16763200	-2.10433100	0.76161600
H	0.77252200	-2.56421800	1.61805200
H	-3.95628300	-2.36984200	1.63229300
H	-4.46473900	0.13672300	1.69025500
H	-4.07969800	1.85623700	1.60834400
H	5.50730900	-3.50190100	1.60880600
H	3.60596400	-3.89101600	-1.52285000
H	-0.48780400	-3.14987800	2.66379500

H	-4.73202600	-3.45648700	2.79306800
H	5.30397600	-3.42646900	-1.43165500
H	-4.97375600	-1.71704600	2.91717700
H	2.86072200	5.05830200	3.09618200
H	4.66414900	-4.64335900	-0.33046400
H	-2.39137700	-3.27408700	3.42578000
H	0.65260800	4.14779900	-1.23853900
H	-2.07151200	1.54016700	2.98939200
H	-4.57035900	0.36395400	4.31044800
H	0.93245100	-1.91099900	4.34815500
H	-4.19600100	2.07526700	4.11373200
H	0.71336000	0.71244300	3.96139600
H	-4.09458600	-3.41200900	5.22267900
H	-0.36276500	-2.76848600	5.19247100
H	3.49090100	6.38737900	1.08347100
H	2.35634000	5.91146400	-1.08338900
H	-0.60738600	1.56234900	4.77365600
H	-4.09780500	-1.65817900	5.39119800
H	-3.20079400	1.07268300	5.17281000
H	-2.64575600	-2.57849700	5.78857100
H	-1.47598600	-0.56385300	5.68684500
H	0.70428200	-1.67681700	6.08043600
H	0.65684900	0.77930400	5.72352500

$TS_{4b\text{-}3b}$ (small core singlet)

H= -2210.523296 au

N	-0.48810100	-2.65865200	-0.76698200
Th	0.18539500	-0.14100400	0.00662400
N	-0.64004700	-1.36223500	1.82479500
Si	-1.51206000	-0.96670700	3.32047900
C	-0.33917200	-0.97127100	4.85613800
C	0.65732800	0.19315500	4.84719700
C	-1.55500600	-2.50248900	-1.78076900
C	-2.27787200	-1.17426400	-1.56526200
N	-1.35973800	-0.03514100	-1.76370700
Si	-1.71923700	0.99745000	-3.16452400
C	-3.23391000	2.15031000	-2.83439500
C	-2.96217700	3.22674400	-1.77776300
C	0.72895300	-3.29187200	-1.31280100
C	1.60757900	-2.26225900	-2.01110200
N	1.93023600	-1.15296200	-1.10879100
Si	3.64178500	-0.80797000	-0.77299100
C	4.35801700	-2.23336800	0.33866200
C	4.74045500	-3.50793300	-0.42795300
C	-0.96148300	-3.36556000	0.44245800
C	-0.27859000	-2.78310000	1.67421100
C	-4.51298900	1.38034600	-2.47847700
C	5.50922500	-1.81545400	1.26501300
C	0.40320400	-2.30198000	5.03652300
C	-2.19328400	-0.08015900	-4.70978400
C	-1.01404400	-0.81586900	-5.36056700
C	-2.98993700	0.67415000	-5.78576200
C	-0.19645500	2.13470000	-3.47194300
C	1.13101900	1.40754900	-3.72392800
C	-0.43898500	3.17996200	-4.57146600
C	3.62546200	0.81187800	0.25103000
C	2.41303000	0.82632400	1.20250300
C	3.67446800	2.09840200	-0.58645900
C	4.69677700	-0.50087800	-2.36359600
C	4.56959200	-1.48935700	-3.52947800

C	6.17726000	-0.28779200	-2.00949600
C	-2.20481300	0.82132500	3.15483300
C	-2.96294300	1.28368000	4.40843700
C	-3.04921100	1.09460100	1.90418600
C	-2.89807400	-2.28336300	3.65447000
C	-3.36306800	-2.35830200	5.11605800
C	-4.10785600	-2.15558300	2.71903100
C	0.16103600	2.54789700	0.59566200
C	0.79545400	3.82817500	1.01950100
C	1.00658900	4.11301300	2.37915400
C	1.62993400	5.29125200	2.78163100
C	2.06416300	6.21857200	1.83490600
C	1.86334500	5.95153000	0.48123300
C	1.23750200	4.77359400	0.08039500
H	-3.25305400	0.00324200	-6.61464600
H	-1.36723700	-1.58064700	-6.06525800
H	-2.41189300	1.49953000	-6.21570000
H	-0.38226700	-0.12762900	-5.93327500
H	-3.92366300	1.09523900	-5.40115900
H	-0.53084400	2.70732600	-5.55593600
H	-0.36989200	-1.31248400	-4.62767600
H	0.40262600	3.88219200	-4.63394700
H	3.61432500	2.98450700	0.05616300
H	-2.86701200	-0.85211800	-4.30637000
H	1.13622100	0.91609000	-4.70156000
H	-1.34515500	3.77094700	-4.40369200
H	4.59974300	2.17644300	-1.16671000
H	2.84027700	2.16329600	-1.29540600
H	-3.41160000	2.66247700	-3.79195600
H	1.96808700	2.11833500	-3.72211900
H	-4.76782600	0.61601500	-3.22140800
H	-1.09437900	-2.48657600	-2.77199200
H	2.58553600	1.55773900	2.00720500
H	1.09236200	-1.89643400	-2.91463800
H	2.49796300	-2.79020700	-2.37813500
H	1.35144300	0.63696200	-2.97606500
H	6.31843600	0.42901400	-1.19295200
H	0.46406300	-4.12866700	-1.98066800
H	-0.09023500	2.69020000	-2.52662400
H	-3.15584300	-1.14370300	-2.22491800
H	4.54979600	0.79688700	0.85006000
H	-5.37327400	2.05885800	-2.40257500
H	-2.24532000	-3.36046600	-1.74628900
H	1.26041600	1.67758200	0.79861800
H	6.73645600	0.08961900	-2.87613100
H	-2.12670600	3.88178800	-2.04681600
H	4.30730100	0.46230800	-2.72548100
H	-3.84145400	3.86897800	-1.63293400
H	-4.41661900	0.87961600	-1.50817200
H	2.30806700	-0.13908000	1.73751900
H	1.29625500	-3.70660400	-0.47312700
H	6.65611800	-1.22596600	-1.70670400
H	-2.70583500	-1.17603100	-0.54627100
H	-2.72960600	2.77878200	-0.80507900
H	-0.67340200	2.31125500	1.27235700
H	5.21614900	-1.18168300	-4.36302300
H	-0.79588000	-4.45098900	0.34383600
H	5.22556600	-0.99900700	1.93619700
H	-2.03817100	-3.20108700	0.54317900
H	3.54880800	-1.54072400	-3.91816100

H	-0.26338600	2.65756900	-0.41252200
H	3.50218900	-2.48656800	0.98458100
H	0.66934700	3.40167900	3.13007200
H	4.87507100	-2.50399300	-3.25040500
H	-2.57455400	0.75988100	0.97273900
H	6.39166400	-1.48922400	0.70357800
H	0.81352500	-2.91492600	1.57653900
H	-3.81613000	-2.03769500	1.66993000
H	-4.01612800	0.58541000	1.95380100
H	-3.25384200	2.16710100	1.79124700
H	5.82536000	-2.65823100	1.89515500
H	3.92283600	-3.89578600	-1.04503900
H	-0.55236000	-3.39590700	2.54389200
H	-4.75506500	-3.04027900	2.78595000
H	5.59526500	-3.33442200	-1.09089800
H	-4.72766500	-1.29165000	2.98477100
H	1.77487600	5.48658100	3.84121900
H	5.03198800	-4.30993600	0.26399100
H	-2.42106600	-3.24932500	3.42858400
H	1.08178000	4.58300900	-0.97903300
H	-1.29912900	1.44455800	3.08970400
H	-3.90284500	0.73393200	4.53194800
H	1.11088100	-2.47352900	4.21761800
H	-3.22201100	2.34808900	4.33921300
H	1.29239800	0.17060600	3.95419600
H	-4.12196900	-3.14201800	5.24281100
H	-0.27478200	-3.16263100	5.07408900
H	2.54841600	7.13908100	2.14835200
H	2.19067700	6.66690900	-0.26905500
H	0.15771600	1.16739700	4.87470500
H	-3.81652900	-1.41817000	5.44867600
H	-2.37907600	1.14877100	5.32470600
H	-2.54279500	-2.58686300	5.80303800
H	-0.99847900	-0.83941100	5.72757600
H	0.98483300	-2.30556800	5.96792400
H	1.32521200	0.14883200	5.71799300

3b (small core singlet)

H= -1939.225086 au

N	-0.60325900	-2.62889500	-0.68461400
Th	-0.12546000	0.00754400	-0.00704300
N	-0.86120100	-1.19505600	1.83523000
Si	-1.86093900	-0.87747800	3.27818900
C	-0.76920900	-0.63208500	4.85095600
C	0.03226100	0.67453400	4.82431300
C	-1.69860900	-2.61606200	-1.67388500
C	-2.56626100	-1.37374300	-1.48967600
N	-1.76043500	-0.14768000	-1.64273700
Si	-2.17582100	0.89838400	-3.02208300
C	-3.81402000	1.88138900	-2.73740900
C	-3.69274400	2.98681200	-1.68262900
C	0.66332500	-3.13033300	-1.25071600
C	1.44207100	-1.98747900	-1.89237400
N	1.79947600	-0.95170200	-0.89861200
Si	3.54245500	-0.89132200	-0.53760800
C	4.09779500	-2.60741800	0.20715500
C	4.42410000	-3.69733400	-0.82569500
C	-0.96176700	-3.31001300	0.57361400
C	-0.32893000	-2.56959600	1.74924700
C	-5.00742800	0.97065000	-2.41622100

C	5.25049200	-2.51138100	1.21925600
C	0.16580500	-1.81690600	5.13134900
C	-2.44820400	-0.17524300	-4.61514900
C	-1.15258200	-0.71790500	-5.23300400
C	-3.29687900	0.50786900	-5.69909000
C	-0.77502900	2.20525800	-3.20574700
C	0.65588200	1.66822800	-3.33203600
C	-1.05547500	3.20487400	-4.33859900
C	3.87543600	0.44173900	0.80636900
C	2.85329500	0.39193200	1.94841300
C	4.03421300	1.87435800	0.28167800
C	4.60334600	-0.37093200	-2.06844700
C	4.33250400	-1.05266200	-3.41542000
C	6.10671900	-0.40892600	-1.75016600
C	-2.84665400	0.75441100	3.02455400
C	-3.74963200	1.07799700	4.22460500
C	-3.64534500	0.85414000	1.72091100
C	-3.02217300	-2.39394200	3.62667500
C	-3.48684400	-2.51367700	5.08675700
C	-4.23350100	-2.48852000	2.68765900
C	-0.22297700	2.46112000	0.74054000
C	0.77718300	3.54785400	0.83487000
C	1.42552200	3.84797300	2.04986400
C	2.38730100	4.85033800	2.13989600
C	2.74005800	5.59928100	1.01710500
C	2.10360000	5.32859500	-0.19449000
C	1.14157100	4.32637100	-0.28237500
H	-3.43913600	-0.16198600	-6.55773100
H	-1.36839800	-1.46671300	-6.00675700
H	-2.81765300	1.41670500	-6.08004700
H	-0.57859700	0.08031800	-5.71640100
H	-4.29114100	0.78850400	-5.33906500
H	-0.97905400	2.72467900	-5.32070700
H	-0.49694700	-1.18774000	-4.49242600
H	-0.32573500	4.02480500	-4.32710300
H	4.20823800	2.57614000	1.10548800
H	-3.02653000	-1.04420500	-4.26517700
H	0.81118400	1.15906100	-4.28817600
H	-2.05139700	3.65352700	-4.26794000
H	4.87765000	1.96566100	-0.40906900
H	3.13879400	2.23040000	-0.23832400
H	-4.02181000	2.36808000	-3.70265500
H	1.38550400	2.48638500	-3.27801000
H	-5.15844100	0.18865100	-3.16960800
H	-1.25769800	-2.57697900	-2.67446600
H	3.20166600	0.94992200	2.82645200
H	0.83591500	-1.55760900	-2.70612500
H	2.31898300	-2.41380000	-2.39532400
H	0.94061300	0.94660200	-2.55460700
H	6.35778500	0.11312200	-0.82043700
H	0.47345500	-3.94832800	-1.96581300
H	-0.83124800	2.76943400	-2.26228500
H	-3.39999800	-1.43211000	-2.20320000
H	4.84408800	0.14571000	1.23315600
H	-5.93951600	1.54843000	-2.35802800
H	-2.29232100	-3.54283500	-1.61105400
H	1.91816100	0.90002300	1.66307600
H	6.68730000	0.06309800	-2.55392600
H	-2.93765800	3.73474300	-1.94439300
H	4.32269200	0.68565200	-2.19322400

H	-4.64583000	3.51888400	-1.56019900
H	-4.87760600	0.47531800	-1.44743500
H	2.61637100	-0.62633000	2.27778800
H	1.26647500	-3.54240800	-0.43627000
H	6.47329300	-1.43764400	-1.65639400
H	-3.04337800	-1.41436200	-0.49681100
H	-3.42662300	2.57847600	-0.70196000
H	-0.68532100	2.29737200	1.72870900
H	4.97987800	-0.62763100	-4.19474700
H	-0.66560600	-4.37149000	0.54203900
H	5.00401800	-1.87935800	2.07787200
H	-2.04813600	-3.27261700	0.69394200
H	3.29939200	-0.91478400	-3.74671500
H	-1.05070500	2.76003700	0.07243200
H	3.21069300	-2.94213200	0.76777400
H	1.15376400	3.28776400	2.94242800
H	4.53787900	-2.12887400	-3.38703300
H	-3.03816700	0.67267000	0.82542300
H	6.16294300	-2.10868200	0.76502700
H	0.76709300	-2.56809900	1.61902900
H	-3.96148300	-2.37184300	1.63319000
H	-4.46968700	0.13507100	1.69207000
H	-4.08331600	1.85425700	1.60972800
H	5.50203600	-3.50585900	1.61240200
H	3.60150000	-3.89512600	-1.51984300
H	-0.49360700	-3.15327500	2.66458700
H	-4.73763100	-3.45834500	2.79383300
H	5.29961400	-3.43103400	-1.42817100
H	-4.97865300	-1.71882000	2.91818300
H	2.85796600	5.05463300	3.09910800
H	4.65910100	-4.64758400	-0.32700100
H	-2.39691900	-3.27696700	3.42657400
H	0.64897900	4.14532100	-1.23541600
H	-2.07546300	1.53721900	2.99076200
H	-4.57459700	0.36193700	4.31209900
H	0.92734200	-1.91496100	4.34904200
H	-4.19965400	2.07311300	4.11529300
H	0.70911900	0.70863800	3.96284500
H	-4.10036600	-3.41435000	5.22338400
H	-0.36804400	-2.77215600	5.19338700
H	3.48755900	6.38441400	1.08669600
H	2.35254300	5.90910800	-1.08006600
H	-0.61137000	1.55881300	4.77525700
H	-4.10254000	-1.66055400	5.39227900
H	-3.20467200	1.07020100	5.17427100
H	-2.65103800	-2.58182500	5.78943300
H	-1.48057700	-0.56728800	5.68814200
H	0.69945000	-1.68095500	6.08138800
H	0.65265200	0.77525200	5.72498300

U(III) complex (small core quartet)

H= -2009.060094 au

U	-0.00383600	-0.69128000	-0.45626700
N	-1.00315900	-1.96601200	1.20887500
Si	-1.30286600	-1.35931900	2.83280000
C	-0.19092200	-2.17804700	4.18808000
C	1.28806500	-2.16775600	3.78799200
C	-0.62562400	-3.59607700	4.58560000
C	-1.35912400	-3.36088200	0.97067700
C	-1.59180800	-3.60626000	-0.51634500

N	-0.49161300	-3.06136200	-1.33497100
C	0.74666100	-3.84903600	-1.18312100
C	1.96470300	-3.07340700	-1.67614300
N	1.96779800	-1.72159000	-1.12826900
Si	3.52964000	-0.91563800	-1.05208900
C	3.17623900	0.76879600	-0.15820500
C	3.02236000	0.62837300	1.36228900
C	4.17807900	1.88694900	-0.47905200
C	-0.88319100	-2.93230200	-2.75215000
C	-1.88387100	-1.79878100	-2.95604800
N	-1.43630400	-0.58726800	-2.27638400
Si	-2.11531200	0.92080100	-2.87931700
C	-4.02860400	1.07659700	-2.63063500
C	-4.45067100	0.78527900	-1.18656000
C	-4.86363000	0.23213800	-3.60430300
C	-1.82267700	1.11203100	-4.78017000
C	-0.40692200	0.76410500	-5.25291200
C	-2.27447200	2.47135800	-5.33054700
C	-1.25948700	2.31375600	-1.83544400
C	0.15730900	2.66129700	-2.31464400
C	-2.08468700	3.60003100	-1.68838400
C	4.28490600	-0.51408500	-2.78498400
C	3.27157600	0.20980100	-3.67845100
C	4.86875000	-1.73254700	-3.51377600
C	4.83693600	-2.00690300	-0.13806900
C	4.33342100	-2.66805500	1.14930400
C	6.17610200	-1.29344500	0.09367100
C	-0.85339700	0.52648700	2.75127600
C	-0.41456200	1.13936000	4.08836000
C	-1.95679000	1.38771400	2.12140200
C	-3.12788900	-1.68275900	3.37773600
C	-3.48091700	-1.04388500	4.72787000
C	-4.18454500	-1.35911100	2.31607800
H	-2.21092400	2.49656200	-6.42682900
H	-0.36299700	0.69709200	-6.34852700
H	-1.64278400	3.28611500	-4.95785200
H	0.32235200	1.52247700	-4.95023400
H	-3.30919600	2.70882100	-5.05961600
H	-2.25677200	4.07324700	-2.66179800
H	-0.06638900	-0.19219400	-4.84362500
H	-1.55945200	4.33374600	-1.06257700
H	5.30475800	-1.43822300	-4.47817800
H	-2.49433400	0.35488300	-5.21417100
H	0.12561100	3.19556500	-3.27044200
H	-3.06267900	3.42019700	-1.23346800
H	5.65950500	-2.22488500	-2.93844900
H	4.10141700	-2.48495300	-3.72807400
H	-4.25824800	2.13243300	-2.84195500
H	0.67211100	3.31644300	-1.59895800
H	-4.66497100	0.47975200	-4.65174100
H	0.02071800	-2.69983900	-3.32182400
H	3.69445700	0.43317800	-4.66740800
H	1.97622200	-3.07511100	-2.78002100
H	2.84726500	-3.66670000	-1.38189800
H	0.78510600	1.77681200	-2.47261300
H	6.58753200	-0.86539100	-0.82705400
H	0.65286700	-4.81973100	-1.70025800
H	-1.17436400	1.89246500	-0.81306500
H	-1.98943000	-1.67471700	-4.04746500
H	5.11828000	0.17854100	-2.59077300

H	-5.93725400	0.39006400	-3.43279800
H	-1.28109700	-3.88985100	-3.13052600
H	2.37284100	-0.39816900	-3.83167600
H	6.92870200	-1.98525800	0.49565900
H	-3.95748300	1.44576500	-0.46488800
H	5.02983900	-2.81804600	-0.85776800
H	-5.53357100	0.91431900	-1.05404000
H	-4.67615800	-0.84023000	-3.47814300
H	2.94560100	1.16206800	-3.24540800
H	0.87698700	-4.05106500	-0.11619900
H	6.07714900	-0.47742300	0.81944800
H	-2.88024700	-2.12315300	-2.60927300
H	-4.20629500	-0.24442900	-0.90275200
H	5.04619100	-3.42209900	1.51019600
H	-1.73715500	-4.67950800	-0.72930500
H	4.23006000	2.10746700	-1.54898500
H	-2.50474100	-3.07949100	-0.80865700
H	3.36778000	-3.16145100	1.00219700
H	2.20490300	1.11215200	-0.57018500
H	4.20304000	-1.93981800	1.95619800
H	-2.33013600	0.97656500	1.17635900
H	5.18825600	1.61956200	-0.14958000
H	-0.58642900	-4.05618600	1.34207300
H	-3.92473200	-1.78565500	1.34208300
H	-2.81938100	1.46482800	2.79224000
H	-1.60739900	2.41121600	1.92971100
H	3.90674100	2.81765800	0.03669100
H	2.35551200	-0.19303100	1.65029900
H	-2.28730500	-3.66975300	1.48121100
H	-5.16831500	-1.75282900	2.60583500
H	3.98976000	0.42047600	1.83252400
H	-4.30135000	-0.28000100	2.17412800
H	2.63793700	1.55171600	1.81621200
H	-3.15294500	-2.77355700	3.52715000
H	0.03578400	0.58134400	2.09045900
H	-1.22267900	1.09707200	4.82713600
H	-0.57129000	-4.29188100	3.74048100
H	-0.14586300	2.19708000	3.96623100
H	1.45183000	-2.72682700	2.86000200
H	-4.47327100	-1.36566000	5.07183700
H	-1.64992600	-3.62601900	4.97067500
H	1.66565100	-1.15248800	3.62426100
H	-3.50938900	0.05018400	4.66128000
H	0.45041500	0.62763100	4.51948800
H	-2.76388700	-1.30574100	5.51370400
H	-0.30056700	-1.54433600	5.08162200
H	0.02819600	-3.99773200	5.37176000
H	1.91637900	-2.62457100	4.56477200

Reactant-Zr

H= -1849.838334 au

Zr	0.07204600	-0.00338800	-0.11451500
N	-0.37923100	-2.51422000	-0.73342400
N	-0.53870400	-0.99132500	1.66246000
Si	-1.56356200	-0.65906100	3.10086000
C	-0.50184200	-0.42918700	4.69881600
C	0.24612300	0.90780000	4.75065400
C	-1.53034500	-2.49433900	-1.64645900
C	-2.32818500	-1.21682400	-1.41320500
N	-1.45015800	-0.04405600	-1.58946000

Si	-1.87031800	0.96781100	-3.01158000
C	-3.47219400	2.01032900	-2.72064100
C	-3.28153000	3.21032000	-1.78449800
C	0.86480100	-2.96579600	-1.37113100
C	1.59363000	-1.76273500	-1.95648900
N	1.88629600	-0.76966900	-0.89657800
Si	3.64429600	-0.75158500	-0.51830400
C	4.18037800	-2.54902300	0.03916400
C	4.53066000	-3.53572000	-1.08611600
C	-0.64630800	-3.17645600	0.55021800
C	0.00763700	-2.36533800	1.66400500
C	-4.68018300	1.17727000	-2.27153300
C	5.31634000	-2.55778800	1.07620300
C	0.46877700	-1.58430400	4.98143200
C	-2.24346600	-0.19001300	-4.53015500
C	-0.98716200	-0.73645700	-5.22213500
C	-3.18091800	0.42594400	-5.58131800
C	-0.46714600	2.22921100	-3.39338700
C	0.95514500	1.67003700	-3.51428700
C	-0.80234300	3.08798500	-4.62369100
C	4.04372400	0.42084600	0.94678500
C	3.03498200	0.28171700	2.08899800
C	4.25278800	1.89096900	0.56831300
C	4.68768600	-0.10055400	-2.01030900
C	4.40301500	-0.64197100	-3.41635300
C	6.19283900	-0.18835600	-1.70720000
C	-2.56840600	0.96336200	2.87695000
C	-3.45700300	1.25891100	4.09576800
C	-3.38974400	1.07154000	1.58860200
C	-2.71999000	-2.18978000	3.42917700
C	-3.15793800	-2.34641100	4.89460400
C	-3.95226500	-2.26754800	2.51593300
C	-0.02970500	2.25616600	0.38189100
C	0.94895000	3.34723200	0.63352900
C	1.34718000	3.69138900	1.93802200
C	2.24598300	4.72753600	2.17872300
C	2.77905600	5.46324900	1.12098200
C	2.39125000	5.14569200	-0.18047300
C	1.49359100	4.10772700	-0.41817300
H	-3.36500900	-0.28830500	-6.39508400
H	-1.25026200	-1.50477100	-5.96143300
H	-2.75124300	1.32421900	-6.03814000
H	-0.45371300	0.05380400	-5.76069700
H	-4.15521300	0.70268900	-5.16814800
H	-0.78154700	2.49678400	-5.54595100
H	-0.27887400	-1.18506200	-4.51833100
H	-0.06525300	3.89243600	-4.74478000
H	4.45455400	2.49477400	1.46124700
H	-2.77622500	-1.05525100	-4.10867300
H	1.05862700	1.01011800	-4.38124700
H	-1.78826200	3.55904900	-4.55549500
H	5.10122700	2.02379300	-0.11000200
H	3.37132100	2.32527600	0.09018100
H	-3.70774700	2.41215700	-3.71810300
H	1.67793100	2.48642400	-3.64610400
H	-4.89231300	0.34139400	-2.94799700
H	-1.15908700	-2.48499200	-2.67561400
H	3.36811000	0.82548200	2.98230900
H	0.97211700	-1.31706400	-2.74625300
H	2.49939500	-2.11235500	-2.46553700

H	1.27583700	1.10362600	-2.63264900
H	6.45428600	0.23501000	-0.73167200
H	0.66344300	-3.73430600	-2.13520800
H	-0.47665000	2.90430600	-2.52639000
H	-3.19384100	-1.20884700	-2.08832300
H	5.00696900	0.04514600	1.32005400
H	-5.58662100	1.79555300	-2.22698700
H	-2.15072400	-3.39675600	-1.52498200
H	2.06416700	0.71801300	1.81845700
H	6.77374000	0.35656400	-2.46302700
H	-2.50719000	3.89934000	-2.13659700
H	4.42036100	0.96653600	-2.02751000
H	-4.21195400	3.78786200	-1.69871600
H	-4.52628000	0.76238900	-1.26966200
H	2.86350400	-0.76063300	2.38060300
H	1.50113800	-3.42231000	-0.60809700
H	6.54842700	-1.22483400	-1.72068600
H	-2.75327800	-1.23864100	-0.39917000
H	-3.00653100	2.89444600	-0.77324700
H	-0.69748100	2.16825700	1.25413500
H	5.04764100	-0.14318300	-4.15286800
H	-0.29749700	-4.22189500	0.53947100
H	5.05164200	-2.02352800	1.99307800
H	-1.72649900	-3.18955100	0.72048400
H	3.36863700	-0.46662200	-3.72449200
H	-0.69132000	2.54855000	-0.44688200
H	3.28762600	-2.93952700	0.55111100
H	0.93094100	3.14130100	2.77848200
H	4.60370700	-1.71642000	-3.49817600
H	-2.79200700	0.90159900	0.68701900
H	6.23479700	-2.10656800	0.68391100
H	1.09702700	-2.35821700	1.50911000
H	-3.70583400	-2.13101500	1.45781000
H	-4.21317900	0.35118300	1.57330700
H	-3.83452200	2.07095300	1.49733800
H	5.56477900	-3.58872300	1.36258600
H	3.72776900	-3.66454100	-1.81767000
H	-0.14156400	-2.88258600	2.62029500
H	-4.45097700	-3.24085700	2.61587100
H	5.42333200	-3.21909500	-1.63608900
H	-4.69377200	-1.50487600	2.77807100
H	2.52448100	4.96667300	3.20252600
H	4.75059100	-4.52914200	-0.67219500
H	-2.10051600	-3.06851500	3.19864300
H	1.20339300	3.88042400	-1.44091100
H	-1.80473700	1.75390800	2.84559800
H	-4.27494200	0.53483900	4.18269500
H	1.25598900	-1.63464400	4.22112400
H	-3.91771500	2.25098400	4.00507500
H	0.96552200	0.99457100	3.93006400
H	-3.77708400	-3.24547700	5.01538000
H	-0.02876900	-2.56073300	5.00876900
H	3.47673000	6.27475800	1.30769100
H	2.78691000	5.71306100	-1.01970000
H	-0.43015200	1.76698600	4.69383800
H	-3.76014800	-1.49791600	5.23741900
H	-2.90109500	1.24338500	5.03875000
H	-2.30990900	-2.44377700	5.57859200
H	-1.24403800	-0.42018500	5.51161100
H	0.96701600	-1.44796600	5.95043800

H	0.81182600	1.00352800	5.68722200

TS-Zr

H= -1849.799084 au

Zr	0.27171600	-0.26456300	-0.04741300
N	-0.43799900	-2.59794200	-0.72904000
N	-0.50156200	-1.20547400	1.71101500
Si	-1.45261100	-0.81051300	3.17659200
C	-0.31450300	-0.73028300	4.73803700
C	0.58503900	0.51008100	4.77040700
C	-1.56263600	-2.41701600	-1.66862700
C	-2.21655200	-1.06902000	-1.39648600
N	-1.23272100	0.02102700	-1.57834900
Si	-1.61856400	1.04610700	-2.99591700
C	-3.14224200	2.19835100	-2.68386900
C	-2.86475600	3.37069300	-1.73564000
C	0.72769500	-3.24570200	-1.35735300
C	1.56909000	-2.19112600	-2.05512200
N	1.89586800	-1.12608900	-1.10727900
Si	3.61655200	-0.85020100	-0.75185800
C	4.29820100	-2.35525300	0.27386500
C	4.64875600	-3.59587200	-0.56100400
C	-0.83105800	-3.29183600	0.51261000
C	-0.09811800	-2.62446000	1.66688100
C	-4.40822300	1.45680200	-2.23297900
C	5.46486100	-2.01556800	1.21325900
C	0.53141200	-1.99148600	4.95677500
C	-2.11702200	-0.08064300	-4.50873400
C	-0.93174000	-0.73126400	-5.23580600
C	-3.03032600	0.60285300	-5.53916500
C	-0.14218800	2.20242500	-3.44155000
C	1.21632600	1.51351700	-3.61582500
C	-0.44875100	3.08633200	-4.66053500
C	3.57351000	0.69285900	0.36671200
C	2.27174000	0.62550900	1.17899900
C	3.71977200	2.03094900	-0.36852900
C	4.68405800	-0.47251500	-2.31579500
C	4.53686200	-1.37604800	-3.54611600
C	6.16790000	-0.32451100	-1.94229100
C	-2.28353600	0.91560000	3.00925000
C	-3.02891800	1.32786000	4.28882100
C	-3.19474600	1.11406500	1.79112000
C	-2.75759300	-2.21757400	3.50787200
C	-3.18201100	-2.34153900	4.97971000
C	-4.00430600	-2.14564700	2.61464300
C	0.04582800	2.24582400	0.33208300
C	0.66327700	3.49911700	0.86763900
C	0.78652800	3.72616300	2.24820700
C	1.37043600	4.89061500	2.74153500
C	1.85336800	5.86245300	1.86635000
C	1.73940900	5.65468600	0.49242900
C	1.15242400	4.49052500	0.00236500
H	-3.28876900	-0.09656300	-6.34575000
H	-1.27811700	-1.50187100	-5.93773800
H	-2.54405500	1.46431000	-6.00982600
H	-0.37108400	0.00258600	-5.82535400
H	-3.96995000	0.95526200	-5.10405000
H	-0.52632900	2.49268800	-5.57799800
H	-0.22257400	-1.20502500	-4.54966300
H	0.35617800	3.81555800	-4.82177500

H	3.61953200	2.87346800	0.32527100
H	-2.70628900	-0.90024900	-4.07174600
H	1.24231400	0.90803900	-4.52700400
H	-1.38085900	3.65009700	-4.55129700
H	4.69593400	2.12157100	-0.85666700
H	2.95490000	2.16131900	-1.14190400
H	-3.35146800	2.62462500	-3.67674200
H	2.01891900	2.25806900	-3.70567200
H	-4.68878100	0.64108600	-2.90930400
H	-1.16764700	-2.41143600	-2.68811700
H	2.28691500	1.38998800	1.97002200
H	1.01661400	-1.79214100	-2.91985500
H	2.45786400	-2.68350900	-2.47031200
H	1.46892100	0.84964300	-2.78232700
H	6.32381400	0.32875300	-1.07657200
H	0.40668400	-4.05265300	-2.03590000
H	-0.05620700	2.88122600	-2.58167300
H	-3.09486500	-0.96797300	-2.04667200
H	4.42182200	0.62034200	1.06409800
H	-5.26479300	2.14236400	-2.18121400
H	-2.27358800	-3.25416500	-1.58663500
H	1.15416100	1.40654300	0.64357800
H	6.74027800	0.09934900	-2.77813700
H	-2.04087200	4.00549200	-2.07807600
H	4.32227600	0.52377400	-2.61034900
H	-3.75000700	4.01417900	-1.64201900
H	-4.28227600	1.02895300	-1.23228000
H	2.18184400	-0.32844700	1.72324500
H	1.33366200	-3.69561100	-0.56442100
H	6.62094900	-1.29412800	-1.70625500
H	-2.62383500	-1.07564300	-0.37325000
H	-2.61230800	3.02057800	-0.72945600
H	-0.86758100	2.01376100	0.89395800
H	5.19933600	-1.03327300	-4.35281200
H	-0.62726800	-4.37139700	0.43697300
H	5.21022300	-1.22269000	1.92301900
H	-1.90554300	-3.16142500	0.66629200
H	3.51821400	-1.36936400	-3.94374000
H	-0.24991500	2.39417400	-0.70652200
H	3.43996100	-2.62189200	0.91131800
H	0.41749300	2.97892000	2.94584000
H	4.80911500	-2.41617400	-3.33333200
H	-2.72240100	0.81378200	0.85028100
H	6.35472300	-1.69145400	0.66283300
H	0.98899200	-2.73063300	1.51339500
H	-3.76169600	-2.00551400	1.55578300
H	-4.12180800	0.54101100	1.88578400
H	-3.47964000	2.16945500	1.68970700
H	5.75686300	-2.89613100	1.80185500
H	3.82132300	-3.93106800	-1.19499300
H	-0.30429700	-3.16809000	2.59716100
H	-4.59966400	-3.06445000	2.69949300
H	5.50565300	-3.40721900	-1.21711200
H	-4.65702300	-1.31729200	2.91028500
H	1.44676800	5.03851500	3.81585600
H	4.92355400	-4.43989300	0.08630900
H	-2.24058300	-3.15499000	3.25596800
H	1.06688800	4.34645100	-1.07194500
H	-1.43531100	1.60716200	2.90104300
H	-3.90870200	0.69746400	4.45917500

H	1.28065000	-2.10676800	4.16540200
H	-3.38810000	2.36204400	4.20984600
H	1.26195100	0.53506800	3.91000000
H	-3.90378300	-3.15985800	5.10475000
H	-0.06907900	-2.90802400	4.98160500
H	2.30790400	6.77154000	2.24993000
H	2.10496700	6.40499300	-0.20413800
H	0.00929100	1.44129200	4.77044000
H	-3.66789700	-1.42992700	5.34432100
H	-2.40180300	1.26858400	5.18418700
H	-2.33807000	-2.55070700	5.64349200
H	-1.01332200	-0.65315400	5.58448900
H	1.07707200	-1.93623000	5.90807200
H	1.20952200	0.51816600	5.67397100

Zr-product

H= -1578.473076 au

Zr	-0.29977000	-1.14771200	-0.19206300
N	-0.73572600	-3.61334500	-1.16435900
N	-1.06486000	-2.58713000	1.48331000
Si	-1.57923100	-2.04581700	3.08757300
C	-0.35793300	-2.55486800	4.49290900
C	1.07802500	-2.12178900	4.17581200
C	-1.51807200	-3.41179000	-2.40333000
C	-2.45005600	-2.20656400	-2.26833200
N	-1.69427800	-0.95752000	-2.08699200
Si	-2.01404900	0.39460100	-3.19462300
C	-2.99338100	1.77631500	-2.26926500
C	-2.18115200	2.39349000	-1.12720500
C	0.57680100	-4.23693500	-1.40922100
C	1.59007300	-3.21757200	-1.92248400
N	1.61761500	-2.02763400	-1.07473000
Si	3.18616000	-1.29228600	-0.62063400
C	3.92139400	-2.32088700	0.84912200
C	4.51236600	-3.67730500	0.44161300
C	-1.51741000	-4.36337100	-0.16093200
C	-1.06994400	-4.03504400	1.25853600
C	-4.34545500	1.26184800	-1.76104000
C	4.90375700	-1.56231400	1.75213800
C	-0.39735700	-4.04758200	4.84979800
C	-3.10324300	-0.15667300	-4.69672300
C	-2.39358900	-1.10486100	-5.67262100
C	-3.74183600	1.01122700	-5.46390800
C	-0.32398900	1.16235500	-3.69822400
C	0.68291400	0.16616500	-4.28495700
C	-0.44085400	2.40764000	-4.58805100
C	2.75416600	0.47052600	0.01274900
C	1.42126600	0.41861200	0.79913800
C	2.67808800	1.51228700	-1.10993700
C	4.41161900	-1.10862800	-2.10731100
C	4.66587700	-2.31603500	-3.01875700
C	5.75021500	-0.52664300	-1.62449300
C	-1.61748900	-0.11613800	2.97852200
C	-1.49286100	0.59702700	4.33319300
C	-2.83481200	0.42749400	2.21630700
C	-3.28943200	-2.82438600	3.53715100
C	-3.86157400	-2.30649700	4.86467600
C	-4.34469200	-2.76659200	2.42658300
H	-4.41555700	0.63614200	-6.24593800
H	-3.10221000	-1.53429400	-6.39345600

H	-2.99111300	1.63308600	-5.96280400
H	-1.63126600	-0.57447900	-6.25359100
H	-4.33161800	1.66612800	-4.81497900
H	-0.78380500	2.14683800	-5.59576000
H	-1.89220800	-1.93654000	-5.16656200
H	0.53346700	2.90045000	-4.70225900
H	2.34353200	2.48010400	-0.71151200
H	-3.93535800	-0.71441500	-4.23902000
H	0.36738400	-0.19490400	-5.26944700
H	-1.13727400	3.15138100	-4.18627700
H	3.64489800	1.67864000	-1.59765100
H	1.96736900	1.22452500	-1.89336600
H	-3.18563800	2.57308700	-3.00246600
H	1.66676700	0.63583400	-4.41650100
H	-4.98427600	0.90286300	-2.57546700
H	-0.81910600	-3.21053500	-3.22049300
H	1.13435400	1.44422800	1.09594200
H	1.35127700	-2.95819400	-2.96797600
H	2.55738600	-3.73589200	-1.96964400
H	0.81750800	-0.70430400	-3.63525500
H	5.62358100	0.35172700	-0.98177900
H	0.47906500	-5.08965300	-2.10260300
H	0.08827300	1.50250300	-2.73360000
H	-3.09019100	-2.19414600	-3.15916600
H	3.58180100	0.78719400	0.67025100
H	-4.90181300	2.04685600	-1.23160400
H	-2.07611700	-4.32999700	-2.65437900
H	6.37535500	-0.22253800	-2.47484400
H	-1.26767000	2.88429000	-1.47724400
H	3.92563600	-0.34043500	-2.72674100
H	-2.76415800	3.14143100	-0.57307600
H	-4.21331600	0.42781200	-1.06110100
H	1.59795100	-0.10617200	1.76074800
H	0.93857800	-4.62774200	-0.45281800
H	6.32392300	-1.26761800	-1.05611300
H	-3.14805800	-2.38728800	-1.43189300
H	-1.88424400	1.63559300	-0.38732000
H	5.39590700	-2.05897600	-3.79886700
H	-1.46238800	-5.44677000	-0.36265400
H	4.47035100	-0.63861700	2.14753200
H	-2.56531100	-4.06546300	-0.26574000
H	3.75827600	-2.65083300	-3.52822700
H	3.02377700	-2.52561400	1.45324200
H	5.07620800	-3.17170400	-2.47099000
H	-2.99808700	-0.05971100	1.24539700
H	5.82574800	-1.29433800	1.22477600
H	-0.07701200	-4.47728200	1.44580900
H	-3.94952600	-3.11645200	1.46773700
H	-3.75515800	0.27811700	2.79086600
H	-2.74217500	1.50529300	2.03309500
H	5.19643900	-2.18006200	2.61236200
H	3.81337000	-4.28106300	-0.14731000
H	-1.75472100	-4.57265200	1.93351300
H	-5.21392500	-3.38933900	2.67716200
H	5.42383300	-3.55418300	-0.15462900
H	-4.71692900	-1.74859300	2.27146600
H	4.78773300	-4.26984800	1.32495800
H	-3.04813400	-3.88777800	3.69133600
H	-0.70821700	0.16238900	2.41455600
H	-2.33574500	0.35954100	4.99162400

H	-0.09172400	-4.67458500	4.00444500
H	-1.48414900	1.68642400	4.19978900
H	1.44660300	-2.61700500	3.27016200
H	-4.75711500	-2.87149300	5.15557000
H	-1.39230900	-4.37944100	5.16473500
H	1.16430900	-1.04234000	4.01115900
H	-4.16125400	-1.25446400	4.79082300
H	-0.57491800	0.32542000	4.86151400
H	-3.14499700	-2.38668200	5.68926700
H	-0.68874400	-1.99805000	5.38326200
H	0.29318200	-4.26853000	5.67463300
H	1.76321700	-2.38238800	4.99339800

Hf-reactant

H= -1850.818700 au

N	-0.37338800	-2.50159600	-0.73106500
Hf	0.06592300	-0.01741700	-0.12053500
N	-0.53892500	-0.98571900	1.66701300
Si	-1.56302300	-0.65207100	3.10321000
C	-0.50441900	-0.42107700	4.70297800
C	0.24403800	0.91560600	4.75503200
C	-1.52260800	-2.49288600	-1.64996000
C	-2.33069700	-1.22160300	-1.41984200
N	-1.45871400	-0.04245300	-1.59135900
Si	-1.88121500	0.96728900	-3.01244000
C	-3.48526300	2.00620400	-2.72169200
C	-3.29536300	3.20847400	-1.78827100
C	0.87289100	-2.95747500	-1.36588000
C	1.60217700	-1.75493000	-1.95174100
N	1.89294600	-0.76026800	-0.89086300
Si	3.64948000	-0.74683800	-0.51140600
C	4.18739600	-2.55098000	0.02603200
C	4.54006300	-3.52593600	-1.10900000
C	-0.64553800	-3.16955100	0.55104000
C	0.00540700	-2.36186500	1.66857100
C	-4.68845200	1.16917000	-2.26701900
C	5.32311700	-2.57036500	1.06334400
C	0.46533500	-1.57671500	4.98668900
C	-2.25117800	-0.19081100	-4.53186200
C	-0.99334200	-0.73443100	-5.22350100
C	-3.19041300	0.42211500	-5.58312800
C	-0.48145800	2.23210100	-3.39722800
C	0.94235900	1.67590100	-3.51284400
C	-0.81681600	3.08339200	-4.63268100
C	4.05167200	0.40675100	0.96827800
C	3.03665700	0.26197300	2.10401200
C	4.27473700	1.87941600	0.60855800
C	4.69162500	-0.08076200	-1.99693600
C	4.39891900	-0.60451400	-3.40807500
C	6.19773800	-0.17570600	-1.70156600
C	-2.56643500	0.97070900	2.87499700
C	-3.45732000	1.26921200	4.09129300
C	-3.38482700	1.07644400	1.58459800
C	-2.72187600	-2.18070300	3.43355400
C	-3.16222500	-2.33435400	4.89855000
C	-3.95297700	-2.25926000	2.51869500
C	-0.02830600	2.23415100	0.36614900
C	0.95718000	3.32147900	0.62023900
C	1.34064200	3.67529700	1.92601500
C	2.24043200	4.71041000	2.16834200

C	2.78815700	5.43500100	1.11056100
C	2.41511300	5.10714400	-0.19259000
C	1.51702900	4.06968500	-0.43165500
H	-3.37233600	-0.29264300	-6.39695700
H	-1.25436100	-1.50369700	-5.96257600
H	-2.76387900	1.32188800	-6.03988000
H	-0.46152500	0.05678300	-5.76228000
H	-4.16554400	0.69555000	-5.16969700
H	-0.79062500	2.48798500	-5.55205800
H	-0.28409500	-1.18105600	-4.51930300
H	-0.08303700	3.89062800	-4.75533200
H	4.48257400	2.46940400	1.50941800
H	-2.78165600	-1.05776100	-4.11104300
H	1.04698000	1.00462100	-4.37086200
H	-1.80509400	3.55028600	-4.56969800
H	5.12482200	2.01259900	-0.06766500
H	3.39790100	2.32838300	0.13581600
H	-3.72561900	2.40550000	-3.71897000
H	1.66271500	2.49250300	-3.65665900
H	-4.90065800	0.33269700	-2.94278900
H	-1.14681800	-2.48014200	-2.67732500
H	3.36554200	0.80006700	3.00236600
H	0.98183800	-1.31079300	-2.74368000
H	2.50854200	-2.10376500	-2.45947600
H	1.26627800	1.12285200	-2.62381200
H	6.46399100	0.23356100	-0.72130500
H	0.67015300	-3.72817900	-2.12684900
H	-0.49394200	2.91254300	-2.53443200
H	-3.19293600	-1.21932500	-2.09882000
H	5.01042200	0.01956100	1.34115100
H	-5.59688300	1.78422000	-2.21824300
H	-2.13291600	-3.40190700	-1.52941000
H	2.06729900	0.69914600	1.83014800
H	6.77693300	0.37821000	-2.45215600
H	-2.52682700	3.90097300	-2.14631000
H	4.42677400	0.98718300	-2.00025000
H	-4.22820900	3.78140800	-1.69771400
H	-4.52827600	0.75456200	-1.26599700
H	2.86366500	-0.78210900	2.38861500
H	1.50726600	-3.41166000	-0.60003200
H	6.55094600	-1.21264800	-1.73054900
H	-2.76136100	-1.24693800	-0.40799500
H	-3.01242000	2.89564400	-0.77825900
H	-0.70745300	2.16631900	1.23150000
H	5.03828400	-0.09580700	-4.14238800
H	-0.29828400	-4.21509100	0.53480200
H	5.05648800	-2.04943200	1.98729100
H	-1.72630800	-3.18094900	0.71731800
H	3.36225200	-0.42668700	-3.70707700
H	-0.68048400	2.53337600	-0.46805700
H	3.29529200	-2.94816800	0.53405500
H	0.91202600	3.13443600	2.76617800
H	4.60027300	-1.67765800	-3.50482000
H	-2.78477400	0.90547200	0.68463000
H	6.24045600	-2.11124600	0.67762300
H	1.09573700	-2.35693100	1.51850900
H	-3.70488400	-2.12529300	1.46060700
H	-4.20773000	0.35551500	1.56842400
H	-3.82998300	2.07546600	1.49056900
H	5.57435800	-3.60436500	1.33591700

H	3.73816600	-3.64962100	-1.84251000
H	-0.14868400	-2.88017800	2.62310900
H	-4.45300800	-3.23177000	2.62006700
H	5.43223600	-3.20171000	-1.65521200
H	-4.69400300	-1.49513400	2.77795900
H	2.50772800	4.95759900	3.19319200
H	4.76213900	-4.52291200	-0.70484600
H	-2.10342800	-3.06092200	3.20569900
H	1.23883500	3.83349000	-1.45560500
H	-1.80202300	1.76064200	2.84357500
H	-4.27595500	0.54586500	4.17777500
H	1.25234400	-1.62841200	4.22626400
H	-3.91718200	2.26147200	3.99816900
H	0.96344300	1.00243500	3.93447600
H	-3.78307300	-3.23216600	5.02005200
H	-0.03317800	-2.55266500	5.01505000
H	3.48612700	6.24600200	1.29841700
H	2.82267100	5.66572900	-1.03199300
H	-0.43220200	1.77489200	4.69827000
H	-3.76336500	-1.48423300	5.23922000
H	-2.90332800	1.25465800	5.03543100
H	-2.31522000	-2.43202400	5.58378300
H	-1.24722300	-0.41142300	5.51516500
H	0.96383800	-1.44000200	5.95553100
H	0.80965900	1.01126200	5.69168400

TS-Hf

H= -1850.775684 au

N	-0.42567800	-2.59087500	-0.72886900
Hf	0.27846400	-0.26790600	-0.05758400
N	-0.50058700	-1.19298300	1.70366200
Si	-1.45050800	-0.79743100	3.16823700
C	-0.31729300	-0.71404600	4.73316200
C	0.57950600	0.52814200	4.77017900
C	-1.55144700	-2.41797300	-1.67048800
C	-2.21627600	-1.07626600	-1.39646100
N	-1.23730800	0.02091400	-1.56941700
Si	-1.62959800	1.04625700	-2.98464800
C	-3.16254700	2.18571100	-2.67235500
C	-2.89159200	3.36270400	-1.72778900
C	0.73876700	-3.24303000	-1.35770100
C	1.57893300	-2.19063100	-2.06108800
N	1.90439000	-1.12286700	-1.11514600
Si	3.62388100	-0.85977300	-0.74808300
C	4.29868300	-2.37907700	0.26137400
C	4.65369900	-3.61022100	-0.58565800
C	-0.82048600	-3.28556600	0.51317500
C	-0.09414600	-2.61258500	1.66782000
C	-4.42142200	1.43518400	-2.21653500
C	5.46106300	-2.05036000	1.21009300
C	0.53049500	-1.97345700	4.95572000
C	-2.11478200	-0.08096600	-4.50123600
C	-0.92069100	-0.71127500	-5.23209600
C	-3.03952600	0.59286600	-5.52787500
C	-0.16552700	2.21906500	-3.43107000
C	1.20341000	1.54854400	-3.59468300
C	-0.47919900	3.09085600	-4.65709800
C	3.57967100	0.66961900	0.38899900
C	2.26783800	0.59792000	1.18658600
C	3.73662300	2.01512200	-0.33019600

C	4.69702300	-0.46681600	-2.30393100
C	4.54165900	-1.35124400	-3.54703100
C	6.18174300	-0.33418600	-1.92887100
C	-2.28436800	0.92680900	2.99707600
C	-3.03349500	1.34051800	4.27390800
C	-3.19290200	1.12053300	1.77624200
C	-2.75496200	-2.20503500	3.50201200
C	-3.18113800	-2.32620800	4.97359400
C	-4.00103000	-2.13663700	2.60752600
C	0.05192800	2.23254200	0.32008700
C	0.67108900	3.48743700	0.85334900
C	0.78938700	3.71941800	2.23321200
C	1.37372900	4.88473900	2.72402500
C	1.86188500	5.85210100	1.84676700
C	1.75289900	5.63894000	0.47336600
C	1.16533600	4.47390200	-0.01416600
H	-3.28870900	-0.10733900	-6.33667700
H	-1.25662000	-1.48328600	-5.93755100
H	-2.56705200	1.46327900	-5.99607000
H	-0.37087800	0.03322900	-5.81832300
H	-3.98370300	0.92958700	-5.09005900
H	-0.54559700	2.49095100	-5.57126400
H	-0.20426200	-1.17812600	-4.54874700
H	0.31646600	3.82987200	-4.81963300
H	3.63206800	2.85011300	0.37209700
H	-2.69144900	-0.91124800	-4.06771800
H	1.24246600	0.93825800	-4.50223200
H	-1.41912000	3.64278300	-4.55452100
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H	2.97930600	2.15679600	-1.10916500
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H	1.99634100	2.30339600	-3.68409300
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H	1.02599000	-1.79591500	-2.92741900
H	2.46736500	-2.68398800	-2.47528300
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Hf-product

H= -1579.44898 au

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C	-2.18115200	2.39349000	-1.12720500
C	0.57680100	-4.23693500	-1.40922100
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N	1.61761500	-2.02763400	-1.07473000
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C	-1.51741000	-4.36337100	-0.16093200
C	-1.06994400	-4.03504400	1.25853600

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C	-0.32398900	1.16235500	-3.69822400
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C	2.75416600	0.47052600	0.01274900
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C	2.67808800	1.51228700	-1.10993700
C	4.41161900	-1.10862800	-2.10731100
C	4.66587700	-2.31603500	-3.01875700
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H	1.59795100	-0.10617200	1.76074800
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H	5.39590700	-2.05897600	-3.79886700
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H	5.19643900	-2.18006200	2.61236200
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H	-1.75472100	-4.57265200	1.93351300
H	-5.21392500	-3.38933900	2.67716200
H	5.42383300	-3.55418300	-0.15462900
H	-4.71692900	-1.74859300	2.27146600
H	4.78773300	-4.26984800	1.32495800
H	-3.04813400	-3.88777800	3.69133600
H	-0.70821700	0.16238900	2.41455600
H	-2.33574500	0.35954100	4.99162400
H	-0.09172400	-4.67458500	4.00444500
H	-1.48414900	1.68642400	4.19978900
H	1.44660300	-2.61700500	3.27016200
H	-4.75711500	-2.87149300	5.15557000
H	-1.39230900	-4.37944100	5.16473500
H	1.16430900	-1.04234000	4.01115900
H	-4.16125400	-1.25446400	4.79082300
H	-0.57491800	0.32542000	4.86151400
H	-3.14499700	-2.38668200	5.68926700
H	-0.68874400	-1.99805000	5.38326200
H	0.29318200	-4.26853000	5.67463300
H	1.76321700	-2.38238800	4.99339800
Hf	-0.29977000	-1.14771200	-0.19206300

KI

H= -39.861349 au

K	-1.14166000	-0.55889600	-0.00022900
I	-4.03329800	0.84454900	-0.00059800

KCH_2Ph

H= -299.056082 au

C	-0.85752400	0.24692100	1.21136800
C	-0.85752400	-1.13697100	1.20165200
C	-0.76985100	-1.87161400	0.00000000
C	-0.85752400	-1.13697100	-1.20165200
C	-0.85752400	0.24692100	-1.21136800
C	-0.69146000	1.02024500	0.00000000
H	-0.89990900	0.77993400	2.16033300
H	-0.93600400	-1.67073600	2.14869100
H	-0.80614100	-2.95646800	0.00000000
H	-0.93600400	-1.67073600	-2.14869100
H	-0.89990900	0.77993400	-2.16033300
C	-0.23291300	2.33917800	0.00000000
H	-0.25790700	2.91577200	-0.92273500
H	-0.25790700	2.91577200	0.92273500
K	1.88103600	0.03475100	0.00000000

Toluene

H= -271.334977 au

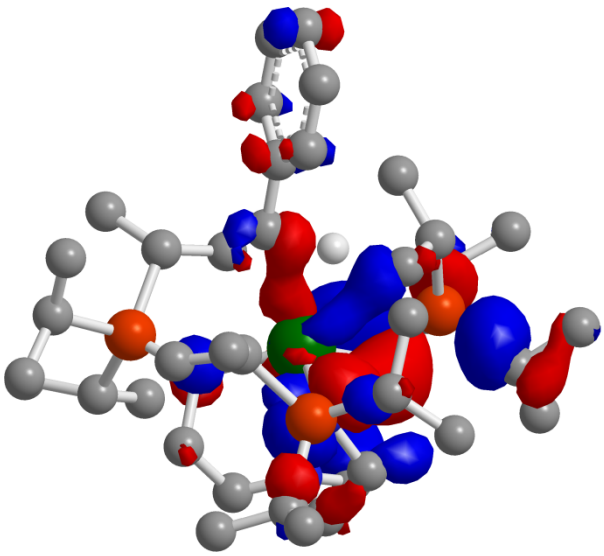
C	-0.90684100	-0.98323100	-0.02723600
C	0.49268300	-0.96113600	-0.02234000
C	1.19205000	0.24413800	-0.00901000
C	0.50112900	1.45481400	-0.00264300
C	-0.89276300	1.44806000	-0.01109700
C	-1.58721900	0.23985100	-0.02439900
H	1.04042400	-1.90107400	-0.03106900
H	2.27889800	0.23727600	-0.00779700
H	1.04445800	2.39568600	0.00456300
H	-1.44196400	2.38597000	-0.01151800
H	-2.67506700	0.24440400	-0.03474700
C	-1.65994300	-2.28795200	-0.00896000
H	-1.10060700	-3.08134700	-0.51411500
H	-1.84364400	-2.62366600	1.01940800
H	-2.63399100	-2.19624600	-0.49915100

bibenzyl

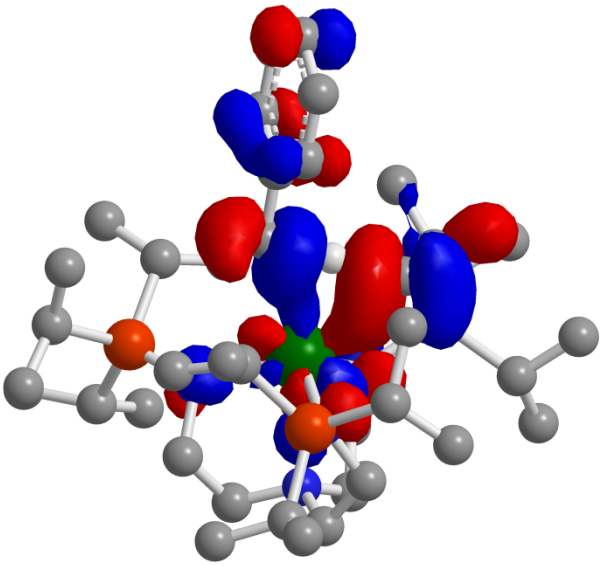
H= -541.484820 au

C	-3.09812200	-0.80689000	-0.07565400
C	-1.70460600	-0.78791500	-0.11336100
C	-1.02198400	0.42689600	-0.12646400
C	-1.71456800	1.64307900	-0.10283700
C	-3.11351600	1.60858600	-0.06632000
C	-3.80130200	0.39670900	-0.05303400
H	-3.63244500	-1.75292700	-0.06867800
H	-1.14760900	-1.72090400	-0.13731200
H	0.06557100	0.43392600	-0.16167400
H	-3.66941300	2.54398900	-0.05434200
H	-4.88791100	0.39240700	-0.02956500
C	-0.97193600	2.95613400	-0.07430600
H	-0.02789700	2.86599000	-0.62478600
H	-1.55665300	3.72978800	-0.58603400
C	-0.66525700	3.43404700	1.36257600
H	-0.08053800	2.66039500	1.87430600
H	-1.60929100	3.52420000	1.91306200
C	0.07738800	4.74709700	1.39109200
C	1.47634300	4.78154700	1.35445000
C	-0.61515000	5.96329300	1.41480400
C	2.16416700	5.99339500	1.34113700
H	2.03220100	3.84612200	1.34239400
C	0.06751600	7.17808600	1.40167600
H	-1.70270300	5.95631000	1.45010200
C	1.46102400	7.19702000	1.36385200
H	3.25077400	5.99766500	1.31757500
H	-0.48945500	8.11108900	1.42569600
H	1.99537600	8.14304000	1.35685400

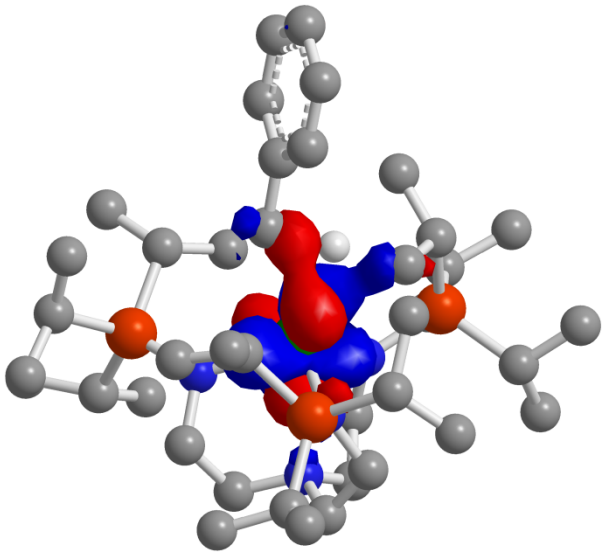
Molecular Orbitals - *Uranium*



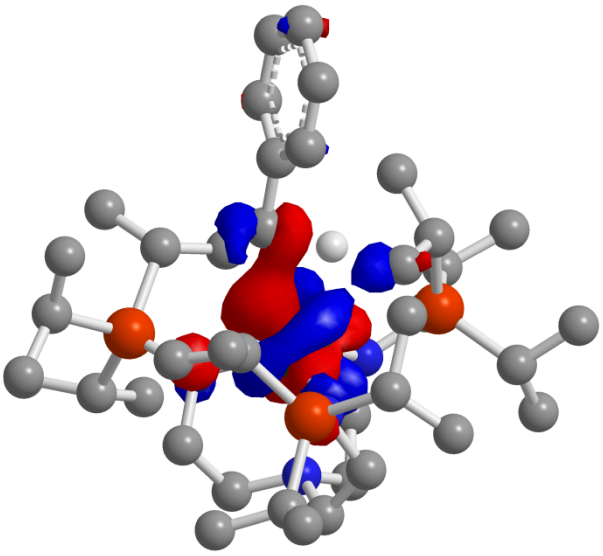
HOMO-3 (195a, -5.65 eV)



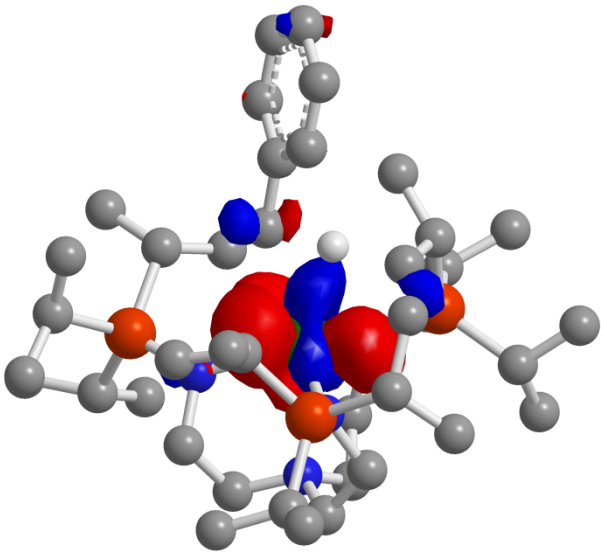
HOMO-2 (196a, -5.05 eV)



HOMO-1 (197a, -4.95 eV)

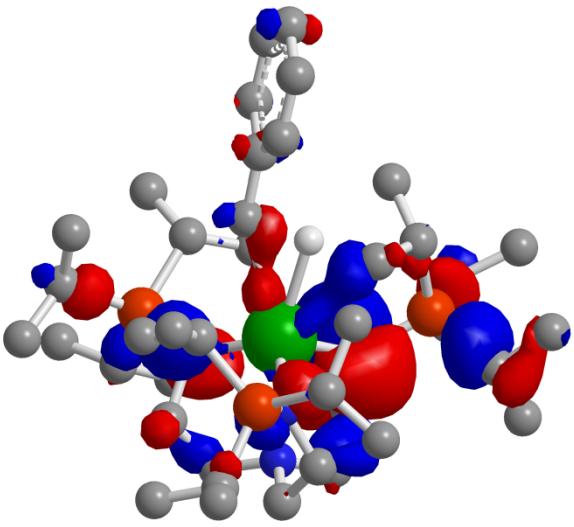


HOMO (198a, -4.83 eV)

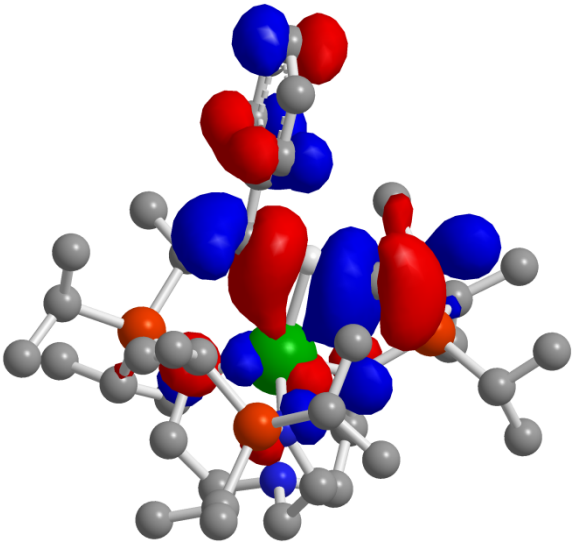


LUMO (199a, -1.45 eV)

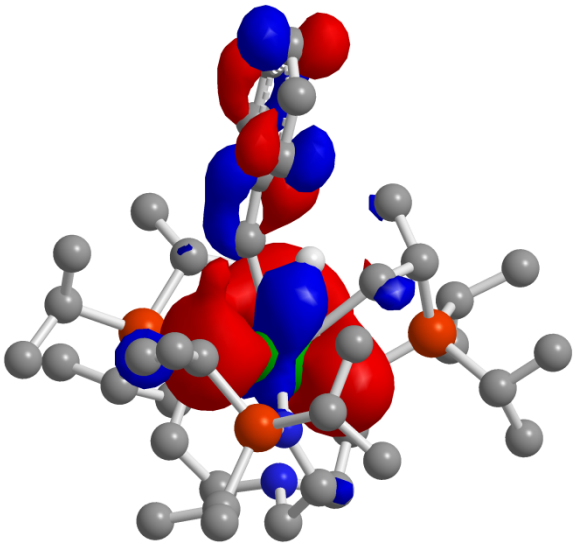
Molecular Orbitals - *Thorium*



HOMO-1 (195, -5.58 eV)

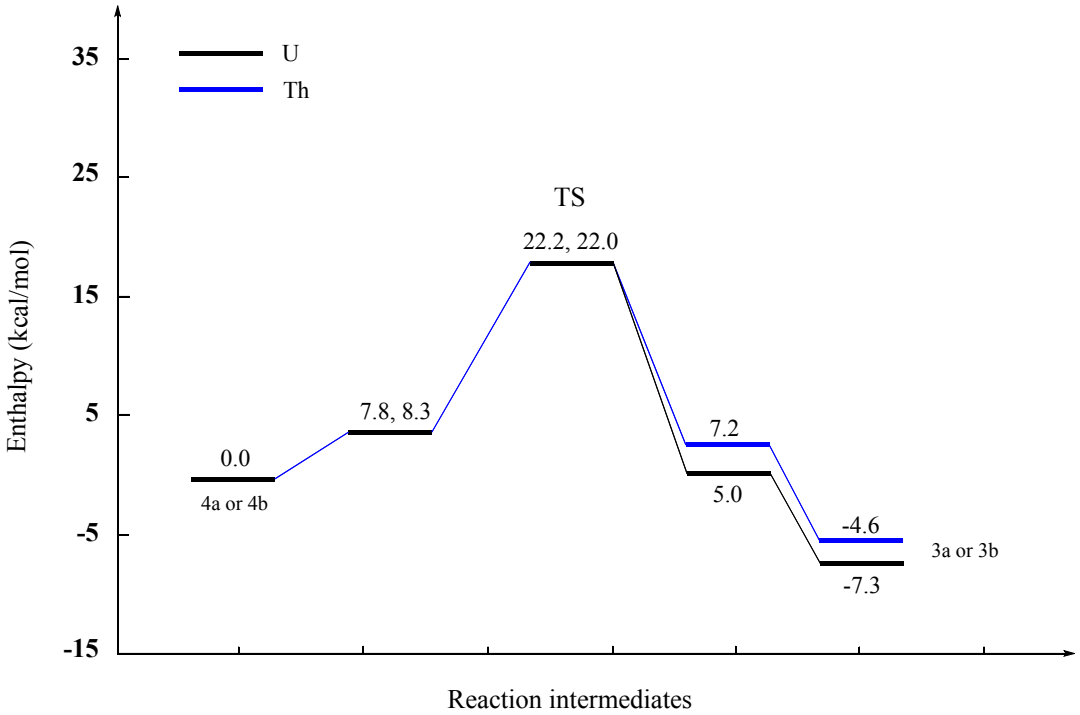


HOMO (196, -4.88 eV)

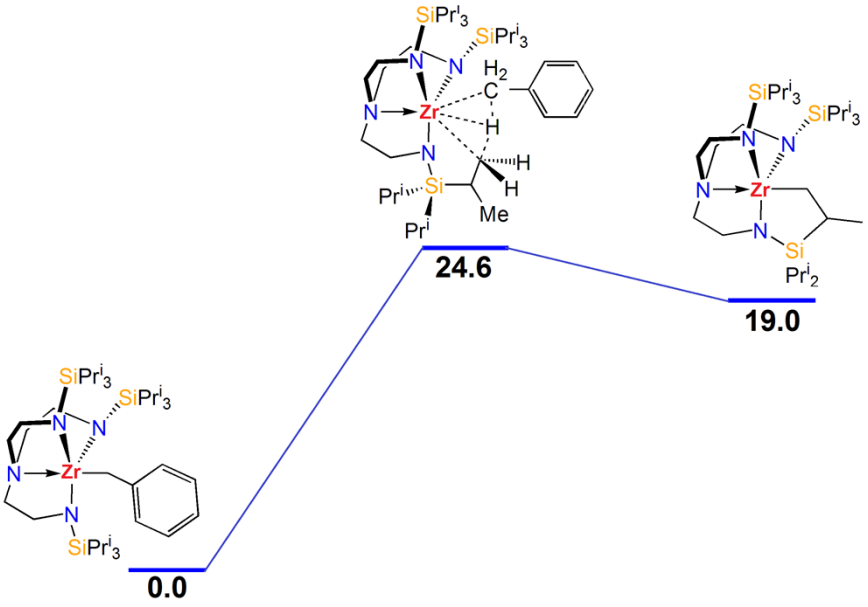


LUMO (197, -0.24 eV)

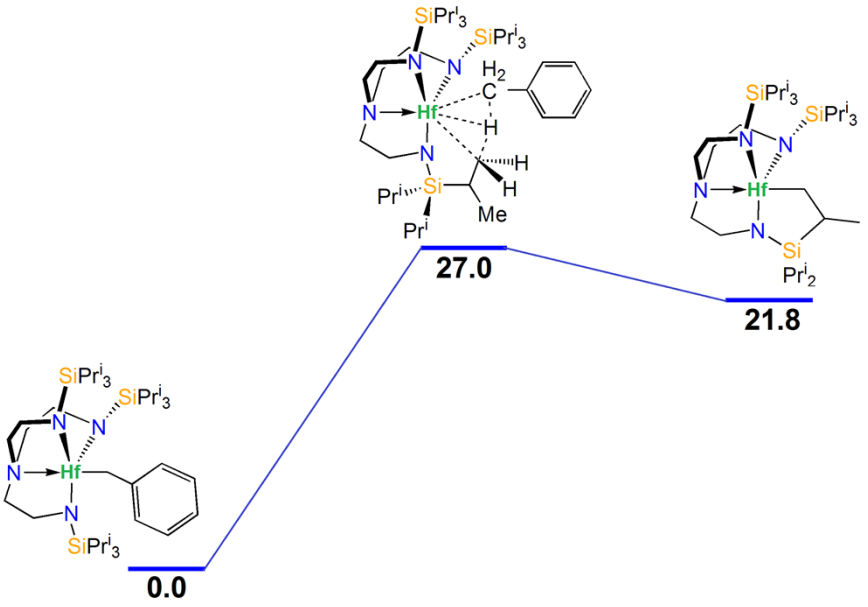
Energy Profile Using f-in-Core RECPs



Energy Profile for Zr



Energy Profile for Hf



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