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# The "Wanderlust" of $Me_3Si$ groups in rare-earth triple-decker complexes: A combined experimental and computational study

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## Supplementary Information

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# 1. Preparation and full characterization for all new compounds

**General procedures:** All operations were performed with rigorous exclusion of air and moisture under an inert atmosphere of dry argon, employing standard Schlenkand glovebox techniques (MBraun MBLab; <1 ppm $O_2$, <1 ppm $H_2O$). THF, DME, TMEDA, and toluene were dried over sodium/benzophenone and freshly distilled under nitrogen atmosphere prior to use. All glassware was oven-dried at 120 °C for at least 24 h, assembled while hot and cooled under high vacuum prior to use. The starting materials, anhydrous $[Li(THF)_4][Ln\{C_8H_6(SiMe_3)_2\}_2]$ (Ln = Y, La, Tb, Tm, Lu),[S1] 1,4-$C_8H_6(SiMe_3)_2$[S2] and anhydrous $CoCl_2$[S3] were prepared according to published procedures. 1.6 M *n*-Butyllithium solution in hexanes was obtained from commercial sources and used as received. The NMR spectra were recorded in $d_8$-THF solutions on a Bruker DPX 600 ($^1$H: 600.1 MHz; $^{13}$C: 150.9 MHz) or a Bruker-AVANCE-DMX400 ($^1$H: 400.1 MHz; $^{13}$C: 100.6 MHz). $^1$H and $^{13}$C shifts are referenced to internal solvent resonances and reported in parts per million (ppm) relative to TMS. IR spectra were measured using an ATR IR spectrometer Bruker Vertex V70. Mass spectra (EI, 70 eV) were recorded on a MAT 95 apparatus. Microanalyses of the compounds were performed using a Leco CHNS 932 apparatus.

***Synthesis of $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (4Y-1,4) and $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,5\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (4Y-1,5)***

0.28 g (2.2 mmol) of anhydrous $CoCl_2$ were added to a stirred solution of 3.8 g (4.33 mmol) $[Li(THF)_4][Y\{C_8H_6(SiMe_3)_2\}_2]$ in toluene (100 mL) at r.t. The reaction mixture was stirred for 24 h and refluxed for an additional 0.5 h. After filtration, the solvent was evaporated *in vacuo*. The solid residue was extracted with 150 mL of *n*-pentane. Upon removal of 100 mL of the *n*-pentane, $Y_2(COT'')_3$ precipitated at r.t. as yellow crystals (1.2 g, 60%). The first fraction of crystals was identified as $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}$**1,5**$\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4Y-1,5**) by single-crystal X-ray crystallography. The more soluble main fraction contains $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}$**1,4**$\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4Y-1,4**). The X-ray analysis of crystals obtained from the main fraction revealed 1,4-substitution of the central COT" ring but also a high degree of disorder in the several times recrystallized compound. The $^1$H and $^{13}$C NMR spectra clearly

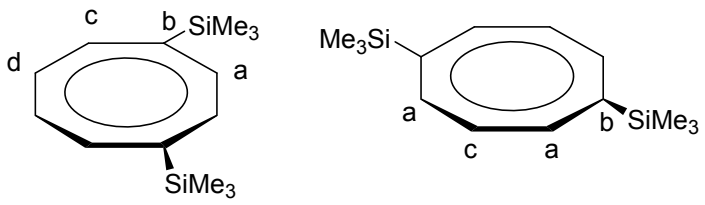
showed the 1,4-substitution of the main fraction. Elemental analysis calcd. for $C_{42}H_{72}Y_2Si_6$ ($M_r$ = 923.4 g·mol$^{-1}$): C 54.63 %, H 7.86 %; Found: C 54.49 %, H 7.61 %. Mass spectrum (EI): *m/z* 921 (100 %) [M+], 907 (5 %) [$Y_2COT"_3$ – $CH_3$], 849 (11 %) [$Y_2COT"_3$ – $SiMe_3$], 824 (10 %), 673 (3 %) [$Y_2COT"_2$], 601 (25 %) [$Y_2COT"_2$ – $SiMe_3$], 585 (5 %) [$YCOT"_2$], 501 (20 %), 479 (2 %), 337 (80 %) [YCOT"].

**4Y-1,4**:

Mp.: 234 °C. IR (ATR): $\nu$ = 3038w, 2994w, 295 m, 2895w, 1777w, 1666w, 1535w, 1487w, 1444w, 1402m, 1320w, 1243s, 1213m, 1124w, 1047m, 1039m (sh), 981m, 937m, 910m, 824vs, 786s (sh), 731vs, 685s, 634s, 549m, 513w, 491m, 434w, 392w, 338s, 309s, 254s, 166m, 118w, 81w cm$^{-1}$. $^1$H NMR (400.1 MHz, $d_8$-toluene, 296 K): $\delta$ = 6.25 (s, 4H, H$^a$-COT), 6.18 – 6.15 (m, 4H, H$^c$-COT), 6.14 (s, 2H, H$^a$-$\mu$-COT), 6.09 - 6.05 (m, 2H, H$^c$-$\mu$-COT), 6.01 – 5.96 (m, 6H, H$^d$-COT + H$^d$-$\mu$-COT), 0.65 (s, 18H, $SiMe_3$), 0.46 (s, 36H, $SiMe_3$) ppm. $^{13}$C NMR (100.2 MHz, $d_8$-toluene, 296 K): $\delta$ = 103.8 (C$^b$-COT), 102.3 (C$^a$-COT), 101.5(C$^c$-COT), 99.9 (C$^d$-COT), 95.2 (C$^b$-$\mu$-COT), 94.2 (C$^c$-$\mu$-COT), 93.7 (C$^a$-$\mu$-COT), 92.8 (C$^d$-$\mu$-COT), 0.9 ($SiMe_3$), 0.7 ($SiMe_3$) ppm. $^{29}$Si NMR (79.5 MHz, $d_8$-toluene, 295 K): $\delta$ = 6.17, 4.11 (1:2) ppm.

**4Y-1,5**:

Mp.: 305 °C. $^1$H NMR (400.1 MHz, $d_8$-THF, 296 K): $\delta$ = 6.68 (s br, 2H, H$^a$-$\mu$-COT), 6.55 (s br, 2H, H$^{a'}$-$\mu$-COT), 6.12 – 6.01 (m, 4H, H$^c$-COT), 5.98 (s, 4H, H$^a$-COT), 5.90 – 5.87 (m, 4H, H$^d$-COT), 5.49 (s br, 2H, H$^c$-COT, 0.46 (s, 18H, $SiMe_3$), 0.44 – 0.33 (2 s, 36H, $SiMe_3$) ppm. $^{13}$C NMR (100.2 MHz, $d_8$-THF, 296 K): $\delta$ = 102.4 (C$^b$-$\mu$-COT), 101.8 and 101.3(C$^a$-$\mu$-COT), 99.3 (C$^c$-COT), 98.0 (C$^b$-COT), 97.5 (C$^c$-$\mu$-COT), 97.2 (C$^d$-COT), 97.1 (C$^a$-COT), 1.4 ($SiMe_3$), 0.8 – 1.0 ($SiMe_3$) ppm. $^{29}$Si NMR (79.5 MHz, $d_8$-THF, 295 K): $\delta$ = 4.77, 1.10 (1:2) ppm.




**Scheme S1.** Numbering Scheme of the COT" rings in the title compounds.

***Synthesis of $La_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (4La)***

From 0.25 g (1.9 mmol) anhydrous $CoCl_2$ and 3.5 g (3.78 mmol) $[Li(THF)_4][La\{C_8H_6(SiMe_3)_2\}_2]$ as described for **4Y**. Compound **4La** precipitated at r.t. as pale yellow plates (1.0 g, 52%), which were suitable for X-ray crystallography after recrystallization from toluene. Elemental analysis calcd. for $C_{42}H_{72}La_2Si_6$ ($M_r$ = 1023.4 g·mol$^{-1}$): C 49.29 %, H 7.09 %; Found: C 48.97 %, H 7.01 %. Mp.: 172–180 °C dec. IR (ATR): $\nu$ = 3030w, 2994w, 2951m, 2892w, 1528w, 1488w, 1445w, 1403m, 1309w, 1243s, 1211s, 1152m, 1046s, 1036m, 979m, 934m, 908w, 827vs, 779m, 747s, 731vs, 684m, 635s, 548m, 513m, 501m, 465w, 446w, 394w, 344m, 300m, 309s, 248s, 229s, 165m, 118w, 84w cm$^{-1}$. Mass spectrum (EI): *m/z* 1021 (100 %) [$La_2COT"_3$ - H], 1006 (5 %) [$La_2COT"_3 – CH_3$], 949 (3 %) [$La_2COT"_3 – SiMe_3$], 774 (6 %) [$La_2COT"_2$], 759 (1%) [$La_2COT"_2 – CH_3$], 701 (15 %) [$La_2COT"_2 – SiMe_3$], 387 (61 %) [$La_2COT"$]. $^1$H NMR (400.1 MHz, $d_8$-toluene, 296 K): $\delta$ = 6.36 (s, 4H, H$^a$-COT), 6.34 – 6.28 (m, 6H, H$^c$-COT + H$^a$-$\mu$-COT), 6.27 - 6.55 (m, 2H, H$^c$-$\mu$-COT), 6.22 – 6.16 (m, 6H, H$^d$-COT + H$^d$-$\mu$-COT), 0.52 (s, 18H, $SiMe_3$), 0.39 (s, 36H, $SiMe_3$) ppm. $^{13}$C NMR (100.2 MHz, $d_8$-toluene, 296 K): $\delta$ = 108.2 (C$^b$-COT), 106.9 (C$^a$-COT), 106.1 (C$^b$-$\mu$-COT), 105.6 (C$^c$-COT), 103.8 (C$^d$-COT), 102.8 (C$^a$-$\mu$-COT), 102.4 (C$^c$-$\mu$-COT), 101.0 (C$^d$-$\mu$-COT), 1.1 ($SiMe_3$), 0.6 ($SiMe_3$) ppm. $^{29}$Si NMR (79.5 MHz, $d_8$-toluene, 295 K): $\delta$ = 5.93, 3.09 (1:2) ppm.

***Synthesis of $Tb_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,5\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (4Tb)***

From 0.21 g (1.60 mmol) anhydrous $CoCl_2$ and 3.1 g (3.27 mmol) $[Li(THF)_4][Tb\{C_8H_6(SiMe_3)_2\}_2]$ as described for **4Y**. Compound **4Tb** precipitated at room temperature as yellow crystals (1.2 g, 69%), which were suitable for X-ray crystallography. Elemental analysis calcd. for $C_{42}H_{72}Tb_2Si_6$ ($M_r$ = 1063.4 g·mol$^{-1}$): C 47.44 %, H 6.82 %; Found: C 47.19 %, H 6.53 %. Mp.: 187 °C. IR (ATR): $\nu$ = 3037w, 2950m, 2894w, 1535vw, 1488vw, 1444w, 1402w, 1365vw, 1319vw, 1243s, 1215m, 1047m, 980m, 937m, 910m, 825vs, 805s (sh), 782m, 748s (sh), 733vs, 685m, 634m, 549m, 523m, 514m, 497w, 466w, 392m, 378m, 356w, 333m, 326m, 308m, 284w, 242m, 224s, 155m, 126w, 73w cm$^{-1}$. Mass spectrum (EI, m < 1025): *m/z* 988 (12 %) [$Tb_2COT"_3 – SiMe_3$], 963 (5 %), 862 (15 %), 814 (6 %) [$Tb_2COT"_2$], 799 (3%) [$Tb_2COT"_2 – CH_3$], 741 (40 %) [$Tb_2COT"_2 – SiMe_3$], 668 (3 %) [$Tb_2COT"_2 – SiMe_3$], 655 (7 %) [$TbCOT"_2$], 614 (10 %), 555 (8 %), 456 (8 %), 407 (100 %) [$TbCOT"$], 391

(10 %) [TbCOT" – $CH_3$], 333 (25 %) [TbCOT" – $SiMe_3$]. Meaningful NMR data could not be obtained for **4Tb** due to the strong paramagnetism of the $Tb^{3+}$ ion.

***Synthesis of $Tm_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,5\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (4Tm)***

From 0.17 g (1.31 mmol) anhydrous $CoCl_2$ and 2.5 g (2.61 mmol) $[Li(THF)_4][Tm\{C_8H_6(SiMe_3)_2\}_2]$ as described for **4Y**. Compound **4Tb** precipitated at r.t. as deep red crystals (1.41 g, 67%). Elemental analysis calcd. for $C_{42}H_{72}Si_6Tm_2$ ($M_r$ = 1083.4 g·mol$^{-1}$): C 46.56 %, H 6.70 %; Found: C 46.37%, H 6.42 %. Mp.: 198 °C. IR (ATR): $\nu$ = 3039w, 2949m, 2894w, 1676vw, 1612vw, 1564vw, 1538vw, 1488vw, 1445w, 1403w, 1366vw, 1342vw, 1318vw, 1242s, 1217m, 1049m, 983s, 938m, 911m, 826vs, 805s (sh), 783m, 760m (sh), 735vs, 685s, 630s, 549m, 522m, 513m, 465w, 391m, 371m, 356w, 325m, 309m, 285w, 241m, 223s, 155m, 102vw, 93vw, 79vw cm$^{-1}$. Mass spectrum (EI, m < 1025): *m/z* 1008 (3 %) [$Tm_2COT"_3$ – $SiMe_3$], 833 (100 %) [$Tm_2COT"_2$], 665 (15 %) [$TmCOT"_2$], 592 (3 %) [$TmCOT"_2$ – $SiMe_3$], 417 (66 %) [TmCOT"]. Meaningful NMR data could not be obtained for **4Tm** due to the strong paramagnetism of the $Tm^{3+}$ ion.

***Synthesis of $Lu_2\{\mu\text{-}\eta^4\text{:}\eta^4\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (4Lu)***

From 0.47 g (3.6 mmol) $CoCl_2$ and 7.0 g (7.27 mmol) $[Li(THF)_4][Lu\{C_8H_6(SiMe_3)_2\}_2]$ as described for **4Y**. Compound **4Lu** precipitated at r.t. as colorless crystals (2.9 g, 72%) which were suitable for X-ray crystallography. Elemental analysis calcd. for $C_{42}H_{72}Lu_2Si_6$ ($M_r$ = 1095.48 g·mol$^{-1}$): C 54.86%, H 7.95%; Found: C 54.59%, H 7.67%. Mp.: 237 °C. IR (KBr disc): $\nu$ = 3044w, 2953m, 2897w, 1443w, 1403m, 1246vs, 1214m, 1198w, 1049s, 1039s, 983m, 938s, 910m, 825vs, 786s, 733vs, 686s, 635s, 552m, 516w, 491m cm$^{-1}$. Mass spectrum (EI): *m/z* 1020 (20 %) [$Lu_2COT"_3$ – $SiMe_3$], 845 (10 %) [$Lu_2COT"_2$], 773 (25 %) [$Lu_2COT"_2$ – $SiMe_3$], 672 (45 %) [$LuCOT"_2$], 599 (10 %), 573 (12 %), 423 (95 %) [LuCOT"], 250 (70 %) [COT"], 207 (85 %), 176 (95 %) [COT" – $SiMe_3$], 162 (100 %). $^1$H NMR (400.1 MHz, $C_6D_6$, 296 K): $\delta$ = 6.32 (s, 4H, $H^a$-COT), 6.28 (m, 4H, $H^c$-COT), 6.10 (m, 2H, $H^c$-$\mu$-COT), 5.97 (s, 2H, $H^a$-$\mu$-COT), 5.91 (m, 4H, $H^d$-COT), 5.71 (m, 2H, $H^d$-$\mu$-COT); 0.53 (s, 18H, $SiMe_3$), 0.46 (s, 36H, $SiMe_3$) ppm. $^{13}$C NMR (100.2 MHz, $C_6D_6$, 296 K): $\delta$ = 100.7 ($C^b$-COT), 100.1 ($C^a$-COT), 98.6 ($C^c$-COT), 98.2 ($C^b$-$\mu$-COT), 97.2 ($C^d$-COT + $C^c$-$\mu$-COT), 94.9 ($C^d$-$\mu$-COT), 94.7 ($C^a$-$\mu$-COT), 0.9 ($SiMe_3$) ppm. $^{29}$Si NMR (79.5 MHz, $C_6D_6$, 295 K): $\delta$ = 4.98, 2.42 (2:1) ppm.

# 2. $^{13}$C NMR spectra for **4Y**, **4La** and **4Lu**

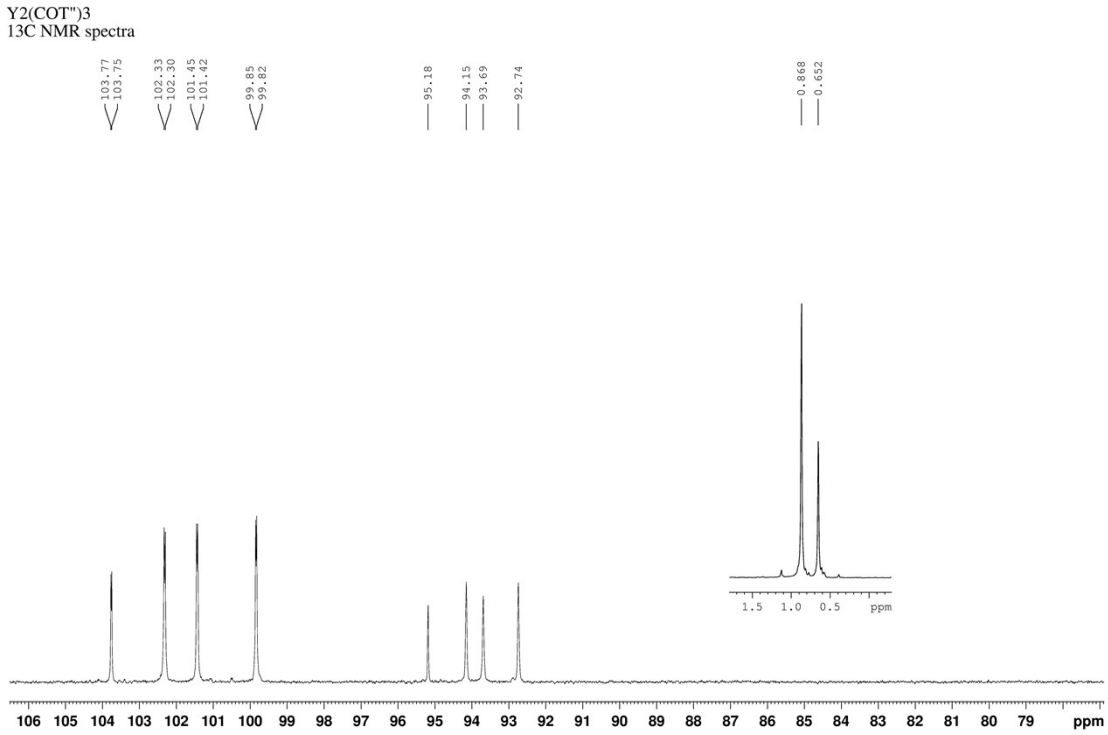



**Figure S1.** $^{13}$C NMR spectrum of $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4Y-1,4**) in $d_8$-toluene.

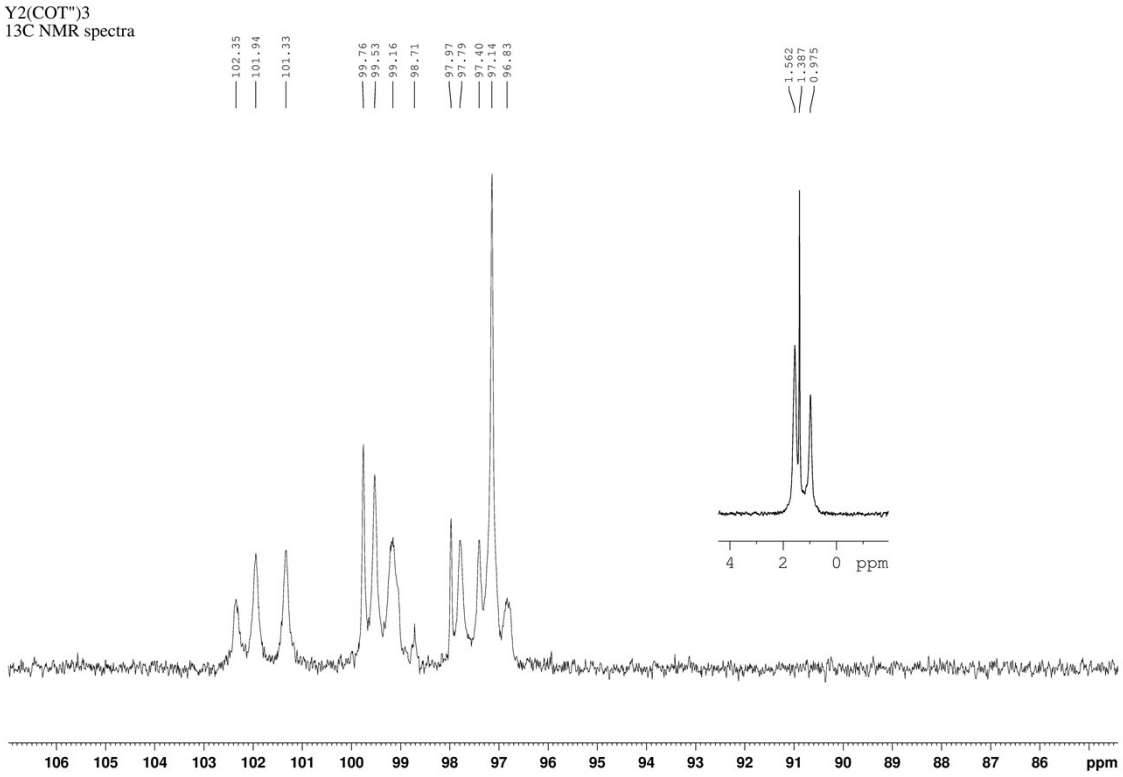



**Figure S2.** $^{13}C$ NMR spectrum of $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,5\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4Y-1,5**) in $d_8$-THF.

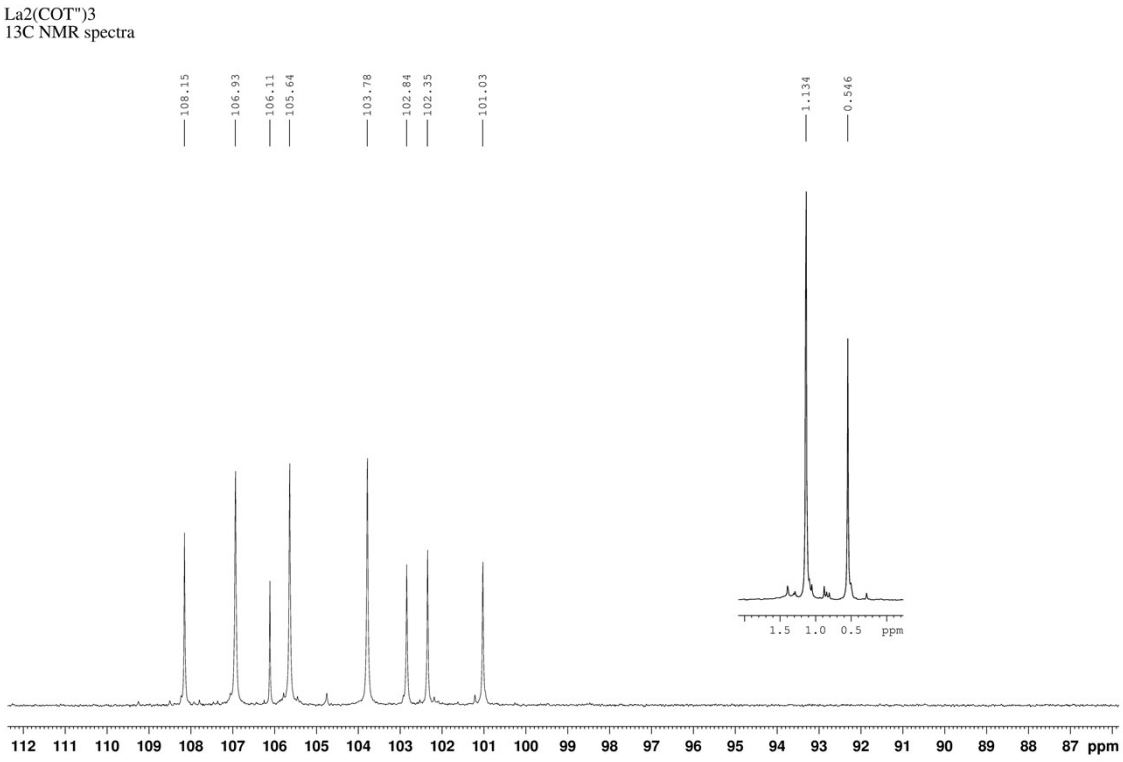



**Figure S3.** $^{13}C$ NMR spectrum of $La_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4La**) in $d_8$-toluene.

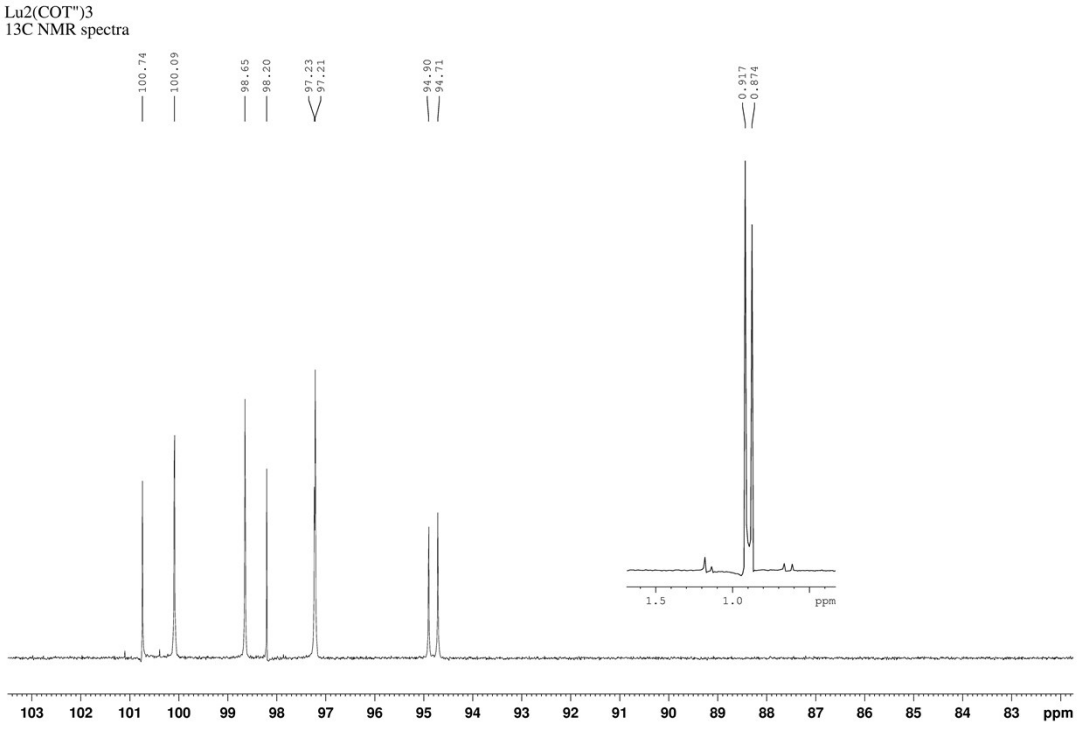



**Figure S4.** $^{13}C$ NMR spectrum of $Lu_2\{\mu\text{-}\eta^4\text{:}\eta^4\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4Lu**) in $C_6D_6$.

# 3. Supporting NMR experiments

Additional NMR experiments have been carried out in order to either establish or rule out an interconversion of isolated triple-decker complexes in solution.

a) In the case of $La_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4La**), the crude reaction mixture has been checked by $^{13}C$ NMR before and after recrystallization. After the reaction, the by-products LiCl and metallic Co were removed by filtration and the filtrate was evaporated to dryness. At this stage the $^{13}C$ NMR spectrum of the remaining solid was not interpretable due to the presence of Co-containing paramagnetic contaminations. Washing with *n*-pentane and crystallization from toluene gave a high yield of **4La**. The $^{13}C$ NMR spectrum (Figure S5) at this stage showed the exclusive formation of the 1,4-isomer (**4La-1,4**) and no indication of the presence of a putative 1,5-isomer.

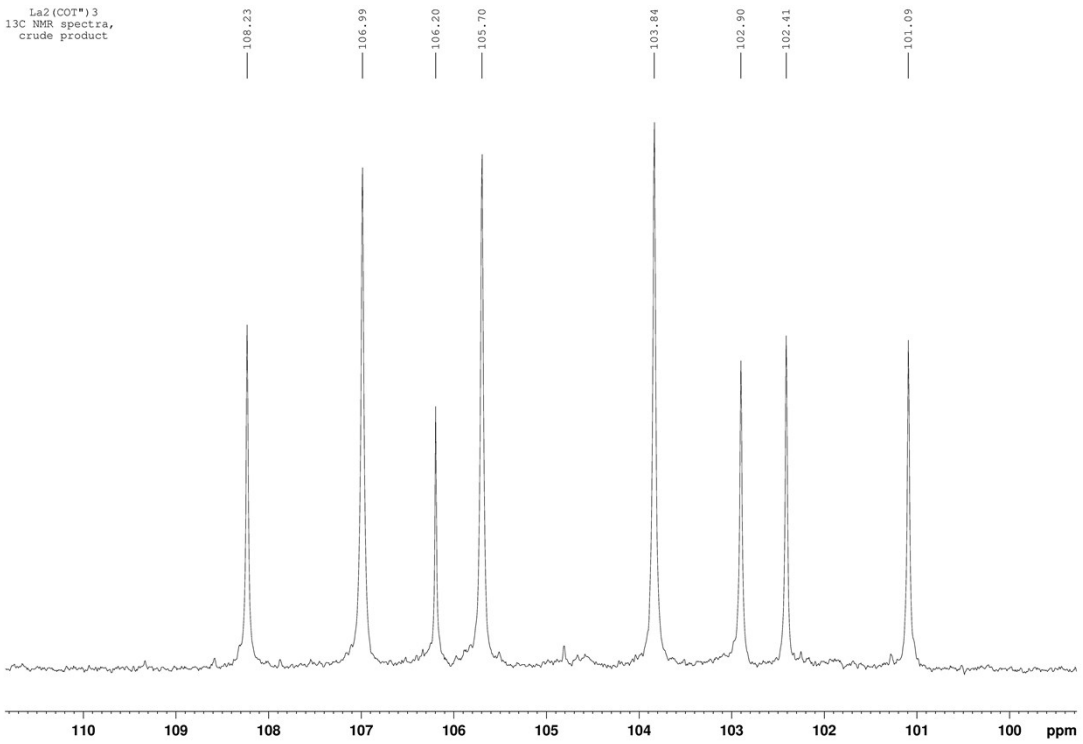



**Figure S5.** $^{13}C$ NMR spectrum of "crude" $La_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4La-1,4**) (COT" ring region).

b) A high-temperature $^{13}C$ NMR study of pure $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4Y-1,4**) in $d_8$-toluene up to 343 K revealed no sign of conversion to **4Y-1,5** in solution (only some line broadening, *cf.* Figure S6). In a second experiment, a sample of pure $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4Y-1,4**) was refluxed in toluene solution for several hours. Once again, the $^{13}C$ NMR spectrum measured after evaporation of the solvent showed only unchanged **4Y-1,4**. After all, the additional NMR experiments clearly indicated that the different isomers of the triple-deckers **4Ln** are formed during the redox reaction of the anionic sandwich complexes with $CoCl_2$ and not within the isolated triple-decker complexes.

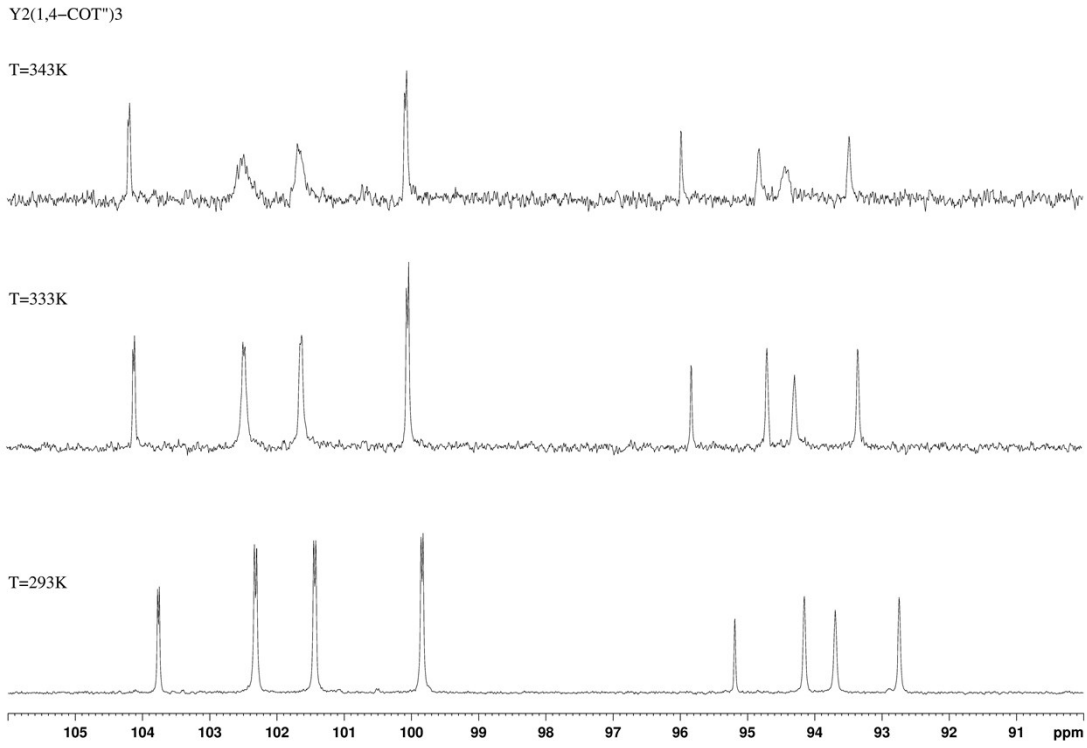



**Figure S6.** High-temperature $^{13}C$ NMR spectra of $Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$ (**4Y-1,4**) in $d_8$-toluene (COT" ring region).

# 4. X-Ray crystallographic data for **4Y, 4La, 4Tb, 4Tm, and 4Lu**

**X-ray crystallographic studies:** Single crystal X-ray intensity data of **4Y**, **4La, 4Tb, 4Tm**, and **4Lu** were collected on a STOE IPDS 2T diffractometer equipped with a 34 cm image plate detector at $T$ = 153(2) K, using graphite-monochromated Mo-$K_\alpha$ radiation. Crystallographic data for the structure reported in this paper have been deposited at the CCDC, 12 Union Road, Cambridge CB21EZ, UK. Copies of the data can be obtained free of charge on quoting the depository numbers 1839498–1839503 (*cf*. Table S1) (Fax: +44-1223-336-033; E-Mail: deposit@ccdc.cam.ac.uk, http://www.ccdc.cam.ac.uk).

**Table S1.** Crystallographic data for all known tripledecker complexes $Ln_2(COT'')_3$

| **Compound** | **$Sc_2(COT'')_3$ (4Sc)** | **$Y_2(COT'')_3$ (4Y)** | **$La_2(COT'')_3$ (4La)** | **$Nd_2(COT'')_3$ (4Nd)** | **$Gd_2(COT'')_3$ (4Gd)** | **$Tb_2(COT'')_3$ (4Tb)** | **$Dy_2(COT'')_3$ (4Dy)** | **$Ho_2(COT'')_3$ (4Ho)** | **$Er_2(COT'')_3$ (4Er)** | **$Tm_2(COT'')_3$ (4Tm)** | **$Lu_2(COT'')_3$ (4Lu)** |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Central COT'' ring | 1,4 non-planar | 1,5 planar | 1,4 planar | 1,4 planar | 1,4 planar | 1,5 planar | 1,4 planar | 1,5 planar | 1,4 planar | 1,5 planar | 1,4 non-planar |
| Solvent used for crystallization | Toluene/*n*-pentane | Toluene/*n*-pentane | Toluene/*n*-pentane | Cyclopentane | Cyclopentane | Toluene/*n*-pentane | Cyclopentane | Cyclopentane | Cyclopentane | Toluene/*n*-pentane | Toluene/*n*-pentane |
| Publication | Angew. Chem. Int. Ed. 2017, 56, 7238–7241 | **this work** | **this work** | OM 2010, 29, 4787 - | JACS 2013, *135*, 3502 - 3510 | **this work** | JACS 2013, *135*, 3502 - 3510 | OM 2013, *32*, 1435 − 1444 | JACS 2014, 136, 8003-8010 | **this work** | **this work** |
| Subst. identifier / CCDC | li0180 / 1537968 | fe109 / 1839500 | fe0160 / 1839501 | ip33 / 740282 | 863405 | fe0044 / 1839502 | 938031 | ip169 / 1839499 | 974992 | fe0094 / 1839503 | li0238 / 1839498 |
| M-M intramol. dist. (Å) | 4.60, $\eta^4/\eta^8$ non-linear | 4.14, $\eta^8/\eta^8$ 4.12, $\eta^8/\eta^8$ | 4.4746(17) $\eta^8/\eta^8$ 4.4631(17) $\eta^8/\eta^8$ | 4.32, $\eta^8/\eta^8$ | 4.21, $\eta^8/\eta^8$ | 4.2012(8) 4.1417(8) | 4.14 $\eta^8/\eta^8$ | 4.127(1) 4.095(1) | 4.11 $\eta^8/\eta^8$ | 4.044(1) 4.036(1) 4.087(1) 4.065(1) | 4.58, $\eta^4/\eta^8$ non-linear |
| Average $C_{cot''(cent.)}$ – M (Å) | 1.52 outer | 1.751 outer 2.067 inner | 1.955 outer 2.239 inner | 1.894 outer 2.164 inner | 1.81 | 1.784, 1.798 outer 2.101, 2.071 inner | 1.79 outer 2.07 inner | 1.751 outer 2.048 inner | 1.76 outer 2.06 inner | 1.717 outer 2.029 inner | 1.65 outer |
| $M_r$ (g/mol) | 835.45 | 923.35 | 1016.29 | 1034.02 | 1060.04 | 1063.37 | 1070.54 | 1075.40 | 1080.06 | 1083.39 | 1095.47 |
| Formula | $C_{42}H_{72}Sc_2Si_6$ | $C_{42}H_{72}Si_6Y_2$ | $C_{42}H_{72}La_2Si_6$ | $C_{42}H_{72}Nd_2Si_6$ | $C_{42}H_{72}Gd_2Si_6$ | $C_{42}H_{72}Si_6Tb_2$ | $C_{42}H_{72}Dy_2Si_6$ | $C_{42}H_{72}Ho_2Si_6$ | $C_{42}H_{72}Er_2Si_6$ | $C_{42}H_{72}Si_6Tm_2$ | $C_{42}H_{72}Lu_2Si_6$ |
| Crystal system | orthorhombic | triclinic | monoclinic | monoclinic | tetragonal | monoclinic | tetragonal | triclinic | tetragonal | triclinic | monoclinic |
| Space group | *Pna*$2_1$ | $P\bar{1}$ | *P*$2_1$ | *P*$2_1$/n | $I\bar{4}$ | *P*$2_1$/n | $I\bar{4}$ | $P\bar{1}$ | $I\bar{4}$ | $P\bar{1}$ | *P*$2_1$/c |
| a (Å) | 18.699(1) | 11.761(8) | 11.700(10) | 13.2914(3) | 16.9774(4) | 20.141(4) | 16.8867(5) | 11.800(2) | 16.8620(4) | 13.092(3) | 9.8651(3) |
| b (Å) | 9.9964(4) | 13.119(6) | 20.285(6) | 17.2442(3) | 16.9774(4) | 12.664(3) | 16.8867(5) | 13.130(3) | 16.8620(4) | 18.108(6) | 39.2173(9) |
| c (Å) | 50.518(2) | 15.744(8) | 20.741(15) | 17.2442(3) | 20.0097(6) | 20.822(4) | 20.1512(6) | 15.747(3) | 20.2149(5) | 20.921(5) | 12.3474(4) |
| $\alpha$ (°) | 90 | 87.01(4) | 90.00 | 90.00 | 90.00 | 90.00 | 90.00 | 87.29(3) | 90.00 | 73.62(2) | 90.00 |
| $\beta$ (°) | 90 | 81.33(5) | 94.16(7) | 102.6801(15) | 90.00 | 116.070(13) | 90.00 | 81.26(3) | 90.00 | 86.14(2) | 92.598(3) |
| $\gamma$ (°) | 90 | 86.58(5) | 90.00 | 90.00 | 90.00 | 90.00 | 90.00 | 86.64(3) | 90.00 | 89.80(2) | 90.00 |
| V (Å$^3$) | 9442.9(8) | 2395(2) | 4910(6) | 5445.65(18) | 5767.44(26) | 4770.6(17) | 5746.3(3) | 2405.4(8) | 5747.6(3) | 4747(2) | 4772.1(2) |
| Density $\rho_{calcd}$ (g cm$^{-3}$) | 1.175 | 1.280 | 1.375 | 1.261 | 1.221 | 1.481 | 1.237 | 1.485 | 1.248 | 1.516 | 1.525 |
| Z | 8 | 2 | 4 | 4 | 4 | 4 | 4 | 2 | 8 | 4 | 4 |
| Reflec. collected | 35180 | 19151 | 49861 | 45485 | 42421 | 48052 | 42231 | 20858 | 28967 | 39793 | 24021 |
| R(int) | 15853, 0.0871 | 8737, 0.0917 | 33493 | 11009, 0.0819 | 7120, 0.0170 | 12657, | 7115, 0.0396 | 9741, 0.0763 | | 15761 | 8445, 0.0423 |
| Final R [I>2sigma(I)] $R_1$ | 0.1048 | 0.0669 | 0.0381 | 0.0394 | 0.0256 | 0.0286 | 0.0324 | 0.0583 | 0.0277 | 0.0572 | 0.0397 |
| *w*$R_2$ | 0.1776 | 0.1544, 0.1432 | 0.1331 | 0.0949 | 0.0755 | 0.0609 | 0.0827 | 0.0906 | 0.0630 | 0.1514, 0.1429 | 0.0661 |
| Crystal color /shape/size | Light yellow plates / 0.30 x 0.20 x 0.02 | Yellow plates / 0.20 x 0.15 x 0.08 | Colorless plates | Green prisms/ 0.30 x 0.20 x 0.10 | Orange blocks / 0.16 x 0.16 x 0.18 | Orange blocks / 0.20 x 0.20 x 0.20 | Orange blocks / 0.11 x 0.13 x 0.15 | Orange prisms / 0.14 x 0.10 x 0.08 | Orange blocks | Red prisms 0.16 x 0.10 x 0.07 | Colorless prisms / 0.41 x 0.25 x 0.16 |

# STRUCTURE REPORT for 4Y-1,5

**Crystallographer:** F. Engelhardt
**ID code:** fe0109
**Date:** 1.11.2017
**Sample by:** Volker Lorenz/Janek Rausch
**Compound:** $Y_2(COT'')_3$ (**4Y-1,5**)
$Y_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,5\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$
**Formula sum:** $C_{42}H_{72}Si_6Y_2$

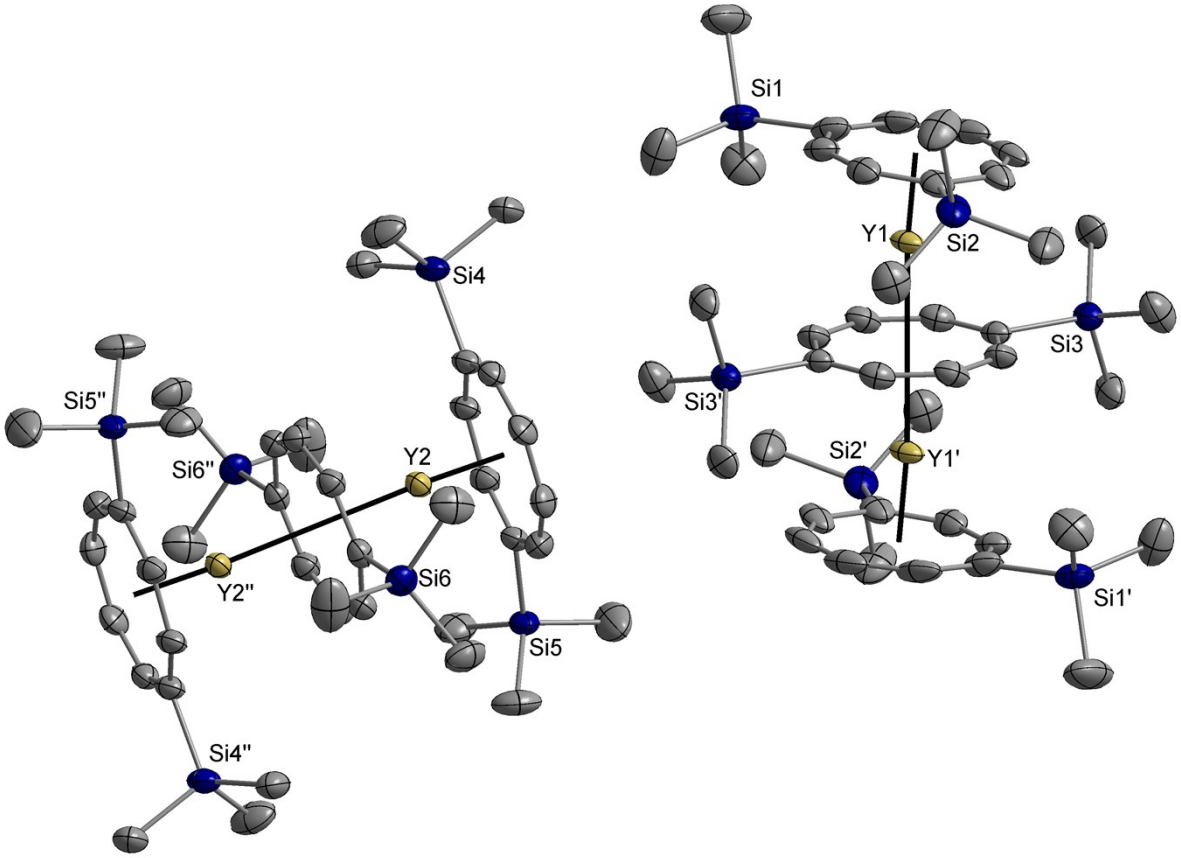



**Figure S7.** Molecular structure of **4Y-1,5** in the crystalline state. Displacement ellipsoids of the heavier atoms with 40% probability, H atoms and disorder of the $SiMe_3$ moieties omitted for clarity.

**Table S2.** Crystallographic Data and Details on Structure Refinement of **4Y-1,5**

| | |
|---|---|
| formula sum | $C_{42}H_{72}Si_6Y_2$ |
| formula weight | 1846.70 |
| crystal size (mm) | 0.20 x 0.15 x 0.08 mm |
| crystal system | Triclinic |
| space group | $P\bar{1}$ |
| unit cell parameters | |
| *a* (Å) | 11.761(8) |
| *b* (Å) | 13.119(6) |
| *c* (Å) | 15.744(8) |
| α (deg) | 87.01(4) |
| *β* (deg) | 81.33(5) |
| γ (deg) | 86.58(5) |
| unit cell volume *V* (Å$^3$) | 2395(2) |
| molecules per cell *z* | 1 |
| crystallographic density $\rho_{calcd}$ (g cm$^{-3}$) | 1.280 |
| absorption coefficient $\mu$ (mm$^{-1}$) | 2.588 |
| | |
| diffractometer | STOE IPDS 2T |
| radiation ($\lambda$[Å]) | graphite-monochromated Mo-$K_\alpha$ (0.71073) |
| temperature (°C) | -173.15 |
| scan type | $\omega$ scan (increment 1.5°, exposure 1 min) |
| completeness of dataset | 99.5% |
| $\theta$ range of data collection (deg) | 1.754 to 25.446 |
| reflections collected | 19151 |
| independent reflections | 8737 |
| independent reflections with $I>2\sigma(I)$ | 6643 |
| structure solution method | dual-space structure solution (SHELXT) |
| refinement method | full-matrix least-squares on $F^2$ (SHELXL 2016/4) |
| absorption correction method | Numerical |
| range of transmission factors | 0.8293 and 0.6043 |
| data / parameters / restraints | 8737 / 596 / 1698 |
| goodness of fit (GooF) [all data] | 1.099 |
| final *R* values | |
| $R_1$ [all data, $I \geq 2\sigma(I)$] | 0.0917, 0.0669 |
| $wR_2$ [all data, $I \geq 2\sigma(I)$]] | 0.1544, 0.1432 |
| largest difference peak and hole | 1.587 and -0.830 eÅ$^{-3}$ |

Refinement special details:
Large residual density peaks due to inefficient absorption correction.

# STRUCTURE REPORT for 4Y-1,4

**Crystallographer:** F. Engelhardt
**ID code:** fe0240
**Date:** 01.11.2017
**Sample by:** Volker Lorenz/Janek Rausch
**Compound:** $Y_2(COT'')_3$ (**4Y-1,4**)
$Y_2\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_3$
**Formula sum:** $C_{126}H_{215}Si_{18}Y_6$

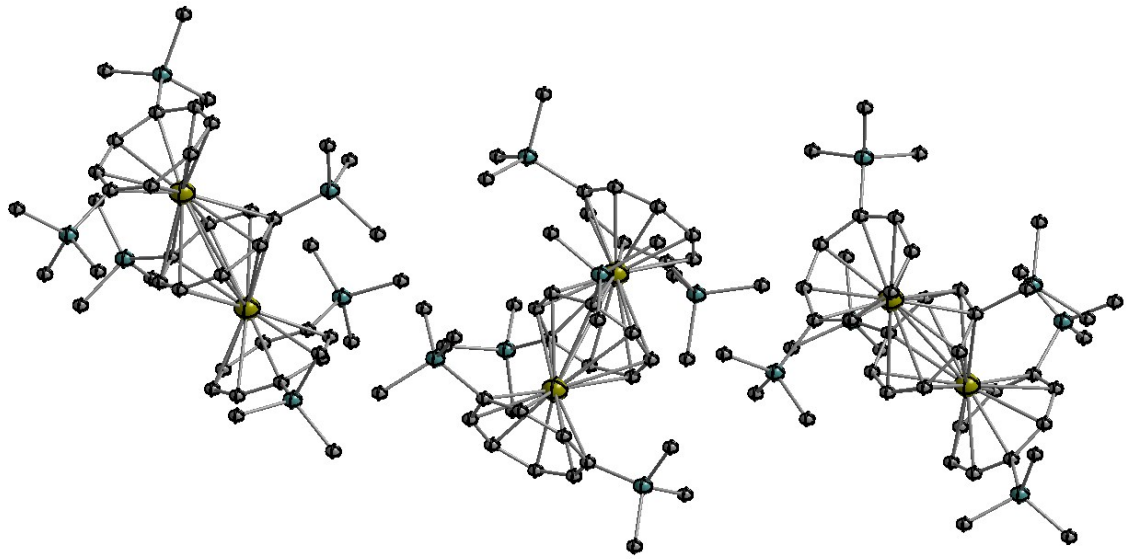


**Figure S8**. Molecular structure of the title compound in the crystalline state. Atoms drawn at arbitrary size, H atoms omitted for clarity.

**Table S3. Crystallographic Data and Details on Structure Refinement of 4Y-1,4**

| | |
|---|---|
| formula sum | $C_{126}\ H_{215}\ Si_{18}\ Y_6$ |
| formula weight | 2769.05 |
| crystal size (mm) | 0.03 x 0.04 x 0.05 mm |
| crystal system | orthorhombic |
| space group | $Pca2_1$ |
| unit cell parameters | |
| a (Å) | 22.405(13) |
| b (Å) | 19.758(11) |
| c (Å) | 32.899(16) |
| *α* (deg) | 90 |
| *β* (deg) | 90 |
| *γ* (deg) | 90 |
| unit cell volume V (Å$^3$) | 14564(14) |
| molecules per cell z | 4 |
| crystallographic density μ calcd (g cm-3) | 1.263 |
| absorption coefficient μ (mm-1) | 2.553 |
| | |
| diffractometer | STOE IPDS 2T |
| radiation (λ [Å]) | graphite-monochromated Mo-$K_\alpha$ (0.71073) |
| temperature (°C) | -173.15 |
| scan type | ω scan (increment 1.5°, exposure 1 min) |
| completeness of dataset | 0.725% |
| θ range of data collection (deg) | 2.090 to 25.349 |
| reflections collected | 15610 |
| independent reflections | 12540 |
| independent reflections with I>2σ(I) | 6490 |
| structure solution method | dual-space structure solution (SHELXT) |
| refinement method | full-matrix least-squares on F2 (SHELXL 2016/4) |
| absorption correction method | none |
| data / parameters / restraints | 12540 / 602 / 3776 |
| goodness of fit (GooF) [all data] | 1.261 |
| final R values | |
| R1 [all data, I ≥ 2σ (I)] | 0.2611, 0.1872 |
| wR2 [all data, I ≥ 2σ (I)]] | 0.4750, 0.4306 |
| largest difference peak and hole | 6.582 and -1.848 eÅ-3 |

Refinement special details:
poor data quality

# STRUCTURE REPORT for 4La

**Crystallographer:** F. Engelhardt
**ID code:** fe0160
**Date:** 25.04.2018
**Sample by:** Volker Lorenz
**Compound:** $La_2(COT'')_3$ (**4La**)
$La_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$
**Formula sum:** $C_{42}H_{72}La_2Si_6$

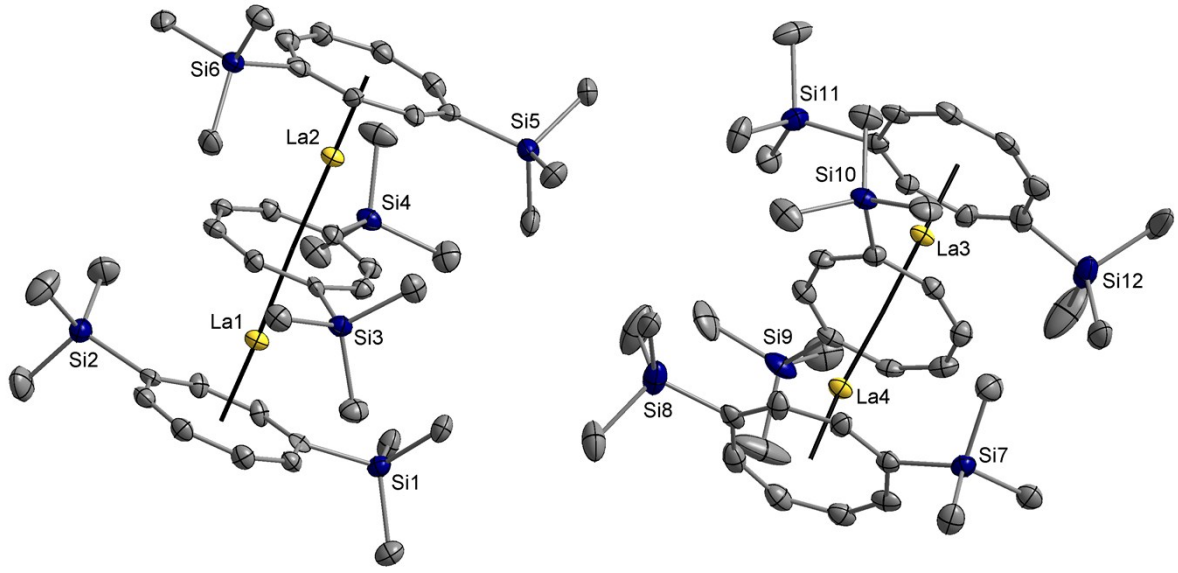



**Figure S9**. Molecular structure of **4La** in the crystalline state. Displacement ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

**Table S4.** Crystallographic Data and Details on Structure Refinement of **4La**

| | |
|---|---|
| formula sum | $C_{42}H_{72}La_2Si_6$ |
| formula weight | 1023.35 |
| crystal size (mm) | 0.09 x 0.15 x 0.21 mm |
| crystal system | monoclinic |
| space group | $P2_1$ |
| unit cell parameters | |
| a (Å) | 11.747(5) |
| b (Å) | 20.280(4) |
| c (Å) | 20.734(8) |
| *α* (deg) | 90 |
| *β* (deg) | 94.11(3) |
| *γ* (deg) | 90 |
| unit cell volume V (Å$^3$) | 4927(3) |
| molecules per cell z | 4 |
| crystallographic density *ρ* calcd (g cm$^{-3}$) | 1.384 |
| absorption coefficient *μ* (mm$^{-1}$) | 1.889 |
| | |
| diffractometer | STOE IPDS 2T |
| radiation (*λ* [Å]) | graphite-monochromated Mo-$K_\alpha$ (0.71073) |
| temperature (°C) | -173.15 |
| scan type | *ω* scan (increment 1.5°, exposure 1 min) |
| completeness of dataset | 0.995% |
| *θ* range of data collection (deg) | 1.935 to 25.203 |
| reflections collected | 33493 |
| independent reflections | 33493 |
| independent reflections with I>2*σ*(I) | 32468 |
| structure solution method | dual-space structure solution (SHELXT) |
| refinement method | full-matrix least-squares on F2 (SHELXL 2016/4) |
| absorption correction method | numerical |
| range of transmission factors | 0.7567 and 0.6186 |
| data / parameters / restraints | 33493 / 963 / 2284 |
| goodness of fit (GooF) [all data] | 0.849 |
| final R values | |
| R1 [all data, I ≥ 2*σ* (I)] | 0.0496, 0.0476 |
| wR2 [all data, I ≥ 2*σ* (I)]] | 0.1331, 0.1299 |
| largest difference peak and hole | 2.672 and -1.141 eÅ$^{-3}$ |

Refinement special details:
Data showed signs of non-merohedral twinning and have been treated accordingly. Additionally, the data are of relatively low quality. Hence, the C-C distance standard uncertainty is relatively high.

# STRUCTURE REPORT for 4Tb

**Crystallographer:** F. Engelhardt
**ID code:** fe0044
**Date:** 21.8.2018
**Sample by:** Volker Lorenz
**Compound:** $Tb_2(COT'')_3$ (**4Tb**)
$Tb_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,5\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$
**Formula sum:** $C_{42}H_{72}Si_6Tb_2$

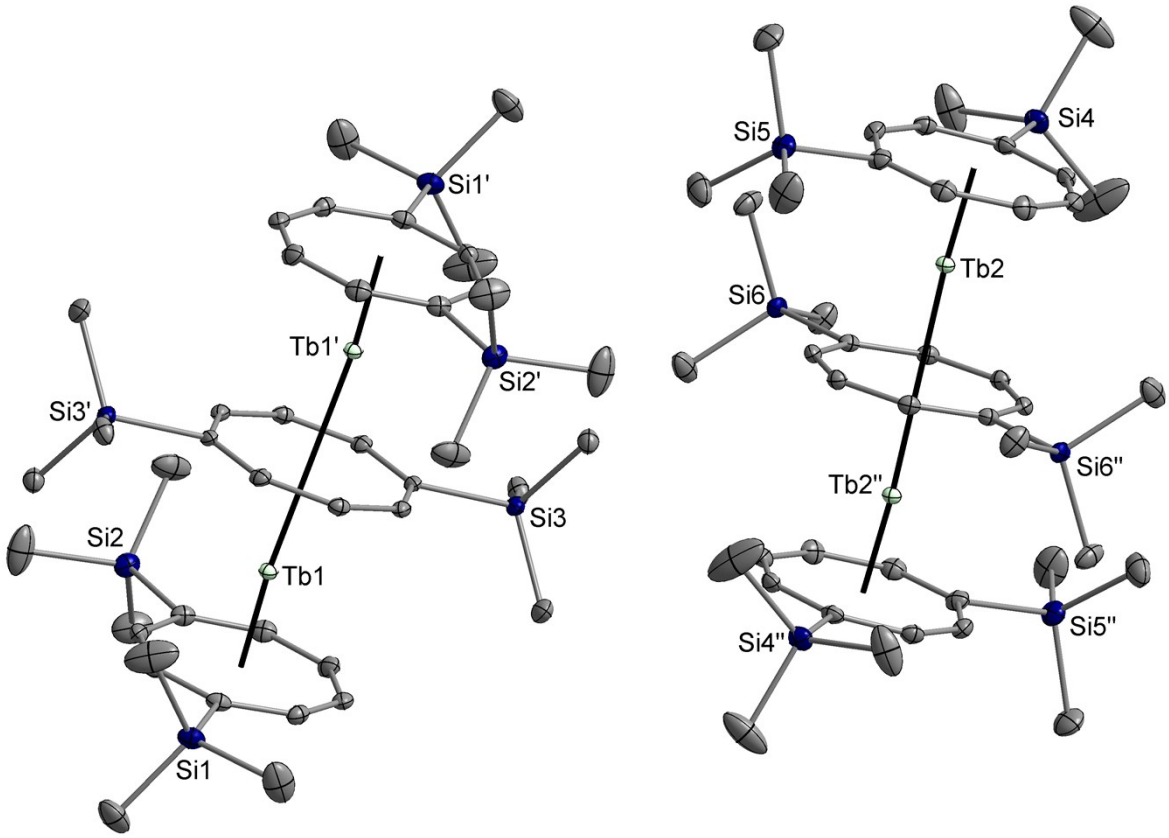



**Figure S10.** Molecular structure of **4Tb** in the crystalline state. Displacement ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

**Table S5.** Crystallographic Data and Details on Structure Refinement of **4Tb**

| | |
|---|---|
| formula sum | $C_{42}H_{72}Si_6Tb_2$ |
| formula weight | 1063.37 |
| crystal size (mm) | 0.2 x 0.2 x 0.2 mm |
| crystal system | Monoclinic |
| space group | $P2_1/n$ |
| unit cell parameters | |
| *a* (Å) | 20.141(4) |
| *b* (Å) | 12.664(3) |
| *c* (Å) | 20.822(4) |
| *α* (deg) | 90 |
| *β* (deg) | 116.070(13) |
| *γ* (deg) | 90 |
| unit cell volume *V* (Å$^3$) | 4770.6(17) |
| molecules per cell *z* | 4 |
| crystallographic density $\rho_{calcd}$ (g cm$^{-3}$) | 1.481 |
| absorption coefficient $\mu$ (mm$^{-1}$) | 3.118 |
| | |
| diffractometer | STOE IPDS 2T |
| radiation ($\lambda$[Å]) | graphite-monochromated Mo-$K_\alpha$ (0.71073) |
| temperature (°C) | -173.15 |
| scan type | $\omega$ scan (increment 1.5°, exposure 15 min) |
| completeness of dataset | 99.7 % |
| $\theta$ range of data collection (deg) | 1.942 to 29.279 |
| reflections collected | 48052 |
| independent reflections | 12657 |
| structure solution method | dual-space structure solution (SHELXT) |
| refinement method | full-matrix least-squares on $F^2$ (SHELXL 2016/4) |
| absorption correction method | empirical |
| range of transmission factors | 1.407 and 0.766 |
| data / parameters / restraints | 12657 / 876 / 470 |
| goodness of fit (GooF) [all data] | 1.037 |
| final *R* values | |
| $R_1$ [all data, $I \geq 2\sigma(I)$] | 0.0388, 0.0286 |
| $wR_2$ [all data, $I \geq 2\sigma(I)$]] | 0.0633, 0.0609 |
| largest difference peak and hole | 1.096 and -1.238 eÅ$^{-3}$ |

Refinement special details: Large positive and negative residual density peaks due to inefficient absorption correction

# STRUCTURE REPORT

**Crystallographer:** F. Engelhardt
**ID code:** fe0074
**Date:** 21.8.2018
**Sample by:** Volker Lorenz
**Compound:** $Tm_2(COT'')_3$ (**4Tm**)
$Tm_2\{\mu\text{-}\eta^8\text{:}\eta^8\text{-}C_8H_6\text{-}1,5\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$
**Formula sum:** $C_{42}H_{72}Si_6Tm_2$

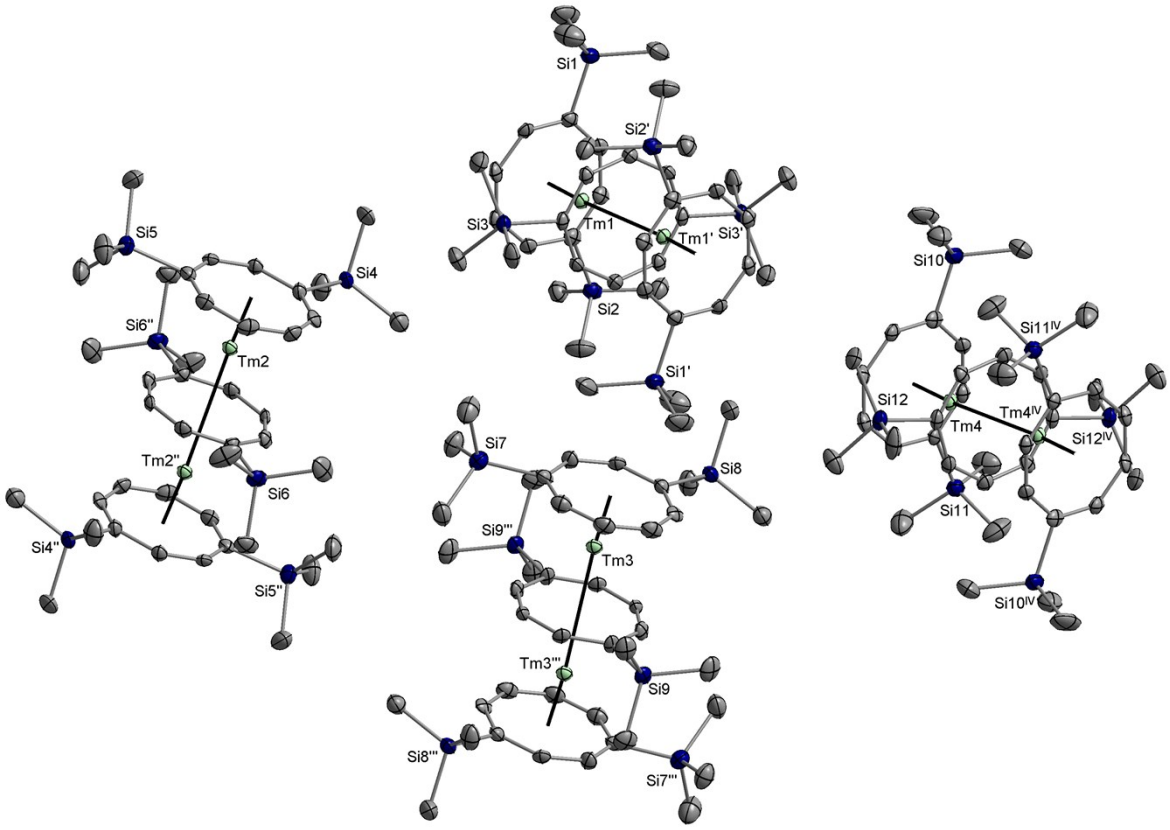



**Figure S11.** Molecular structure of **4Tm** in the crystalline state. Displacement ellipsoids of the heavier atoms with 50% probability, H atoms and disorder of $SiMe_3$ moieties omitted for clarity.

**Table S6.** Crystallographic Data and Details on Structure Refinement of **4Tm**

| | |
|---|---|
| formula sum | $C_{42}H_{72}Si_6Tm_2$ |
| formula weight | 1083.39 |
| crystal size (mm) | 0.16 x 0.10 x 0.07 mm |
| crystal system | Triclinic |
| space group | $P\bar{1}$ |
| unit cell parameters | |
| *a* (Å) | 13.092(3) |
| *b* (Å) | 18.108(6) |
| *c* (Å) | 20.921(5) |
| *α* (deg) | 73.62(2) |
| *β* (deg) | 86.14(2) |
| *γ* (deg) | 89.80(2) |
| unit cell volume *V* (Å$^3$) | 4747(2) |
| molecules per cell *z* | 4 |
| crystallographic density $\rho_{calcd}$ (g cm$^{-3}$) | 1.516 |
| absorption coefficient $\mu$ (mm$^{-1}$) | 3.892 |
| | |
| diffractometer | STOE IPDS 2T |
| radiation ($\lambda$[Å]) | graphite-monochromated Mo-$K_\alpha$ (0.71073) |
| temperature (°C) | -173.15 |
| scan type | $\omega$ scan (increment 1.5°, exposure 1 min) |
| completeness of dataset | 99.5% |
| $\theta$ range of data collection (deg) | 1.920 to 26.371 |
| reflections collected | 39793 |
| independent reflections | 19326 |
| independent reflections with $I>2\sigma(I)$ | 15761 |
| structure solution method | dual-space structure solution (SHELXT) |
| refinement method | full-matrix least-squares on $F^2$ (SHELXL 2016/4) |
| absorption correction method | Numerical |
| range of transmission factors | 0.5492 and 0.4573 |
| data / parameters / restraints | 19326 / 937 /0 |
| goodness of fit (GooF) [all data] | 1.158 |
| final *R* values | |
| $R_1$ [all data, $I \geq 2\sigma(I)$] | 0.0725, 0.0572 |
| $wR_2$ [all data, $I \geq 2\sigma(I)$]] | 0.1514, 0.1429 |
| largest difference peak and hole | 5.079 and -2.082 eÅ$^{-3}$ |

Refinement special details:
The large residual density peaks are related to a very low-occupied disorder (~2.3 %). Due to the large number of electrons in thulium, the disorder is not resolvable for the organic components.

# STRUCTURE REPORT

**Crystallographer:** P. Liebing
**ID code:** li0238
**Date:** 10.02.16
**Sample by:** Volker Lorenz
**Compound:** $Lu_2(COT")_3$ (**4Lu**)
$Lu_2\{\mu\text{-}\eta^4\text{:}\eta^4\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}\{\eta^8\text{-}C_8H_6\text{-}1,4\text{-}(SiMe_3)_2\}_2$
**Formula sum:** $C_{42}H_{72}Lu_2Si_6$

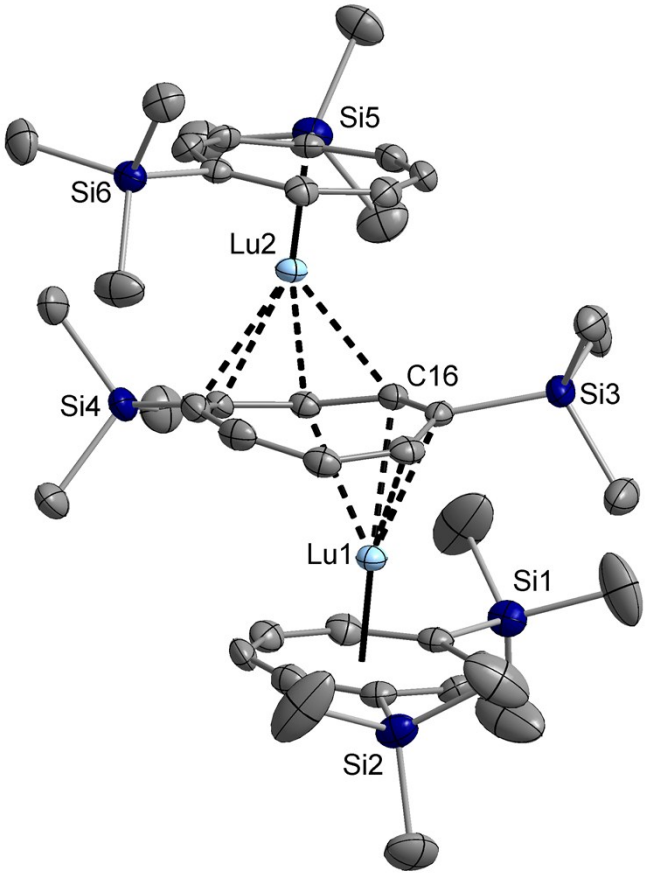



**Figure S12.** Molecular structure of **4Lu** in the crystalline state. Displacement ellipsoids drawn at the 50% probability level, H atoms omitted for clarity.

**Table S7. Crystallographic Data and Details on Structure Refinement**

| | |
|---|---|
| formula sum | $C_{42}H_{72}Lu_2Si_6$ |
| formula weight | 1095.47 |
| crystal color / shape / size (mm) | colorless prisms / 0.41 × 0.25 × 0.16 |
| crystal system | monoclinic |
| space group | $P2_1/c$ |
| unit cell parameters | |
| *a* (Å) | 9.8651(3) |
| *b* (Å) | 39.2173(9) |
| *c* (Å) | 12.3474(4) |
| *α* (deg) | 90 |
| *β* (deg) | 92.598(3) |
| *γ* (deg) | 90 |
| unit cell volume *V* (Å$^3$) | 4772.1(2) |
| molecules per cell *z* | 4 |
| crystallographic density $\rho_{calcd}$ (g cm$^{-3}$) | 1.525 |
| absorption coefficient $\mu$ (mm$^{-1}$) | 4.291 |
| | |
| diffractometer | STOE IPDS 2T |
| radiation ($\lambda$[Å]) | graphite-monochromated Mo-$K_\alpha$ (0.71073) |
| temperature (°C) | –120 |
| scan type | ω scan (increment 1.5°, exposure 1 min) |
| completeness of dataset | 99.4% |
| *θ* range of data collection (deg) | 2.067 … 25.084 |
| reflections collected | 24021 ($-11 \le h \le 11$, $-46 \le k \le 41$, $-14 \le l \le 14$) |
| independent reflections | 8445 ($R_{int}$ = 0.0423) |
| independent reflections with $I>2\sigma(I)$ | 7340 |
| structure solution method | heavy atom methods (SIR-97) |
| refinement method | full-matrix least-squares on $F^2$ (SHELXL 2016/4) |
| absorption correction method | numerical |
| range of transmission factors | 0.2449 – 0.5579 |
| data / parameters / restraints | 8445 / 470 / 0 |
| goodness of fit (GooF) [all data] | 1.080 |
| final *R* values [a] | |
| $R_1$ [all data, $I \ge 2\sigma(I)$] | 0.0397, 0.0322 |
| $wR_2$ [all data, $I \ge 2\sigma(I)$]] | 0.0661, 0.0643 |
| largest difference peak and hole | 0.913 and –1.059 e Å$^{-3}$ |
| Extinction coefficient | 0.00082(5) |
| Flack parameter | – |

Refinement special details: Six reflections are strongly disagreeing with the structural model and were therefore omitted for refinement.

# 5. Details on the Analysis of Close Interactions in **4Y-1,5** and **4Y-1,4**

The Hirshfeld surfaces and condensed 2-dimensional fingerprint plots have been calculated with Crystal Explorer by Spackman et al.[S4] The crystallographic information files (CIFs) used as input have been modified to only contain the major part if disorder was present.

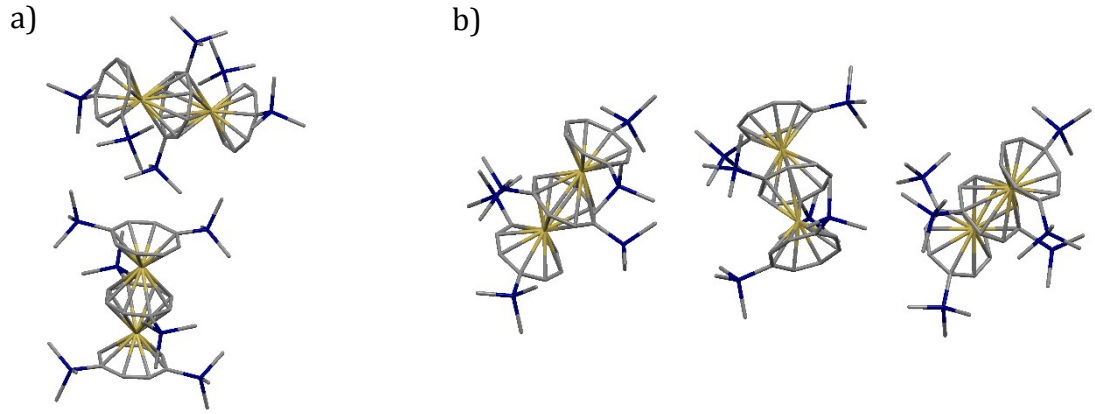



**Figure S13.** Asymmetric units of **4Y-1,5** (a) and **4Y-1,4** (b). Disorder of the methyl groups and hydrogen atoms have been omitted for clarity.

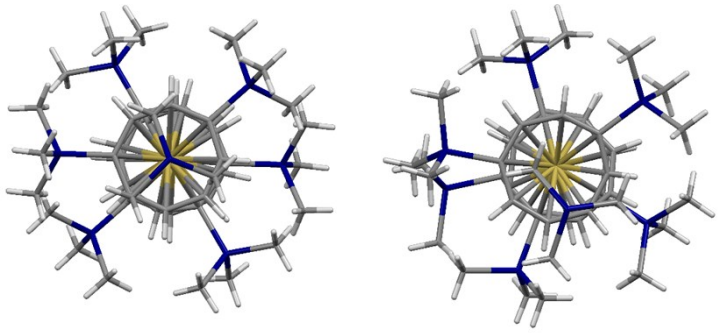


**Figure S14.** View along the Y-Y axis of the structures **4Y-1,5** (left) and **4Y-1,4** (right). Also shown is the $SiMe_3$ group facing the top-deck COT" ring.

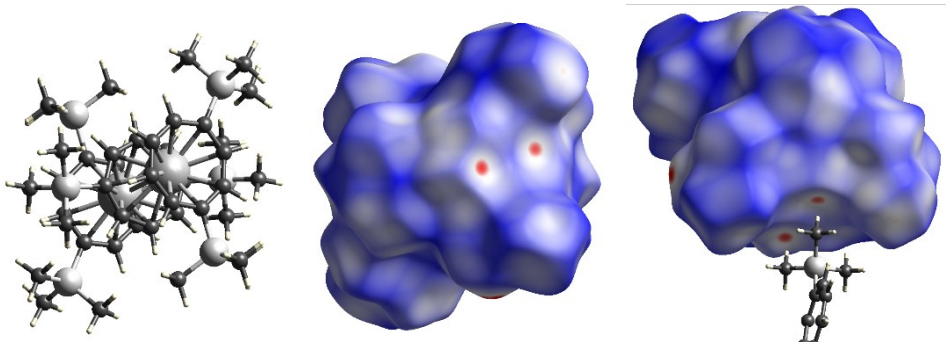


**Figure S15.** Orientation of a triple decker of **4Y-1,5** (left), corresponding Hirshfeld surface with $d_{norm}$ mapped on it (middle) and neighboring $SiMe_3$ group matching the C-H regions of high hydrogen interactions donor and acceptor capability marked in red (right)

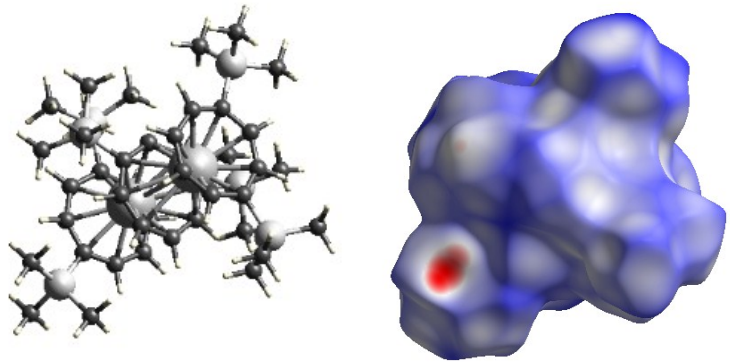


**Figure S16.** Orientation of a triple decker of **4Y-1,4**(left) and corresponding Hirshfeld surface with $d_{norm}$ mapped on it. Red regions indicate hydrogen interactions donor and acceptor capability

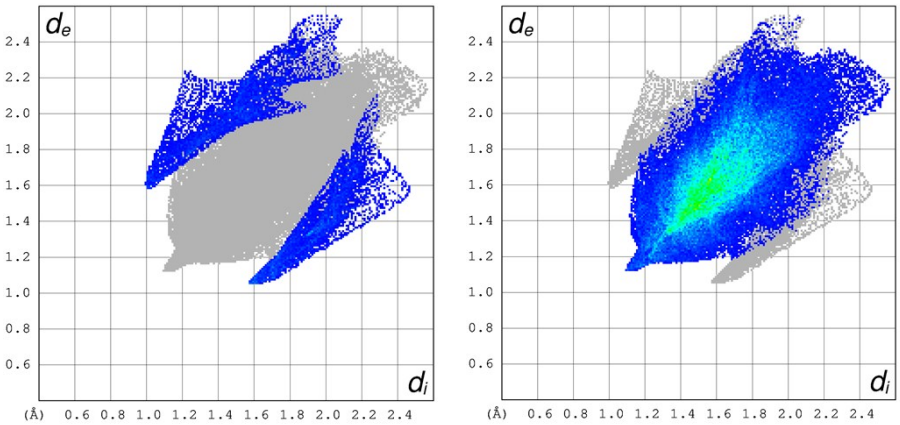



**Figure S17.** Fingerprint plots for **4Y-1,5**. Left: Interactions from C to H or Vice versa are highlighted; right: Interactions from H to H are highlighted.

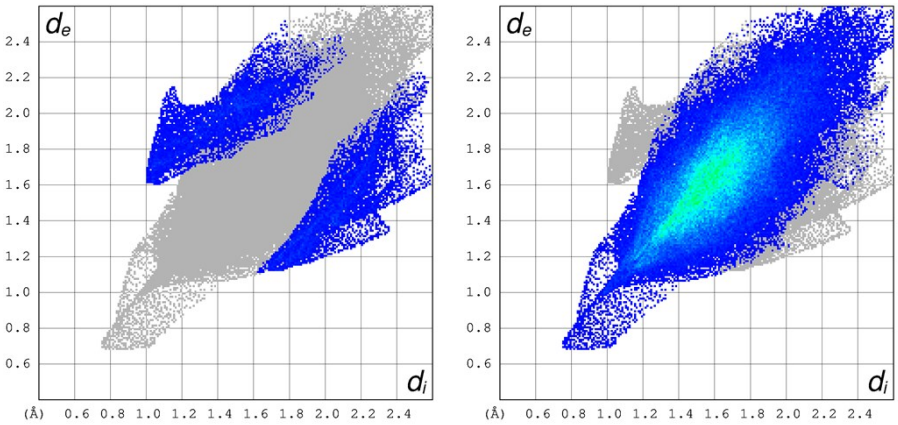



**Figure S18.** Fingerprint plots for **4Y-1,4**. Left: Interactions from C to H or *vice versa* are highlighted; right: Interactions from H to H are highlighted.

# 6. Computational details

**Computational details**

Calculations were carried out at the DFT level using the hybrid functional B3PW91[S5] with the Gaussian 09[S6] suite of programs. The rare earth center was treated with a small-core relativistic pseudopotential (RECP) ([Ar] + 3d)[S7] in combination with its adapted basis set (segmented basis set that includes up to g functions). Silicon atoms have been treated with the small core Stuttgart-Dresden effective core potential associated with its adapted basis set and additional *d* polarization functions.[S8] Polarized all-electron triple-ζ 6-311G(d,p)[S9] basis sets were used for C, H. Geometry optimization was carried out without any symmetry restriction. The nature of the extrema (minimum) was verified with analytical frequency calculations. The NBO analysis[S10] was finally carried out on the optimized geometry.

**$Sc_2$(1,4-COT)3:**

| | | | |
|---|---|---|---|
| Si | 5.929265 | 7.312739 | 25.091833 |
| C | 7.294516 | 6.298804 | 25.930301 |
| C | 6.713881 | 8.891867 | 24.385651 |
| C | 5.205617 | 6.309337 | 23.652634 |
| C | 4.494204 | 7.685035 | 26.296534 |
| C | 4.554527 | 7.002997 | 27.536921 |
| C | 3.728044 | 6.901586 | 28.677077 |
| C | 2.482855 | 7.437615 | 29.066289 |
| C | 1.559578 | 8.346411 | 28.509470 |
| C | 1.466201 | 9.100498 | 27.310638 |
| Si | -0.138779 | 10.130265 | 27.215391 |
| C | -0.116296 | 11.325124 | 25.742572 |
| Sc | 3.760795 | 9.197060 | 28.058444 |
| C | 4.790241 | 11.301076 | 28.399851 |
| C | 5.897485 | 10.489587 | 28.031786 |
| C | 6.756341 | 9.643389 | 28.752394 |
| C | 6.902961 | 9.268592 | 30.097326 |
| C | 6.055888 | 9.157493 | 31.212330 |
| C | 4.664859 | 9.381998 | 31.409272 |
| Si | 3.899090 | 8.326707 | 32.808680 |
| C | 4.788537 | 8.584349 | 34.465504 |
| C | 3.540510 | 8.589618 | 25.761248 |
| C | 2.317482 | 9.172471 | 26.175357 |
| C | 3.943326 | 11.156145 | 29.546422 |
| C | 3.800256 | 10.223371 | 30.634721 |
| Sc | 5.510911 | 11.547667 | 31.803227 |
| C | 7.716714 | 12.476432 | 31.836871 |
| C | 6.929097 | 13.267809 | 30.973510 |
| C | 5.627697 | 13.810092 | 31.024907 |
| C | 4.541778 | 13.745515 | 31.922977 |
| C | 4.279834 | 13.116839 | 33.167108 |

| | | | |
|---|---|---|---|
| C | 5.100838 | 12.317559 | 34.006437 |
| C | 6.433481 | 11.835503 | 33.992881 |
| C | 7.546728 | 11.886793 | 33.116128 |
| Si | 9.140728 | 11.037924 | 33.745341 |
| C | 10.456200 | 12.391134 | 33.940390 |
| Si | 2.530576 | 13.502314 | 33.828560 |
| C | 2.119829 | 12.480186 | 35.372218 |
| C | 1.205575 | 13.176240 | 32.508103 |
| C | 2.486328 | 15.341321 | 34.292949 |
| C | -1.584883 | 8.922319 | 26.997277 |
| C | -0.419431 | 11.130198 | 28.805238 |
| Si | 4.534679 | 12.797519 | 27.233119 |
| C | 6.096846 | 13.880073 | 27.224911 |
| C | 4.283717 | 12.265330 | 25.429497 |
| C | 3.049841 | 13.844282 | 27.776574 |
| C | 4.077514 | 6.474812 | 32.419806 |
| C | 2.061672 | 8.735566 | 33.041505 |
| C | 9.787512 | 9.731034 | 32.531375 |
| C | 8.868610 | 10.208116 | 35.428654 |
| H | 2.000111 | 9.930637 | 25.465281 |
| H | 3.872440 | 9.043539 | 24.828922 |
| H | 5.504217 | 6.504375 | 27.704669 |
| H | 4.212979 | 6.361418 | 29.484587 |
| H | 2.239505 | 7.194129 | 30.096166 |
| H | 0.783724 | 8.596157 | 29.231019 |
| H | -1.358644 | 11.690163 | 28.734749 |
| H | 0.387898 | 11.849470 | 28.973646 |
| H | -0.488233 | 10.489691 | 29.689993 |
| H | -1.044077 | 11.908014 | 25.740923 |
| H | -0.063303 | 10.795694 | 24.785877 |
| H | 0.717149 | 12.033147 | 25.788741 |
| H | -2.541672 | 9.453716 | 26.950503 |

| | | | |
|---|---|---|---|
| H | -1.632891 | 8.212061 | 27.828969 |
| H | -1.470766 | 8.344481 | 26.074521 |
| H | 7.221771 | 9.468809 | 25.165064 |
| H | 5.978622 | 9.543362 | 23.903182 |
| H | 7.460384 | 8.626484 | 23.628469 |
| H | 7.715778 | 6.818536 | 26.796800 |
| H | 8.107577 | 6.130688 | 25.215444 |
| H | 6.938442 | 5.317260 | 26.258420 |
| H | 5.975688 | 6.056527 | 22.915612 |
| H | 4.418628 | 6.871610 | 23.139588 |
| H | 4.762827 | 5.376619 | 24.016532 |
| H | 3.093304 | 11.835715 | 29.524620 |
| H | 2.801784 | 10.301352 | 31.060414 |
| H | 6.545494 | 8.669025 | 32.055437 |
| H | 7.893951 | 8.865430 | 30.299353 |
| H | 7.577738 | 9.279073 | 28.135909 |
| H | 6.227548 | 10.639898 | 27.004069 |
| H | 3.172527 | 14.232344 | 28.792764 |
| H | 2.112701 | 13.280021 | 27.739802 |
| H | 2.943184 | 14.703624 | 27.105556 |
| H | 6.272352 | 14.382680 | 28.179522 |
| H | 6.011067 | 14.653615 | 26.453401 |
| H | 6.981789 | 13.277622 | 26.995852 |
| H | 4.261512 | 13.153586 | 24.787951 |
| H | 3.346365 | 11.721440 | 25.292349 |
| H | 5.101037 | 11.626645 | 25.081070 |
| H | 1.650091 | 8.116708 | 33.846306 |
| H | 1.475862 | 8.534295 | 32.138943 |
| H | 1.908586 | 9.782920 | 33.319785 |
| H | 4.396147 | 7.874853 | 35.202894 |
| H | 4.636691 | 9.595543 | 34.849865 |
| H | 5.865707 | 8.410599 | 34.382059 |

| | | | |
|---|---|---|---|
| H | 3.803495 | 5.884463 | 33.301406 |
| H | 5.111749 | 6.226377 | 32.160657 |
| H | 3.436070 | 6.153167 | 31.595231 |
| H | 4.554936 | 11.902300 | 34.849328 |
| H | 6.598110 | 11.167910 | 34.833885 |
| H | 8.649613 | 12.191833 | 31.353491 |
| H | 7.399659 | 13.415234 | 30.005493 |
| H | 5.349802 | 14.287992 | 30.090844 |
| H | 3.658192 | 14.210319 | 31.488544 |
| H | 1.499576 | 15.631084 | 34.670442 |
| H | 2.715471 | 15.972065 | 33.428093 |
| H | 3.226012 | 15.562073 | 35.069241 |
| H | 1.105877 | 12.729175 | 35.704428 |
| H | 2.798673 | 12.702365 | 36.201775 |
| H | 2.148945 | 11.402243 | 35.184954 |
| H | 0.214484 | 13.439262 | 32.894093 |
| H | 1.183837 | 12.121238 | 32.218249 |
| H | 1.371674 | 13.770057 | 31.603866 |
| H | 8.556187 | 10.925798 | 36.193826 |
| H | 9.811428 | 9.760675 | 35.762464 |
| H | 8.123188 | 9.407507 | 35.385237 |
| H | 10.124272 | 13.154467 | 34.651396 |
| H | 10.654436 | 12.890472 | 32.986737 |
| H | 11.401045 | 11.973470 | 34.304875 |
| H | 10.771381 | 9.372428 | 32.853930 |
| H | 9.893480 | 10.127017 | 31.516906 |
| H | 9.113215 | 8.870136 | 32.489158 |

**$Sc_2$(1,5-COT)(1,4-COT)$_2$:**

| | | | |
|---|---|---|---|
| C | 7.073005 | 6.332443 | 26.905068 |
| Si | 5.724030 | 6.934224 | 25.715202 |
| C | 4.211043 | 7.615787 | 26.662179 |

| | | | |
|---|---|---|---|
| C | 3.423148 | 8.536961 | 25.924590 |
| C | 2.239679 | 9.286482 | 26.137264 |
| Sc | 3.485505 | 9.371984 | 28.156672 |
| C | 5.955897 | 10.517537 | 28.020126 |
| C | 6.816577 | 9.897146 | 28.941604 |
| C | 6.779769 | 9.476355 | 30.283410 |
| C | 5.729180 | 9.148742 | 31.188715 |
| Sc | 5.724954 | 11.467118 | 31.767441 |
| C | 6.872902 | 11.751746 | 33.849487 |
| C | 7.839159 | 12.089803 | 32.866873 |
| Si | 9.657040 | 11.665536 | 33.279640 |
| C | 9.804913 | 10.725298 | 34.921394 |
| C | 6.487646 | 8.225576 | 24.551881 |
| C | 5.121002 | 5.469119 | 24.669240 |
| C | 4.047720 | 7.067249 | 27.961439 |
| C | 3.089097 | 7.165220 | 28.993579 |
| C | 1.897613 | 7.889214 | 29.197694 |
| C | 1.168236 | 8.841918 | 28.457759 |
| C | 1.285605 | 9.447713 | 27.178117 |
| Si | -0.179356 | 10.613738 | 26.800485 |
| C | -0.442201 | 11.873803 | 28.197033 |
| C | 0.064372 | 11.532055 | 25.158936 |
| C | -1.737530 | 9.540070 | 26.658653 |
| C | 4.813253 | 11.361290 | 28.143915 |
| Si | 4.714686 | 12.728440 | 26.816158 |
| C | 3.137461 | 13.763386 | 27.008410 |
| C | 3.938914 | 11.447479 | 29.255102 |
| C | 3.704069 | 10.617960 | 30.398036 |
| C | 4.381677 | 9.582238 | 31.118054 |
| C | 7.732320 | 12.770862 | 31.626203 |
| C | 6.717613 | 13.459507 | 30.929386 |
| C | 5.367236 | 13.767571 | 31.189873 |

| | | | |
|---|---|---|---|
| C | 4.439628 | 13.458777 | 32.208712 |
| C | 4.446937 | 12.690596 | 33.399673 |
| Si | 2.782697 | 12.581192 | 34.332061 |
| C | 3.013911 | 13.389075 | 36.032877 |
| C | 5.486868 | 11.971775 | 34.052247 |
| C | 10.566018 | 13.319927 | 33.477248 |
| C | 10.504750 | 10.680489 | 31.895893 |
| C | 2.237903 | 10.778952 | 34.571864 |
| C | 1.407908 | 13.500512 | 33.403871 |
| C | 6.204313 | 13.889748 | 27.020749 |
| C | 4.785302 | 12.024027 | 25.057136 |
| H | 2.083892 | 9.986967 | 25.321103 |
| H | 3.900067 | 8.845085 | 24.997431 |
| H | 4.906258 | 6.489505 | 28.291769 |
| H | 3.411595 | 6.651495 | 29.893072 |
| H | 1.527906 | 7.789208 | 30.215270 |
| H | 0.368165 | 9.268636 | 29.060486 |
| H | -1.304540 | 12.511440 | 27.972403 |
| H | 0.430392 | 12.521608 | 28.323171 |
| H | -0.639839 | 11.384264 | 29.155978 |
| H | -0.790293 | 12.196460 | 24.990074 |
| H | 0.110068 | 10.837506 | 24.313832 |
| H | 0.968504 | 12.147871 | 25.143609 |
| H | -2.622156 | 10.152389 | 26.452107 |
| H | -1.920498 | 8.983835 | 27.583611 |
| H | -1.631768 | 8.811114 | 25.848847 |
| H | 6.885435 | 9.081287 | 25.105741 |
| H | 5.776277 | 8.599206 | 23.809098 |
| H | 7.318160 | 7.767705 | 24.002705 |
| H | 7.347459 | 7.111544 | 27.623100 |
| H | 7.968453 | 6.066837 | 26.332303 |
| H | 6.768807 | 5.440785 | 27.462154 |

| | | | |
|---|---|---|---|
| H | 5.942657 | 5.020653 | 24.099975 |
| H | 4.351065 | 5.788150 | 23.959167 |
| H | 4.684478 | 4.692163 | 25.305178 |
| H | 3.182042 | 12.224564 | 29.176809 |
| H | 2.742443 | 10.845899 | 30.854004 |
| H | 7.756999 | 9.138953 | 30.622570 |
| H | 7.786345 | 9.682146 | 28.489965 |
| H | 6.389303 | 10.535514 | 27.020398 |
| H | 3.104491 | 14.288898 | 27.968599 |
| H | 2.233569 | 13.154371 | 26.921623 |
| H | 3.103015 | 14.523723 | 26.220407 |
| H | 6.132319 | 14.468411 | 27.947000 |
| H | 6.256422 | 14.600339 | 26.188362 |
| H | 7.142978 | 13.327405 | 27.044303 |
| H | 4.831703 | 12.844958 | 24.332779 |
| H | 3.900752 | 11.421729 | 24.834466 |
| H | 5.667880 | 11.396613 | 24.901367 |
| H | 5.129326 | 11.385281 | 34.897678 |
| H | 7.266231 | 11.073672 | 34.603134 |
| H | 8.634127 | 12.698480 | 31.021168 |
| H | 7.023914 | 13.743464 | 29.927250 |
| H | 4.889672 | 14.247226 | 30.339809 |
| H | 3.444851 | 13.796266 | 31.932128 |
| H | 2.089800 | 13.346421 | 36.619582 |
| H | 3.299703 | 14.440224 | 35.924043 |
| H | 3.800264 | 12.889863 | 36.607859 |
| H | 1.308869 | 10.736261 | 35.151190 |
| H | 2.988656 | 10.188465 | 35.105146 |
| H | 2.054555 | 10.297242 | 33.605739 |
| H | 0.481072 | 13.436953 | 33.984711 |
| H | 1.207340 | 13.067915 | 32.418225 |
| H | 1.640567 | 14.561916 | 33.272191 |

| | | | |
|---|---|---|---|
| H | 9.403914 | 11.314272 | 35.752635 |
| H | 10.864935 | 10.542566 | 35.130352 |
| H | 9.301609 | 9.754068 | 34.916302 |
| H | 10.118740 | 13.912471 | 34.281777 |
| H | 10.512712 | 13.913496 | 32.559168 |
| H | 11.623140 | 13.161982 | 33.717639 |
| H | 11.577072 | 10.593163 | 32.103762 |
| H | 10.396799 | 11.170472 | 30.923118 |
| H | 10.094468 | 9.670467 | 31.811481 |
| H | 3.727884 | 9.144193 | 31.870096 |
| Si | 6.115844 | 7.763994 | 32.445520 |
| C | 5.146187 | 7.984281 | 34.060837 |
| C | 5.649444 | 6.074668 | 31.710134 |
| C | 7.965427 | 7.710068 | 32.846971 |
| H | 5.359384 | 7.148267 | 34.736188 |
| H | 5.430815 | 8.911491 | 34.566985 |
| H | 4.064372 | 8.004598 | 33.896909 |
| H | 8.143730 | 6.978528 | 33.642833 |
| H | 8.565822 | 7.407105 | 31.983635 |
| H | 8.325566 | 8.681596 | 33.193939 |
| H | 6.016752 | 5.267811 | 32.354403 |
| H | 4.565276 | 5.956091 | 31.620905 |
| H | 6.092501 | 5.941589 | 30.718307 |

**$Y_2$(1,4-COT)$_3$:**

| | | | |
|---|---|---|---|
| C | 8.797991 | 12.516967 | 12.526997 |
| Si | 7.333471 | 13.415286 | 11.722640 |
| C | 7.560157 | 13.357512 | 9.839188 |
| C | 5.672561 | 12.577186 | 12.139654 |
| C | 5.755144 | 11.349033 | 12.852144 |
| C | 4.850893 | 10.366756 | 13.330543 |
| C | 3.445460 | 10.143644 | 13.294211 |

| | | | |
|---|---|---|---|
| Si | 2.915363 | 8.503858 | 14.110920 |
| C | 3.252102 | 7.095663 | 12.884097 |
| Y | 3.819329 | 12.583587 | 13.952996 |
| C | 2.272905 | 12.082439 | 11.958611 |
| C | 3.170268 | 13.072128 | 11.499223 |
| C | 4.564518 | 13.280974 | 11.589033 |
| C | 4.060732 | 12.262772 | 16.580438 |
| C | 2.668714 | 12.195460 | 16.381969 |
| C | 1.685085 | 12.982913 | 15.725567 |
| C | 1.655399 | 14.178977 | 14.955070 |
| C | 2.591398 | 15.222405 | 14.693939 |
| C | 3.938954 | 15.360414 | 15.159227 |
| Y | 2.164688 | 15.278893 | 17.256516 |
| C | 0.579414 | 17.016008 | 18.119976 |
| C | 1.881125 | 17.547652 | 18.321020 |
| C | 3.133943 | 17.082530 | 18.814224 |
| C | 3.536102 | 15.819748 | 19.326932 |
| C | 2.906483 | 14.576104 | 19.575924 |
| C | 1.600875 | 14.057397 | 19.416010 |
| C | 0.378362 | 14.548220 | 18.903544 |
| C | -0.080089 | 15.772745 | 18.340633 |
| Si | -1.925655 | 15.704342 | 17.855421 |
| C | -2.944845 | 15.517582 | 19.444241 |
| C | 5.048410 | 13.251196 | 16.343413 |
| C | 4.923470 | 14.556482 | 15.802847 |
| C | 7.347881 | 15.231938 | 12.279142 |
| C | -2.469484 | 17.283027 | 16.954954 |
| C | -2.279785 | 14.219339 | 16.723540 |
| Si | 1.987450 | 16.632271 | 13.541032 |
| C | 1.597244 | 18.214042 | 14.515109 |
| C | 3.335114 | 17.058586 | 12.278803 |
| C | 0.420371 | 16.096212 | 12.618554 |

| | | | |
|---|---|---|---|
| Si | 4.476992 | 18.439825 | 18.832039 |
| C | 4.042428 | 19.676667 | 20.203586 |
| C | 4.560107 | 19.373789 | 17.179637 |
| C | 6.194324 | 17.712165 | 19.176379 |
| C | 2.385942 | 10.886284 | 12.704275 |
| C | 3.889808 | 8.157019 | 15.704907 |
| C | 1.065807 | 8.511326 | 14.543962 |
| H | 6.762126 | 11.138986 | 13.202978 |
| H | 5.375581 | 9.643574 | 13.951351 |
| H | 1.403655 | 10.485554 | 12.940156 |
| H | 4.841657 | 14.244735 | 11.164341 |
| H | 1.235254 | 12.354626 | 11.779149 |
| H | 2.654248 | 13.914626 | 11.044422 |
| H | 4.313939 | 7.058076 | 12.619639 |
| H | 2.685271 | 7.246160 | 11.959593 |
| H | 2.970926 | 6.123171 | 13.302831 |
| H | 3.730432 | 8.944394 | 16.448183 |
| H | 4.966065 | 8.071532 | 15.525932 |
| H | 3.556394 | 7.209065 | 16.141870 |
| H | 0.432092 | 8.531551 | 13.651673 |
| H | 0.800650 | 9.368926 | 15.171032 |
| H | 0.818010 | 7.600062 | 15.099340 |
| H | 6.746082 | 13.878801 | 9.325281 |
| H | 7.564749 | 12.321179 | 9.486147 |
| H | 8.504021 | 13.825380 | 9.538459 |
| H | 8.885254 | 11.485124 | 12.171276 |
| H | 8.730470 | 12.497869 | 13.619181 |
| H | 9.726149 | 13.035686 | 12.262366 |
| H | 7.220343 | 15.309488 | 13.363438 |
| H | 6.544204 | 15.805340 | 11.806551 |
| H | 8.297118 | 15.709279 | 12.011664 |
| H | -0.048136 | 17.736414 | 17.602067 |

| | | | |
|---|---|---|---|
| H | 1.940981 | 18.552653 | 17.906637 |
| H | 4.603071 | 15.758616 | 19.521128 |
| H | -0.364467 | 13.753422 | 18.856177 |
| H | 3.614212 | 13.814373 | 19.891747 |
| H | 1.553906 | 12.995205 | 19.642793 |
| H | 0.770730 | 18.067227 | 15.217138 |
| H | 1.312514 | 19.014255 | 13.822118 |
| H | 2.466659 | 18.557996 | 15.083170 |
| H | 2.976575 | 17.841276 | 11.601304 |
| H | 3.602180 | 16.183321 | 11.680595 |
| H | 4.245844 | 17.428559 | 12.759815 |
| H | 4.022634 | 19.179096 | 21.178574 |
| H | 3.054139 | 20.116820 | 20.035369 |
| H | 4.773343 | 20.491252 | 20.250174 |
| H | 3.611005 | 19.855269 | 16.924167 |
| H | 4.834327 | 18.701274 | 16.360061 |
| H | 5.320030 | 20.161405 | 17.235590 |
| H | 6.464939 | 16.950941 | 18.437584 |
| H | 6.264417 | 17.265432 | 20.173142 |
| H | 6.942527 | 18.510514 | 19.121347 |
| H | 0.574407 | 15.163897 | 12.066314 |
| H | 0.145480 | 16.872775 | 11.896285 |
| H | -0.434233 | 15.960068 | 13.289451 |
| H | -2.788482 | 16.377527 | 20.103548 |
| H | -2.651246 | 14.619006 | 19.996349 |
| H | -4.015480 | 15.444901 | 19.224356 |
| H | -1.905388 | 17.448870 | 16.031192 |
| H | -2.365419 | 18.172048 | 17.585238 |
| H | -3.527339 | 17.195335 | 16.683855 |
| H | -1.980533 | 13.272968 | 17.185290 |
| H | -1.744783 | 14.314607 | 15.772785 |
| H | -3.350927 | 14.154767 | 16.502137 |

| | | | |
|---|---|---|---|
| H | 0.689975 | 14.321844 | 14.478814 |
| H | 0.713557 | 12.496354 | 15.733973 |
| H | 2.237087 | 11.277699 | 16.772947 |
| H | 5.860644 | 15.106428 | 15.840008 |
| H | 4.379979 | 16.307323 | 14.853310 |
| H | 4.439397 | 11.356050 | 17.047572 |
| Si | 6.745933 | 12.798537 | 17.095685 |
| C | 8.090229 | 14.034290 | 16.585101 |
| C | 6.601305 | 12.819188 | 18.989696 |
| C | 7.278360 | 11.056835 | 16.565569 |
| H | 8.231158 | 10.794786 | 17.039178 |
| H | 6.544965 | 10.298330 | 16.856621 |
| H | 7.409219 | 10.998145 | 15.481162 |
| H | 7.551735 | 12.542715 | 19.459409 |
| H | 6.325777 | 13.816683 | 19.346303 |
| H | 5.838409 | 12.114197 | 19.335933 |
| H | 9.054924 | 13.700456 | 16.983079 |
| H | 8.188609 | 14.111755 | 15.498183 |
| H | 7.905235 | 15.037154 | 16.983540 |

**$Y_2$(1,5-COT)(1,4-COT)$_2$:**

| | | | |
|---|---|---|---|
| C | 5.326367 | 9.339080 | 16.653977 |
| Si | 5.173882 | 11.028311 | 17.503968 |
| C | 4.334105 | 10.758353 | 19.184894 |
| C | 6.914624 | 11.719589 | 17.803136 |
| C | 4.128409 | 12.236278 | 16.456299 |
| C | 4.637254 | 13.548458 | 16.260930 |
| C | 4.224029 | 14.683977 | 15.489717 |
| Y | 4.415468 | 12.509980 | 13.900062 |
| C | 6.695292 | 12.133137 | 12.840630 |
| Si | 8.545056 | 12.252723 | 13.298491 |
| C | 9.151466 | 10.682651 | 14.174090 |

| | | | |
|---|---|---|---|
| Y | 2.313082 | 15.261038 | 17.312671 |
| C | 0.272254 | 15.684783 | 18.837565 |
| Si | -1.626033 | 15.503228 | 18.936449 |
| C | -2.514111 | 16.948343 | 18.084394 |
| C | 2.840508 | 11.734906 | 16.108548 |
| C | 1.589823 | 12.320870 | 15.825838 |
| C | 1.088741 | 13.579804 | 15.436801 |
| C | 1.661430 | 14.750660 | 14.864385 |
| Si | 0.487347 | 15.895735 | 13.882166 |
| C | 0.796931 | 15.692382 | 12.020317 |
| C | 3.033573 | 15.122520 | 14.821988 |
| C | 0.751533 | 16.943086 | 18.377853 |
| C | 2.013203 | 17.575410 | 18.213620 |
| C | 3.377852 | 17.260518 | 18.483211 |
| Si | 4.564385 | 18.685131 | 18.028859 |
| C | 4.304715 | 19.244773 | 16.231748 |
| C | 3.694016 | 13.214681 | 11.556117 |
| C | 3.106080 | 11.949962 | 11.800121 |
| C | 3.546068 | 10.696883 | 12.311328 |
| Si | 2.219689 | 9.323699 | 12.268233 |
| C | 2.395861 | 8.131532 | 13.735399 |
| C | 4.967106 | 13.793583 | 11.757938 |
| C | 6.195037 | 13.352993 | 12.301300 |
| C | 6.090135 | 10.854203 | 13.014632 |
| C | 4.814666 | 10.270407 | 12.795861 |
| C | 0.470569 | 10.059509 | 12.317263 |
| C | 2.436436 | 8.342076 | 10.658220 |
| C | 8.880115 | 13.750480 | 14.419908 |
| C | 9.529310 | 12.471705 | 11.691673 |
| C | 0.949501 | 14.532834 | 19.327976 |
| C | 2.291109 | 14.185493 | 19.610286 |
| C | 3.538296 | 14.844101 | 19.509045 |

| | | | |
|---|---|---|---|
| C | 3.983359 | 16.105770 | 19.048147 |
| C | -1.326386 | 15.470427 | 14.223878 |
| C | 0.789118 | 17.719153 | 14.318220 |
| C | 6.379023 | 18.169881 | 18.231664 |
| C | 4.206263 | 20.147048 | 19.183321 |
| C | -2.219631 | 13.870897 | 18.167858 |
| C | -2.101161 | 15.514110 | 20.773497 |
| H | 6.747151 | 10.149961 | 13.518292 |
| H | 4.792939 | 9.258687 | 13.194987 |
| H | 2.040406 | 11.973600 | 11.588043 |
| H | 6.903820 | 14.176544 | 12.375410 |
| H | 2.965147 | 13.942133 | 11.212310 |
| H | 4.974371 | 14.857779 | 11.533126 |
| H | 5.870856 | 8.645501 | 17.304622 |
| H | 5.871395 | 9.418870 | 15.708940 |
| H | 4.349148 | 8.894963 | 16.442204 |
| H | 4.334740 | 11.678501 | 19.777119 |
| H | 4.858656 | 9.987657 | 19.760346 |
| H | 3.295220 | 10.437702 | 19.058743 |
| H | 3.431197 | 7.886847 | 10.611828 |
| H | 2.330412 | 8.997827 | 9.787889 |
| H | 1.692174 | 7.542488 | 10.575121 |
| H | 2.293789 | 8.661538 | 14.687488 |
| H | 3.355250 | 7.604963 | 13.738900 |
| H | 1.607988 | 7.371544 | 13.686439 |
| H | 0.223915 | 10.613601 | 11.405949 |
| H | 0.348816 | 10.731755 | 13.172680 |
| H | -0.262014 | 9.250550 | 12.413907 |
| H | 7.496264 | 10.997112 | 18.386244 |
| H | 6.895836 | 12.656137 | 18.370096 |
| H | 7.450154 | 11.895930 | 16.865271 |
| H | 9.208488 | 13.369530 | 11.153705 |

| | | | |
|---|---|---|---|
| H | 9.376285 | 11.614580 | 11.027999 |
| H | 10.602417 | 12.562047 | 11.892309 |
| H | 9.079059 | 9.803742 | 13.525201 |
| H | 8.597150 | 10.474513 | 15.094539 |
| H | 10.206295 | 10.805013 | 14.443660 |
| H | 8.355541 | 13.657733 | 15.376222 |
| H | 8.564254 | 14.688792 | 13.952579 |
| H | 9.952091 | 13.833295 | 14.631146 |
| H | -0.039904 | 17.566850 | 17.969577 |
| H | 1.893375 | 18.528177 | 17.698844 |
| H | 5.068788 | 16.154250 | 19.049692 |
| H | 0.290163 | 13.680116 | 19.478779 |
| H | 4.368288 | 14.186338 | 19.754529 |
| H | 2.395286 | 13.145198 | 19.906499 |
| H | 0.585338 | 17.917248 | 15.375520 |
| H | 0.131375 | 18.360064 | 13.720294 |
| H | 1.820362 | 18.022193 | 14.111316 |
| H | 0.118759 | 16.334272 | 11.446955 |
| H | 0.628532 | 14.657205 | 11.707490 |
| H | 1.822231 | 15.968324 | 11.754571 |
| H | 4.384025 | 19.866064 | 20.226427 |
| H | 3.162378 | 20.466165 | 19.099487 |
| H | 4.842840 | 21.006744 | 18.947562 |
| H | 3.272969 | 19.556756 | 16.042402 |
| H | 4.546184 | 18.436048 | 15.533655 |
| H | 4.955629 | 20.095167 | 15.999890 |
| H | 6.638232 | 17.313667 | 17.599999 |
| H | 6.621674 | 17.917325 | 19.268817 |
| H | 7.024839 | 19.004625 | 17.937664 |
| H | -1.583123 | 14.463919 | 13.878729 |
| H | -1.967154 | 16.176426 | 13.684163 |
| H | -1.574508 | 15.542310 | 15.286484 |

| | | | |
|---|---|---|---|
| H | -1.786294 | 16.451019 | 21.244529 |
| H | -1.614143 | 14.693568 | 21.310073 |
| H | -3.183645 | 15.411574 | 20.907276 |
| H | -2.244995 | 17.048513 | 17.028329 |
| H | -2.303681 | 17.900441 | 18.582486 |
| H | -3.596229 | 16.784812 | 18.135261 |
| H | -1.750317 | 13.001605 | 18.639225 |
| H | -2.000887 | 13.830222 | 17.096624 |
| H | -3.303084 | 13.769144 | 18.295833 |
| H | 0.001611 | 13.585916 | 15.424544 |
| H | 0.782965 | 11.596479 | 15.938227 |
| H | 2.741780 | 10.663111 | 16.278983 |
| H | 5.627186 | 13.710002 | 16.681085 |
| H | 5.029519 | 15.409069 | 15.385912 |
| H | 3.230615 | 16.032404 | 14.256065 |

**$La_2$(1,4-COT)$_3$:**

| | | | |
|---|---|---|---|
| La | 10.091115 | 20.492679 | -1.281210 |
| C | 11.587972 | 19.295291 | 0.983869 |
| C | 10.292559 | 19.541925 | 1.523418 |
| La | 10.362656 | 16.586917 | 1.271583 |
| C | 9.790914 | 15.478931 | 3.706383 |
| C | 11.208413 | 15.604059 | 3.718736 |
| Si | 11.973591 | 16.373231 | 5.287835 |
| C | 12.962825 | 17.941501 | 4.861906 |
| C | 12.142887 | 18.619820 | -0.143401 |
| C | 11.517792 | 17.877192 | -1.188980 |
| H | 12.224590 | 17.463303 | -1.905854 |
| C | 8.935632 | 19.235250 | 1.194858 |
| C | 8.382362 | 18.491650 | 0.113589 |
| C | 8.898011 | 17.791300 | -1.008571 |
| C | 10.187794 | 17.533212 | -1.540499 |

| | | | |
|---|---|---|---|
| C | 11.536250 | 22.490875 | -2.467954 |
| C | 11.139117 | 21.633144 | -3.526959 |
| C | 9.934073 | 21.024758 | -3.984335 |
| Si | 10.177011 | 20.023891 | -5.588697 |
| C | 8.652693 | 18.967529 | -5.997987 |
| C | 10.910678 | 23.133058 | -1.361966 |
| Si | 12.034197 | 24.225814 | -0.276326 |
| C | 11.428899 | 26.021045 | -0.388292 |
| Si | 7.680643 | 19.951846 | 2.456040 |
| C | 7.991595 | 21.805659 | 2.704426 |
| C | 7.903869 | 19.080806 | 4.125117 |
| C | 5.900348 | 19.705705 | 1.856812 |
| C | 8.767536 | 14.358324 | 1.534072 |
| Si | 7.012007 | 13.835334 | 1.006900 |
| C | 6.920965 | 13.441307 | -0.848496 |
| C | 8.803599 | 14.979843 | 2.817147 |
| C | 9.807234 | 13.982776 | 0.638054 |
| C | 11.220738 | 14.061439 | 0.633458 |
| C | 12.205995 | 14.564429 | 1.515128 |
| C | 12.198431 | 15.212800 | 2.772299 |
| C | 9.553923 | 23.156066 | -0.927466 |
| C | 8.330988 | 22.603283 | -1.375398 |
| C | 7.938206 | 21.747847 | -2.431727 |
| C | 8.598536 | 21.092469 | -3.499160 |
| C | 10.474497 | 21.235194 | -7.018884 |
| C | 11.674248 | 18.859107 | -5.457312 |
| C | 6.529084 | 12.285439 | 1.989915 |
| C | 5.737938 | 15.200908 | 1.366500 |
| C | 13.152130 | 15.110005 | 6.073426 |
| C | 10.647371 | 16.832276 | 6.564115 |
| C | 13.843619 | 24.163577 | -0.845972 |
| C | 11.963533 | 23.676285 | 1.543184 |

| | | | |
|---|---|---|---|
| H | 10.378664 | 20.140056 | 2.429027 |
| H | 12.347390 | 19.756234 | 1.609024 |
| Si | 14.051077 | 18.702094 | -0.326835 |
| H | 7.762824 | 17.999645 | 4.026533 |
| H | 8.907150 | 19.255833 | 4.527020 |
| H | 7.181375 | 19.453240 | 4.859350 |
| H | 5.628242 | 18.648972 | 1.774238 |
| H | 5.216494 | 20.162471 | 2.581244 |
| H | 5.722500 | 20.185965 | 0.889196 |
| H | 7.857951 | 22.356330 | 1.768788 |
| H | 7.287218 | 22.209882 | 3.439991 |
| H | 9.002748 | 22.006171 | 3.072606 |
| H | 7.808129 | 15.177746 | 3.213114 |
| H | 9.322310 | 15.935429 | 4.575219 |
| H | 13.208517 | 15.504194 | 3.062152 |
| H | 13.205070 | 14.498381 | 1.090927 |
| H | 11.649331 | 13.706273 | -0.301634 |
| H | 9.438194 | 13.576259 | -0.300205 |
| H | 7.537474 | 12.579682 | -1.123286 |
| H | 5.886223 | 13.199064 | -1.116179 |
| H | 7.231463 | 14.293096 | -1.462534 |
| H | 6.578219 | 12.478040 | 3.066564 |
| H | 5.511845 | 11.958216 | 1.749151 |
| H | 7.214046 | 11.460138 | 1.770815 |
| H | 5.704921 | 15.478451 | 2.424537 |
| H | 5.958247 | 16.102346 | 0.785449 |
| H | 4.735028 | 14.858735 | 1.087727 |
| H | 12.303692 | 18.717628 | 4.458444 |
| H | 13.456200 | 18.347252 | 5.751989 |
| H | 13.738365 | 17.737344 | 4.116677 |
| H | 13.619619 | 15.518222 | 6.976277 |
| H | 12.609837 | 14.200802 | 6.351749 |

| | | | |
|---|---|---|---|
| H | 13.950817 | 14.820639 | 5.383387 |
| H | 9.947963 | 17.585328 | 6.187899 |
| H | 10.069087 | 15.958190 | 6.880359 |
| H | 11.131661 | 17.247221 | 7.454981 |
| H | 10.142948 | 16.930075 | -2.443289 |
| H | 8.111487 | 17.344973 | -1.610454 |
| H | 7.297773 | 18.444587 | 0.134957 |
| H | 12.612998 | 22.644439 | -2.487613 |
| H | 12.009835 | 21.321438 | -4.103047 |
| H | 7.911265 | 20.451304 | -4.046122 |
| H | 6.885567 | 21.478670 | -2.373064 |
| H | 7.503216 | 22.836625 | -0.709299 |
| H | 9.410559 | 23.708561 | 0.000565 |
| H | 11.485295 | 26.382685 | -1.419796 |
| H | 12.035504 | 26.682899 | 0.239428 |
| H | 10.387526 | 26.109659 | -0.063079 |
| H | 14.267247 | 23.155895 | -0.786515 |
| H | 14.446125 | 24.812044 | -0.200346 |
| H | 13.960097 | 24.523088 | -1.873280 |
| H | 12.344875 | 22.655682 | 1.656198 |
| H | 10.941261 | 23.698397 | 1.933386 |
| H | 12.572538 | 24.334727 | 2.172464 |
| H | 8.409601 | 18.262338 | -5.196406 |
| H | 8.852989 | 18.383588 | -6.903207 |
| H | 7.766788 | 19.579360 | -6.194640 |
| H | 10.634282 | 20.705262 | -7.964104 |
| H | 11.352404 | 21.860723 | -6.828509 |
| H | 9.614862 | 21.901894 | -7.142761 |
| H | 11.535381 | 18.137423 | -4.645727 |
| H | 12.607122 | 19.400473 | -5.271823 |
| H | 11.801163 | 18.297879 | -6.389751 |
| C | 14.489808 | 19.426100 | -2.024288 |

| | | | |
|---|---|---|---|
| C | 14.816846 | 19.792483 | 1.020061 |
| C | 14.795235 | 16.963193 | -0.201743 |
| H | 15.875664 | 16.995916 | -0.379882 |
| H | 14.627997 | 16.539024 | 0.793038 |
| H | 14.355837 | 16.281663 | -0.936720 |
| H | 15.901626 | 19.830251 | 0.871723 |
| H | 14.444950 | 20.821323 | 0.980564 |
| H | 14.638279 | 19.401011 | 2.026505 |
| H | 15.577300 | 19.475767 | -2.147696 |
| H | 14.091393 | 18.817495 | -2.842180 |
| H | 14.091080 | 20.439422 | -2.136234 |

**$La_2$(1,5-COT)(1,4-$COT)_2$:**

| | | | |
|---|---|---|---|
| C | 6.755368 | 18.363389 | 3.238386 |
| Si | 7.255763 | 19.710512 | 2.001112 |
| C | 7.624894 | 21.308415 | 2.953101 |
| C | 8.799996 | 19.164131 | 1.000800 |
| La | 10.173470 | 20.532277 | -1.292018 |
| C | 11.721721 | 22.245697 | -2.736869 |
| C | 10.941627 | 21.560270 | -3.704617 |
| C | 9.566731 | 21.241362 | -3.893370 |
| Si | 9.128933 | 20.306685 | -5.496350 |
| C | 10.676219 | 19.693315 | -6.408784 |
| C | 10.049927 | 19.610206 | 1.521912 |
| La | 10.502121 | 16.661119 | 1.292008 |
| C | 12.531595 | 14.919497 | 1.933533 |
| C | 11.751854 | 14.236771 | 0.970582 |
| C | 10.372912 | 13.972655 | 0.790829 |
| C | 9.178621 | 14.254142 | 1.510911 |
| Si | 7.595440 | 13.474476 | 0.789550 |
| C | 6.133018 | 14.688999 | 0.838161 |
| C | 8.508729 | 18.361545 | -0.141027 |

| | | | |
|---|---|---|---|
| C | 9.255550 | 17.720159 | -1.166876 |
| C | 10.625668 | 17.583191 | -1.521923 |
| C | 11.875599 | 18.029265 | -1.000811 |
| Si | 13.419829 | 17.482880 | -2.001124 |
| C | 13.050709 | 15.884949 | -2.953069 |
| C | 11.420045 | 19.473237 | 1.166864 |
| C | 12.166866 | 18.831852 | 0.141015 |
| C | 8.953885 | 14.947695 | 2.736870 |
| C | 9.733962 | 15.633146 | 3.704615 |
| C | 11.108853 | 15.952078 | 3.893372 |
| Si | 11.546625 | 16.886776 | 5.496347 |
| C | 9.999325 | 17.500144 | 6.408759 |
| C | 12.264976 | 15.637108 | 3.122683 |
| C | 5.795442 | 20.018391 | 0.830779 |
| C | 7.834259 | 12.934886 | -1.015445 |
| C | 7.150602 | 11.950258 | 1.828528 |
| C | 12.645219 | 18.395451 | 5.131392 |
| C | 12.495934 | 15.706551 | 6.640084 |
| C | 11.497005 | 22.939237 | -1.510899 |
| Si | 13.080201 | 23.718874 | -0.789540 |
| C | 14.542621 | 22.504354 | -0.838234 |
| C | 10.302724 | 23.220732 | -0.790804 |
| C | 8.923776 | 22.956640 | -0.970551 |
| C | 8.144018 | 22.273938 | -1.933506 |
| C | 8.410618 | 21.556339 | -3.122668 |
| C | 13.920193 | 18.829976 | -3.238439 |
| C | 14.880165 | 17.175051 | -0.830796 |
| C | 12.841419 | 24.258393 | 1.015482 |
| C | 13.525015 | 25.243137 | -1.828464 |
| C | 8.030331 | 18.798014 | -5.131401 |
| C | 8.179621 | 21.486930 | -6.640063 |
| H | 9.947504 | 20.222540 | 2.413678 |

| | | | |
|---|---|---|---|
| H | 12.068454 | 19.997243 | 1.864309 |
| H | 13.231087 | 18.998635 | 0.284765 |
| H | 6.519169 | 17.425971 | 2.725276 |
| H | 7.558146 | 18.160976 | 3.954040 |
| H | 5.868678 | 18.670555 | 3.803937 |
| H | 5.458712 | 19.105026 | 0.330624 |
| H | 4.945164 | 20.404212 | 1.403893 |
| H | 6.046141 | 20.755516 | 0.062100 |
| H | 7.989365 | 22.098068 | 2.288914 |
| H | 6.704708 | 21.666818 | 3.427400 |
| H | 8.362150 | 21.163895 | 3.749113 |
| H | 7.895630 | 15.031513 | 2.981811 |
| H | 9.092644 | 16.078219 | 4.461984 |
| H | 13.178161 | 16.082260 | 3.516649 |
| H | 13.583581 | 14.957575 | 1.657812 |
| H | 12.351693 | 13.879467 | 0.135900 |
| H | 10.194214 | 13.464175 | -0.153465 |
| H | 8.582514 | 12.142839 | -1.118783 |
| H | 6.887479 | 12.539643 | -1.400042 |
| H | 8.130295 | 13.770120 | -1.658700 |
| H | 7.000422 | 12.224312 | 2.877653 |
| H | 6.233738 | 11.471267 | 1.467707 |
| H | 7.957831 | 11.211608 | 1.793124 |
| H | 5.876842 | 14.993217 | 1.857757 |
| H | 6.350966 | 15.592229 | 0.258670 |
| H | 5.242269 | 14.219802 | 0.405819 |
| H | 12.110759 | 19.123500 | 4.512025 |
| H | 12.931787 | 18.893600 | 6.064276 |
| H | 13.566922 | 18.121275 | 4.608569 |
| H | 12.801874 | 16.207792 | 7.564939 |
| H | 11.873683 | 14.846598 | 6.907662 |
| H | 13.395918 | 15.322771 | 6.149285 |

| | | | |
|---|---|---|---|
| H | 9.413216 | 18.200723 | 5.805170 |
| H | 9.343593 | 16.677767 | 6.711417 |
| H | 10.305392 | 18.026734 | 7.319556 |
| H | 10.728091 | 16.970856 | -2.413688 |
| H | 8.607140 | 17.196153 | -1.864320 |
| H | 7.444507 | 18.194762 | -0.284776 |
| H | 14.156376 | 19.767414 | -2.725360 |
| H | 13.117409 | 19.032351 | -3.954096 |
| H | 14.806887 | 18.522810 | -3.803985 |
| H | 15.216898 | 18.088438 | -0.330683 |
| H | 15.730437 | 16.789210 | -1.403906 |
| H | 14.629479 | 16.437957 | -0.062085 |
| H | 12.686250 | 15.095309 | -2.288861 |
| H | 13.970895 | 15.526543 | -3.427366 |
| H | 12.313447 | 16.029442 | -3.749080 |
| H | 12.779972 | 22.161866 | -2.981818 |
| H | 11.582933 | 21.115198 | -4.461996 |
| H | 7.497423 | 21.111207 | -3.516633 |
| H | 7.092033 | 22.235873 | -1.657778 |
| H | 8.323948 | 23.313941 | -0.135860 |
| H | 10.481436 | 23.729196 | 0.153496 |
| H | 12.093174 | 25.050444 | 1.118864 |
| H | 13.788209 | 24.653609 | 1.400080 |
| H | 12.545383 | 23.423135 | 1.658707 |
| H | 13.675168 | 24.969128 | -2.877604 |
| H | 14.441888 | 25.722112 | -1.467645 |
| H | 12.717787 | 25.981786 | -1.793008 |
| H | 14.798770 | 22.200172 | -1.857847 |
| H | 14.324690 | 21.601103 | -0.258768 |
| H | 15.433382 | 22.973536 | -0.405900 |
| H | 8.564796 | 18.069947 | -4.512060 |
| H | 7.743738 | 18.299887 | -6.064288 |

| | | | |
|---|---|---|---|
| H | 7.108643 | 19.072190 | -4.608553 |
| H | 7.873667 | 20.985701 | -7.564921 |
| H | 8.801876 | 22.346881 | -6.907639 |
| H | 7.279645 | 21.870712 | -6.149250 |
| H | 11.262327 | 18.992724 | -5.805209 |
| H | 11.331955 | 20.515690 | -6.711438 |
| H | 10.370139 | 19.166738 | -7.319584 |

**$Nd_2$(1,4-COT)$_3$:**

| | | | |
|---|---|---|---|
| C | 4.703790 | 12.925637 | 6.155256 |
| Si | 6.059288 | 14.253956 | 6.044744 |
| C | 5.642138 | 15.424199 | 4.610952 |
| C | 7.779192 | 13.458707 | 5.829589 |
| C | 8.109481 | 12.579756 | 6.901212 |
| C | 9.233040 | 11.808115 | 7.278629 |
| C | 10.510859 | 11.550837 | 6.729807 |
| C | 11.214840 | 11.967880 | 5.574821 |
| C | 10.950123 | 12.832707 | 4.477758 |
| Si | 12.400315 | 13.091448 | 3.267077 |
| C | 11.836811 | 12.928469 | 1.458690 |
| C | 6.054738 | 15.258699 | 7.654809 |
| Nd | 8.791386 | 11.199822 | 4.684445 |
| C | 6.621166 | 10.148568 | 3.048294 |
| C | 7.674050 | 10.317272 | 2.096654 |
| Si | 7.148020 | 11.348670 | 0.566247 |
| C | 8.471178 | 11.265810 | -0.786973 |
| C | 8.523213 | 13.876617 | 4.690661 |
| C | 9.806693 | 13.617110 | 4.143304 |
| C | 6.424901 | 9.491550 | 4.297813 |
| C | 7.191678 | 8.689196 | 5.193499 |
| C | 8.552765 | 8.267628 | 5.134590 |
| C | 9.634107 | 8.435731 | 4.233273 |

| | | | |
|---|---|---|---|
| C | 9.824120 | 9.081086 | 2.983909 |
| C | 9.019278 | 9.850263 | 2.102940 |
| Nd | 7.478589 | 7.384724 | 2.552668 |
| C | 7.277894 | 4.756832 | 3.028463 |
| C | 5.942363 | 5.195590 | 2.834117 |
| C | 5.237761 | 5.989160 | 1.885245 |
| C | 5.669767 | 6.641090 | 0.694290 |
| C | 6.888404 | 6.769303 | -0.012465 |
| C | 8.219239 | 6.331969 | 0.184284 |
| C | 8.896523 | 5.568376 | 1.165249 |
| C | 8.532361 | 4.895528 | 2.364529 |
| Si | 9.929829 | 3.909684 | 3.207700 |
| C | 9.646266 | 2.062870 | 2.874239 |
| C | 9.946344 | 4.188449 | 5.088155 |
| C | 11.637578 | 4.397535 | 2.536709 |
| C | 13.094042 | 14.837812 | 3.532220 |
| C | 13.788554 | 11.829856 | 3.555909 |
| Si | 6.277533 | 8.053189 | 6.756314 |
| C | 4.442800 | 8.522068 | 6.708286 |
| C | 7.055650 | 8.783971 | 8.323299 |
| C | 6.420718 | 6.164555 | 6.851335 |
| C | 6.874671 | 13.156988 | 1.065901 |
| C | 5.518456 | 10.671846 | -0.128118 |
| Si | 3.362228 | 6.177951 | 2.177682 |
| C | 2.442992 | 5.382474 | 0.720084 |
| C | 2.811862 | 5.317608 | 3.777263 |
| C | 2.861722 | 8.008845 | 2.283917 |
| H | 7.947791 | 14.514003 | 4.023791 |
| H | 9.913841 | 14.123212 | 3.184241 |
| H | 12.168340 | 11.451978 | 5.493290 |
| H | 11.056885 | 10.798949 | 7.295832 |
| H | 9.041188 | 11.209071 | 8.165363 |

| | | | |
|---|---|---|---|
| H | 7.282227 | 12.419311 | 7.592628 |
| H | 3.721890 | 13.382169 | 6.321497 |
| H | 4.889956 | 12.230920 | 6.980655 |
| H | 4.654115 | 12.344169 | 5.228751 |
| H | 5.072823 | 15.710121 | 7.834591 |
| H | 6.795658 | 16.063181 | 7.606837 |
| H | 6.301584 | 14.633738 | 8.518667 |
| H | 5.608747 | 14.911448 | 3.644586 |
| H | 6.363636 | 16.243962 | 4.535715 |
| H | 4.655483 | 15.868323 | 4.783181 |
| H | 12.325016 | 15.596885 | 3.357255 |
| H | 13.931562 | 15.041766 | 2.856074 |
| H | 13.448652 | 14.958148 | 4.560841 |
| H | 5.407959 | 9.648041 | 4.645520 |
| H | 5.700213 | 10.641316 | 2.742881 |
| H | 9.580195 | 10.143763 | 1.221067 |
| H | 10.834762 | 8.950942 | 2.607454 |
| H | 10.538258 | 7.941910 | 4.578006 |
| H | 8.854889 | 7.665608 | 5.989252 |
| H | 6.919524 | 9.868734 | 8.360675 |
| H | 8.129015 | 8.576337 | 8.376461 |
| H | 6.587566 | 8.353148 | 9.215263 |
| H | 7.463121 | 5.834531 | 6.898791 |
| H | 5.958738 | 5.690348 | 5.979963 |
| H | 5.914283 | 5.791564 | 7.748470 |
| H | 3.950418 | 8.116208 | 7.598920 |
| H | 3.933895 | 8.104482 | 5.833891 |
| H | 4.284799 | 9.605081 | 6.713133 |
| H | 6.532978 | 13.748300 | 0.209307 |
| H | 7.796873 | 13.608375 | 1.444104 |
| H | 6.114672 | 13.236049 | 1.849829 |
| H | 4.699264 | 10.749500 | 0.593397 |

| | | | |
|---|---|---|---|
| H | 5.621443 | 9.619435 | -0.408462 |
| H | 5.225273 | 11.235150 | -1.020872 |
| H | 7.362180 | 4.221659 | 3.973531 |
| H | 5.316646 | 4.888884 | 3.668893 |
| H | 4.882589 | 7.222962 | 0.215540 |
| H | 6.795986 | 7.420841 | -0.878964 |
| H | 8.899087 | 6.738072 | -0.561913 |
| H | 9.964810 | 5.540942 | 0.965326 |
| H | 9.000805 | 3.904754 | 5.560266 |
| H | 10.140810 | 5.239304 | 5.326041 |
| H | 10.736864 | 3.586930 | 5.550537 |
| H | 12.409363 | 3.838659 | 3.077555 |
| H | 11.842384 | 5.464298 | 2.674886 |
| H | 11.751033 | 4.163093 | 1.473649 |
| H | 8.670572 | 1.741934 | 3.252883 |
| H | 10.415627 | 1.448398 | 3.354574 |
| H | 9.667357 | 1.857694 | 1.799212 |
| H | 3.024419 | 4.244005 | 3.757542 |
| H | 1.729024 | 5.436139 | 3.894580 |
| H | 3.286859 | 5.743115 | 4.667132 |
| H | 3.332745 | 8.492998 | 3.145977 |
| H | 1.776045 | 8.107201 | 2.394191 |
| H | 3.154348 | 8.562812 | 1.386480 |
| H | 2.719593 | 5.850703 | -0.229820 |
| H | 1.357947 | 5.476861 | 0.838486 |
| H | 2.686857 | 4.317801 | 0.646947 |
| H | 8.108999 | 11.800228 | -1.672140 |
| H | 9.410777 | 11.738095 | -0.483873 |
| H | 8.684213 | 10.235137 | -1.088136 |
| H | 12.673010 | 13.129782 | 0.780021 |
| H | 11.476907 | 11.914087 | 1.258788 |
| H | 11.033898 | 13.628518 | 1.207223 |

| | | | |
|---|---|---|---|
| H | 14.576073 | 11.982420 | 2.809660 |
| H | 14.248639 | 11.939037 | 4.542937 |
| H | 13.433471 | 10.798743 | 3.456810 |

**$Nd_2$(1,5-COT)(1,4-$COT)_2$:**

| | | | |
|---|---|---|---|
| C | 4.489273 | 13.191242 | 5.336120 |
| Si | 5.923858 | 14.439610 | 5.300480 |
| C | 5.696775 | 15.663774 | 6.732491 |
| C | 5.828810 | 15.400021 | 3.666481 |
| C | 7.605028 | 13.565200 | 5.513991 |
| C | 8.598719 | 13.862880 | 4.538757 |
| C | 9.948251 | 13.500664 | 4.287922 |
| Nd | 8.682943 | 11.186976 | 4.765111 |
| C | 7.712659 | 10.361906 | 2.073488 |
| Nd | 7.412557 | 7.423174 | 2.522829 |
| C | 6.150855 | 5.107598 | 2.999117 |
| C | 5.155988 | 5.926641 | 2.388210 |
| Si | 3.481292 | 5.882739 | 3.300408 |
| C | 2.333968 | 7.280787 | 2.722141 |
| C | 7.647961 | 12.760996 | 6.688755 |
| C | 8.623296 | 11.980302 | 7.350561 |
| C | 9.969467 | 11.624282 | 7.100908 |
| C | 10.918417 | 11.899626 | 6.087068 |
| C | 10.942201 | 12.680347 | 4.898579 |
| Si | 12.616775 | 12.722492 | 3.986064 |
| C | 13.762963 | 11.323470 | 4.564188 |
| C | 12.391596 | 12.544016 | 2.106942 |
| C | 13.456387 | 14.387558 | 4.337782 |
| C | 6.596941 | 10.215115 | 2.947880 |
| C | 6.335194 | 9.561174 | 4.183162 |
| C | 7.057283 | 8.757386 | 5.107293 |
| C | 8.384419 | 8.248260 | 5.213702 |

| | | | |
|---|---|---|---|
| C | 9.500050 | 8.394968 | 4.339213 |
| C | 9.761750 | 9.048902 | 3.103982 |
| C | 9.039747 | 9.852770 | 2.179956 |
| Si | 7.418637 | 11.404775 | 0.488305 |
| C | 5.578465 | 11.812088 | 0.290316 |
| C | 7.994707 | 10.440499 | -1.038932 |
| C | 8.412725 | 13.016113 | 0.571124 |
| C | 7.501002 | 4.747286 | 2.748755 |
| C | 8.494716 | 5.046551 | 1.774047 |
| Si | 10.177393 | 4.175321 | 1.988809 |
| C | 11.609483 | 5.426671 | 1.956340 |
| C | 5.179114 | 6.707407 | 1.199714 |
| C | 6.128106 | 6.984086 | 0.186261 |
| C | 7.474945 | 6.630130 | -0.062771 |
| C | 8.451148 | 5.850849 | 0.599394 |
| C | 10.408957 | 2.952978 | 0.555971 |
| C | 10.272284 | 3.213615 | 3.622052 |
| C | 2.643288 | 4.216894 | 2.948571 |
| C | 3.705868 | 6.061430 | 5.179596 |
| H | 8.216132 | 14.478639 | 3.728072 |
| H | 10.275993 | 13.918974 | 3.337201 |
| H | 11.830773 | 11.329331 | 6.243133 |
| H | 10.345704 | 10.908188 | 7.828606 |
| H | 8.218267 | 11.470490 | 8.221762 |
| H | 6.686955 | 12.690952 | 7.197551 |
| H | 3.526603 | 13.711923 | 5.283891 |
| H | 4.488971 | 12.589675 | 6.250721 |
| H | 4.547497 | 12.506380 | 4.483693 |
| H | 4.733562 | 16.180961 | 6.662409 |
| H | 6.490189 | 16.417988 | 6.723586 |
| H | 5.736542 | 15.154247 | 7.700369 |
| H | 5.944099 | 14.749851 | 2.793225 |

| | | | |
|---|---|---|---|
| H | 6.586863 | 16.187496 | 3.608676 |
| H | 4.848311 | 15.882901 | 3.590259 |
| H | 12.823774 | 15.219623 | 4.012552 |
| H | 14.417027 | 14.467745 | 3.817254 |
| H | 13.638388 | 14.510003 | 5.410249 |
| H | 5.309334 | 9.717035 | 4.505858 |
| H | 5.706141 | 10.722529 | 2.590442 |
| H | 9.678040 | 10.137806 | 1.346241 |
| H | 10.787542 | 8.892853 | 2.781175 |
| H | 10.390809 | 7.887481 | 4.696638 |
| Si | 8.678407 | 7.205568 | 6.799019 |
| H | 8.299393 | 13.584957 | -0.358428 |
| H | 9.479105 | 12.814804 | 0.711908 |
| H | 8.078364 | 13.649278 | 1.397952 |
| H | 5.198705 | 12.447569 | 1.096701 |
| H | 4.962728 | 10.908027 | 0.246194 |
| H | 5.432628 | 12.356904 | -0.648836 |
| H | 7.884105 | 4.132006 | 3.559561 |
| H | 5.823352 | 4.688775 | 3.949693 |
| H | 4.266031 | 7.276449 | 1.043300 |
| H | 5.751163 | 7.699696 | -0.541554 |
| H | 7.879608 | 7.140727 | -0.933680 |
| H | 9.412293 | 5.922412 | 0.091054 |
| H | 9.515377 | 2.424942 | 3.678477 |
| H | 10.155191 | 3.862883 | 4.495741 |
| H | 11.253457 | 2.732183 | 3.698796 |
| H | 12.573198 | 4.907984 | 2.009127 |
| H | 11.548722 | 6.110360 | 2.809537 |
| H | 11.609561 | 6.029363 | 1.042479 |
| H | 9.617070 | 2.197151 | 0.563008 |
| H | 11.373124 | 2.437704 | 0.627016 |
| H | 10.369615 | 3.463323 | -0.411489 |

| | | | |
|---|---|---|---|
| H | 4.297229 | 5.246160 | 5.607639 |
| H | 2.729512 | 6.052395 | 5.676760 |
| H | 4.200925 | 7.006385 | 5.426631 |
| H | 2.789804 | 8.267223 | 2.857770 |
| H | 1.411272 | 7.257258 | 3.312464 |
| H | 2.049093 | 7.178067 | 1.670384 |
| H | 2.461971 | 4.094050 | 1.876039 |
| H | 1.682441 | 4.136050 | 3.468613 |
| H | 3.276406 | 3.385429 | 3.274356 |
| H | 7.864211 | 11.053203 | -1.937741 |
| H | 9.052084 | 10.164376 | -0.979432 |
| H | 7.413466 | 9.523046 | -1.166256 |
| H | 13.367884 | 12.550790 | 1.609612 |
| H | 11.894372 | 11.600140 | 1.860193 |
| H | 11.801972 | 13.360545 | 1.678894 |
| H | 14.686066 | 11.346913 | 3.974497 |
| H | 14.047208 | 11.425351 | 5.616199 |
| H | 13.306711 | 10.337361 | 4.427630 |
| C | 10.518730 | 6.799284 | 6.997624 |
| H | 6.418990 | 8.472398 | 5.941022 |
| C | 8.101402 | 8.169757 | 8.325963 |
| C | 7.685045 | 5.593795 | 6.716068 |
| H | 7.798845 | 5.024797 | 7.645463 |
| H | 6.618544 | 5.794726 | 6.575627 |
| H | 8.019412 | 4.960958 | 5.888993 |
| H | 10.664534 | 6.254136 | 7.936593 |
| H | 10.899292 | 6.164413 | 6.191134 |
| H | 11.133821 | 7.703752 | 7.042389 |
| H | 8.232457 | 7.557458 | 9.224967 |
| H | 8.681841 | 9.087759 | 8.452967 |
| H | 7.043781 | 8.444939 | 8.266428 |

**$Tb_2$(1,4-COT)$_3$:**

| | | | |
|---|---|---|---|
| C | 5.609183 | 18.677469 | 9.124547 |
| Si | 6.393310 | 18.713532 | 7.394792 |
| C | 5.982635 | 17.136561 | 6.406510 |
| C | 4.842798 | 16.420480 | 6.866160 |
| C | 4.126091 | 15.274252 | 6.448816 |
| C | 4.247247 | 14.335677 | 5.398612 |
| C | 5.139556 | 14.143514 | 4.319004 |
| C | 6.279349 | 14.819493 | 3.797367 |
| Si | 6.916880 | 14.017498 | 2.189179 |
| C | 7.270216 | 12.165261 | 2.432400 |
| C | 8.268492 | 18.939225 | 7.610636 |
| C | 5.711655 | 20.210323 | 6.447910 |
| C | 6.840632 | 16.929466 | 5.286963 |
| Tb | 6.660715 | 14.590741 | 6.415054 |
| C | 8.019683 | 14.871648 | 8.900606 |
| C | 9.067029 | 14.750693 | 7.954988 |
| C | 9.406620 | 13.833862 | 6.919926 |
| Si | 11.014701 | 14.316120 | 5.991738 |
| C | 12.497359 | 14.293114 | 7.173500 |
| C | 6.957408 | 15.994748 | 4.226089 |
| C | 8.759819 | 12.640207 | 6.486759 |
| C | 7.587543 | 11.899619 | 6.813758 |
| Tb | 8.844049 | 12.185937 | 9.361492 |
| C | 10.503427 | 10.121224 | 9.436532 |
| C | 9.290396 | 9.722250 | 10.069470 |
| C | 8.408820 | 10.251311 | 11.046747 |
| C | 8.318257 | 11.433036 | 11.835796 |
| Si | 6.879000 | 11.486588 | 13.084956 |
| C | 5.946748 | 13.142020 | 13.015220 |
| C | 6.488879 | 12.003686 | 7.721030 |
| C | 6.207561 | 12.971855 | 8.727130 |

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|---|---|---|---|
| C | 6.841617 | 14.145904 | 9.212231 |
| Si | 5.185900 | 10.606927 | 7.524605 |
| C | 4.861687 | 10.292501 | 5.682831 |
| C | 5.791651 | 8.983817 | 8.293103 |
| C | 3.556821 | 11.112599 | 8.353197 |
| C | 5.575553 | 14.202255 | 0.858744 |
| C | 8.501535 | 14.852351 | 1.562356 |
| C | 9.160324 | 12.577550 | 11.928574 |
| C | 10.369052 | 13.001267 | 11.330702 |
| C | 11.251683 | 12.467330 | 10.364074 |
| C | 11.304369 | 11.286715 | 9.585491 |
| Si | 11.212204 | 8.779184 | 8.283444 |
| C | 12.616858 | 9.452401 | 7.197833 |
| C | 9.877967 | 8.064826 | 7.133464 |
| C | 11.895931 | 7.374208 | 9.360567 |
| C | 7.603855 | 11.275703 | 14.826337 |
| C | 5.620509 | 10.097679 | 12.784605 |
| C | 11.355972 | 13.115645 | 4.565498 |
| C | 10.845623 | 16.072544 | 5.299194 |
| H | 7.676094 | 17.626931 | 5.263928 |
| H | 7.844694 | 16.202632 | 3.633110 |
| H | 4.912669 | 13.218777 | 3.789686 |
| H | 3.530034 | 13.523133 | 5.491069 |
| H | 3.343783 | 15.001517 | 7.153769 |
| H | 4.453872 | 16.796030 | 7.809237 |
| H | 5.913355 | 17.793083 | 9.693678 |
| H | 4.515508 | 18.698273 | 9.086737 |
| H | 5.931221 | 19.561734 | 9.685639 |
| H | 8.793332 | 19.031718 | 6.654793 |
| H | 8.708002 | 18.098801 | 8.157185 |
| H | 8.468871 | 19.852910 | 8.181273 |
| H | 5.930568 | 21.147858 | 6.970717 |

| | | | |
|---|---|---|---|
| H | 4.626253 | 20.131277 | 6.329477 |
| H | 6.150018 | 20.269433 | 5.446559 |
| H | 5.278980 | 12.787156 | 9.257773 |
| H | 7.512123 | 11.028320 | 6.167570 |
| H | 9.289740 | 12.153645 | 5.673517 |
| H | 4.063268 | 9.551126 | 5.568407 |
| H | 5.744061 | 9.902808 | 5.165994 |
| H | 4.550962 | 11.209702 | 5.174967 |
| H | 5.047383 | 8.194437 | 8.139366 |
| H | 5.960416 | 9.084515 | 9.369003 |
| H | 6.727996 | 8.654677 | 7.832399 |
| H | 3.186229 | 12.068810 | 7.970988 |
| H | 3.642091 | 11.188719 | 9.441867 |
| H | 2.797318 | 10.351861 | 8.141828 |
| H | 8.887908 | 8.795821 | 9.662808 |
| H | 7.544325 | 9.603716 | 11.167179 |
| H | 8.754769 | 13.356031 | 12.573122 |
| H | 10.639742 | 14.014450 | 11.619636 |
| H | 12.036311 | 13.169731 | 10.094939 |
| H | 12.140820 | 11.317268 | 8.892314 |
| H | 12.288240 | 10.293402 | 6.578983 |
| H | 13.479045 | 9.778586 | 7.787982 |
| H | 12.963158 | 8.660417 | 6.524668 |
| H | 9.048135 | 7.616298 | 7.688492 |
| H | 9.468575 | 8.838420 | 6.475756 |
| H | 10.308627 | 7.280095 | 6.501662 |
| H | 12.297794 | 6.560007 | 8.747494 |
| H | 12.697958 | 7.741241 | 10.008843 |
| H | 11.113499 | 6.960240 | 10.004535 |
| H | 8.137562 | 15.743521 | 9.537043 |
| H | 6.285209 | 14.604690 | 10.023391 |
| H | 5.177353 | 13.172938 | 13.794694 |

| | | | |
|---|---|---|---|
| H | 6.606945 | 14.000580 | 13.172749 |
| H | 5.449822 | 13.271814 | 12.048500 |
| H | 4.814589 | 10.179442 | 13.522415 |
| H | 5.164493 | 10.157828 | 11.791215 |
| H | 6.065141 | 9.103849 | 12.897293 |
| H | 6.820240 | 11.316603 | 15.590921 |
| H | 8.117807 | 10.313290 | 14.915975 |
| H | 8.333669 | 12.061150 | 15.046987 |
| H | 5.887887 | 13.739867 | -0.084113 |
| H | 4.638668 | 13.730488 | 1.171534 |
| H | 5.365261 | 15.259301 | 0.667211 |
| H | 8.824628 | 14.360238 | 0.638358 |
| H | 8.343500 | 15.910742 | 1.332014 |
| H | 9.324960 | 14.778694 | 2.279515 |
| H | 7.595838 | 11.711968 | 1.489484 |
| H | 8.061043 | 12.008306 | 3.173282 |
| H | 6.383266 | 11.620397 | 2.770574 |
| H | 9.776710 | 15.568506 | 8.060804 |
| H | 12.270967 | 13.428611 | 4.050757 |
| H | 11.513786 | 12.089959 | 4.913699 |
| H | 10.549901 | 13.105666 | 3.825417 |
| H | 13.397056 | 14.644410 | 6.656118 |
| H | 12.336445 | 14.944163 | 8.038622 |
| H | 12.693198 | 13.282588 | 7.543073 |
| H | 11.752929 | 16.355396 | 4.754223 |
| H | 9.997932 | 16.144347 | 4.611854 |
| H | 10.693469 | 16.809308 | 6.093987 |

**$Tb_2$(1,5-COT)(1,4-COT)$_2$:**

| | | | |
|---|---|---|---|
| C | 3.777519 | 17.596316 | 8.959995 |
| Si | 4.901117 | 18.170743 | 7.540832 |
| C | 6.487955 | 18.880928 | 8.308764 |

| | | | |
|---|---|---|---|
| C | 4.016509 | 19.554126 | 6.588712 |
| C | 5.283314 | 16.751454 | 6.326777 |
| C | 6.407397 | 17.008129 | 5.488786 |
| C | 7.083213 | 16.356045 | 4.424794 |
| Tb | 6.730329 | 14.546426 | 6.281195 |
| C | 9.362023 | 13.497472 | 6.692898 |
| C | 8.539273 | 12.359917 | 6.467071 |
| C | 7.333300 | 11.822502 | 6.993582 |
| C | 6.390091 | 12.191714 | 7.994472 |
| Si | 4.937762 | 10.950371 | 8.185930 |
| C | 5.564219 | 9.327020 | 8.935109 |
| C | 4.365457 | 15.665694 | 6.363532 |
| C | 4.188810 | 14.462626 | 5.639860 |
| C | 4.865733 | 13.808497 | 4.585035 |
| C | 6.012791 | 14.075894 | 3.804040 |
| C | 6.960513 | 15.133423 | 3.707007 |
| Si | 8.205682 | 14.862774 | 2.289642 |
| C | 7.267664 | 14.988418 | 0.644335 |
| C | 9.588739 | 16.162612 | 2.302198 |
| C | 9.015062 | 13.145343 | 2.393889 |
| C | 7.192580 | 14.460246 | 9.085316 |
| Tb | 9.001523 | 12.273749 | 9.271187 |
| C | 8.771352 | 11.686759 | 11.845378 |
| C | 9.719066 | 12.744293 | 11.748339 |
| C | 10.866119 | 13.011696 | 10.967338 |
| C | 11.543044 | 12.357570 | 9.912512 |
| C | 11.366402 | 11.154499 | 9.188844 |
| C | 10.448554 | 10.068732 | 9.225606 |
| Si | 10.830770 | 8.649445 | 8.011556 |
| C | 9.243949 | 7.939247 | 7.243600 |
| C | 8.398554 | 14.997660 | 8.558803 |
| C | 9.341761 | 14.628451 | 7.557912 |

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|---|---|---|---|
| Si | 10.794051 | 15.869837 | 7.366412 |
| C | 10.167517 | 17.493169 | 6.617252 |
| C | 6.369828 | 13.322693 | 8.859486 |
| C | 9.324474 | 9.812051 | 10.063603 |
| C | 8.648657 | 10.464134 | 11.127594 |
| Si | 7.526185 | 11.957399 | 13.262746 |
| C | 8.464210 | 11.831771 | 14.908050 |
| C | 6.143143 | 10.657546 | 13.250199 |
| C | 6.716786 | 13.674821 | 13.158495 |
| C | 3.587406 | 11.677399 | 9.299251 |
| C | 4.178916 | 10.542022 | 6.497446 |
| C | 11.715379 | 7.266069 | 8.963685 |
| C | 11.954383 | 9.223883 | 6.592409 |
| C | 12.144396 | 15.142856 | 6.253045 |
| C | 11.552935 | 16.278210 | 9.054873 |
| H | 6.946798 | 17.908575 | 5.776853 |
| H | 7.970704 | 16.916401 | 4.141758 |
| H | 6.243083 | 13.232161 | 3.155064 |
| H | 4.457305 | 12.821613 | 4.383545 |
| H | 3.386115 | 13.854379 | 6.050948 |
| H | 3.656217 | 15.731857 | 7.184583 |
| H | 4.212502 | 16.758345 | 9.514371 |
| H | 2.784578 | 17.295612 | 8.611244 |
| H | 3.636895 | 18.424004 | 9.663966 |
| H | 7.160951 | 19.308104 | 7.558894 |
| H | 7.037467 | 18.110736 | 8.859592 |
| H | 6.235448 | 19.681897 | 9.012451 |
| H | 3.781811 | 20.402243 | 7.241341 |
| H | 3.079467 | 19.186495 | 6.158246 |
| H | 4.636314 | 19.921924 | 5.764661 |
| H | 5.509360 | 13.340049 | 9.520928 |
| H | 7.079109 | 10.896027 | 6.483924 |

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|---|---|---|---|
| H | 8.942654 | 11.730351 | 5.679080 |
| H | 3.408949 | 9.772031 | 6.618814 |
| H | 4.919542 | 10.156387 | 5.789968 |
| H | 3.709874 | 11.421467 | 6.049655 |
| H | 4.745345 | 8.604760 | 9.024816 |
| H | 5.989003 | 9.485953 | 9.929985 |
| H | 6.339866 | 8.878310 | 8.306763 |
| H | 3.209961 | 12.630980 | 8.916545 |
| H | 3.928698 | 11.831076 | 10.327808 |
| H | 2.744186 | 10.979113 | 9.338028 |
| H | 8.785079 | 8.911601 | 9.775541 |
| H | 7.761170 | 9.903774 | 11.410635 |
| H | 9.488773 | 13.588026 | 12.397314 |
| H | 11.274541 | 13.998583 | 11.168826 |
| H | 12.345732 | 12.965823 | 9.501419 |
| H | 12.075637 | 11.088337 | 8.367789 |
| H | 11.519399 | 10.061849 | 6.038028 |
| H | 12.947315 | 9.524597 | 6.941176 |
| H | 12.095026 | 8.396196 | 5.888440 |
| H | 8.570946 | 7.512065 | 7.993459 |
| H | 8.694440 | 8.709433 | 6.692762 |
| H | 9.496474 | 7.138279 | 6.539917 |
| H | 11.950092 | 6.417955 | 8.311058 |
| H | 12.652412 | 7.633707 | 9.394163 |
| H | 11.095566 | 6.898264 | 9.787728 |
| H | 10.222490 | 13.480112 | 6.031455 |
| H | 8.652744 | 15.924136 | 9.068461 |
| H | 6.789201 | 15.089811 | 9.873308 |
| H | 12.322872 | 17.048226 | 8.933482 |
| H | 10.812317 | 16.663822 | 9.762372 |
| H | 12.022019 | 15.398781 | 9.502651 |
| H | 10.986364 | 18.215456 | 6.527510 |

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|---|---|---|---|
| H | 9.742700 | 17.334220 | 5.622392 |
| H | 9.391879 | 17.941855 | 7.245625 |
| H | 12.521880 | 14.189284 | 6.635735 |
| H | 11.803077 | 14.989176 | 5.224498 |
| H | 12.987594 | 15.841167 | 6.214244 |
| H | 6.058528 | 13.837480 | 14.019142 |
| H | 7.455321 | 14.482719 | 13.152303 |
| H | 6.111972 | 13.765775 | 12.250491 |
| H | 5.461035 | 10.852610 | 14.085092 |
| H | 5.553675 | 10.691094 | 12.328420 |
| H | 6.527937 | 9.640288 | 13.373570 |
| H | 7.797879 | 12.006860 | 15.759887 |
| H | 8.912082 | 10.839591 | 15.023340 |
| H | 9.273781 | 12.567006 | 14.955152 |
| H | 7.933996 | 14.813326 | -0.207500 |
| H | 6.458085 | 14.253193 | 0.597228 |
| H | 6.819803 | 15.980604 | 0.529048 |
| H | 10.270848 | 15.967543 | 1.467307 |
| H | 9.203957 | 17.179875 | 2.178828 |
| H | 10.178205 | 16.129055 | 3.223979 |
| H | 9.673322 | 12.982679 | 1.533245 |
| H | 9.619870 | 13.054378 | 3.301896 |
| H | 8.276517 | 12.337454 | 2.400074 |

**$Ho_2$(1,4-COT)$_3$:**

| | | | |
|---|---|---|---|
| C | 5.669784 | 18.744124 | 9.082718 |
| Si | 6.421306 | 18.767166 | 7.338626 |
| C | 8.294339 | 19.039136 | 7.515532 |
| C | 5.688975 | 20.231717 | 6.378682 |
| C | 6.023665 | 17.167272 | 6.382864 |
| C | 6.849076 | 16.975884 | 5.236806 |
| C | 6.968151 | 16.028842 | 4.187659 |

| | | | |
|---|---|---|---|
| Ho | 6.775275 | 14.678232 | 6.380370 |
| C | 9.438299 | 14.002273 | 6.774978 |
| C | 8.868501 | 12.735049 | 6.480104 |
| C | 7.738593 | 11.953300 | 6.867521 |
| C | 6.607061 | 12.068122 | 7.740772 |
| Si | 5.293332 | 10.683587 | 7.536553 |
| C | 5.856569 | 9.065013 | 8.350723 |
| C | 4.925283 | 16.419290 | 6.890536 |
| C | 4.227301 | 15.251663 | 6.503250 |
| C | 4.342725 | 14.308617 | 5.457265 |
| C | 5.211782 | 14.125540 | 4.358185 |
| C | 6.318487 | 14.824722 | 3.797500 |
| Si | 6.936850 | 14.014885 | 2.186014 |
| C | 5.539927 | 14.104199 | 0.903501 |
| C | 8.449234 | 14.913954 | 1.474969 |
| C | 7.391848 | 12.189876 | 2.458474 |
| C | 6.331981 | 13.054235 | 8.736223 |
| Ho | 8.595244 | 11.931785 | 9.504960 |
| C | 8.367643 | 10.066286 | 11.214171 |
| C | 8.227314 | 11.267094 | 11.970096 |
| C | 9.005622 | 12.459462 | 11.997333 |
| C | 10.143449 | 12.948870 | 11.315361 |
| C | 10.995188 | 12.462357 | 10.296066 |
| C | 11.095029 | 11.262659 | 9.550026 |
| C | 10.389853 | 10.029290 | 9.502614 |
| Si | 11.111415 | 8.706875 | 8.331819 |
| C | 9.763744 | 7.928419 | 7.240675 |
| C | 7.009343 | 14.214403 | 9.205418 |
| C | 8.129055 | 14.990468 | 8.804240 |
| C | 9.090613 | 14.946614 | 7.774465 |
| C | 9.250107 | 9.563637 | 10.220732 |
| Si | 6.804157 | 11.285303 | 13.241555 |

| | | | |
|---|---|---|---|
| C | 7.556244 | 11.116443 | 14.975014 |
| C | 5.588056 | 9.855094 | 12.961635 |
| C | 5.821458 | 12.909901 | 13.157714 |
| C | 3.656491 | 11.223709 | 8.325668 |
| C | 5.012161 | 10.327364 | 5.696831 |
| C | 11.889210 | 7.343141 | 9.397220 |
| C | 12.439593 | 9.432447 | 7.188550 |
| H | 7.662959 | 17.696619 | 5.181582 |
| H | 7.835686 | 16.251599 | 3.571823 |
| H | 4.995082 | 13.189729 | 3.844354 |
| H | 3.648617 | 13.479599 | 5.575820 |
| H | 3.475421 | 14.963203 | 7.234483 |
| H | 4.561689 | 16.789602 | 7.845521 |
| H | 6.007026 | 17.878058 | 9.661274 |
| H | 4.575419 | 18.736435 | 9.064302 |
| H | 5.979680 | 19.646335 | 9.621585 |
| H | 8.801428 | 19.110883 | 6.548443 |
| H | 8.760533 | 18.226428 | 8.081599 |
| H | 8.484230 | 19.974980 | 8.052929 |
| H | 5.896687 | 21.183388 | 6.880120 |
| H | 4.603554 | 20.126377 | 6.282813 |
| H | 6.106382 | 20.282388 | 5.367925 |
| H | 5.402210 | 12.893191 | 9.273069 |
| H | 7.695484 | 11.049421 | 6.263283 |
| H | 9.408027 | 12.213142 | 5.694065 |
| H | 4.217225 | 9.582657 | 5.580035 |
| H | 5.908709 | 9.927256 | 5.213444 |
| H | 4.715122 | 11.231862 | 5.159721 |
| H | 5.102367 | 8.285883 | 8.191730 |
| H | 6.000476 | 9.177527 | 9.429512 |
| H | 6.797062 | 8.710051 | 7.918600 |
| H | 3.309549 | 12.180284 | 7.923383 |

| | | | |
|---|---|---|---|
| H | 3.724399 | 11.314485 | 9.414509 |
| H | 2.889089 | 10.471784 | 8.111650 |
| H | 8.902475 | 8.592307 | 9.871790 |
| H | 7.556280 | 9.365056 | 11.390152 |
| H | 8.584920 | 13.228413 | 12.642698 |
| H | 10.355723 | 13.985902 | 11.564002 |
| H | 11.697760 | 13.217923 | 9.954544 |
| H | 11.869194 | 11.340805 | 8.791723 |
| H | 12.042182 | 10.239110 | 6.564239 |
| H | 13.300491 | 9.819423 | 7.742574 |
| H | 12.806765 | 8.646053 | 6.520056 |
| H | 8.967385 | 7.462674 | 7.829783 |
| H | 9.307825 | 8.677330 | 6.584674 |
| H | 10.198164 | 7.147959 | 6.606072 |
| H | 12.306208 | 6.541717 | 8.777570 |
| H | 12.694482 | 7.749054 | 10.017703 |
| H | 11.146470 | 6.900062 | 10.068237 |
| Si | 11.030187 | 14.465721 | 5.822787 |
| H | 8.231766 | 15.876473 | 9.425243 |
| H | 6.486453 | 14.667857 | 10.042582 |
| H | 5.044780 | 12.917580 | 13.930556 |
| H | 6.451792 | 13.789752 | 13.319638 |
| H | 5.327837 | 13.023479 | 12.187033 |
| H | 4.786569 | 9.917978 | 13.706069 |
| H | 5.121108 | 9.895736 | 11.972120 |
| H | 6.061347 | 8.874853 | 13.076640 |
| H | 6.781056 | 11.142513 | 15.748660 |
| H | 8.100352 | 10.171257 | 15.069540 |
| H | 8.263945 | 11.926642 | 15.177314 |
| H | 5.836581 | 13.628143 | -0.037631 |
| H | 4.634994 | 13.604519 | 1.263332 |
| H | 5.279092 | 15.145961 | 0.691138 |

| | | | |
|---|---|---|---|
| H | 8.759648 | 14.415606 | 0.549870 |
| H | 8.222799 | 15.955569 | 1.225820 |
| H | 9.305768 | 14.904905 | 2.156084 |
| H | 7.705863 | 11.727932 | 1.515830 |
| H | 8.215545 | 12.094712 | 3.173260 |
| H | 6.546956 | 11.611185 | 2.844603 |
| H | 9.719102 | 15.834823 | 7.783790 |
| C | 11.350432 | 13.267646 | 4.388055 |
| C | 10.915798 | 16.230005 | 5.136674 |
| C | 12.511969 | 14.392093 | 7.007796 |
| H | 12.249584 | 13.588255 | 3.850412 |
| H | 11.527819 | 12.243557 | 4.731886 |
| H | 10.525466 | 13.248819 | 3.669463 |
| H | 13.432310 | 14.695131 | 6.496329 |
| H | 12.371292 | 15.059242 | 7.864385 |
| H | 12.658990 | 13.377709 | 7.391145 |
| H | 11.848251 | 16.495797 | 4.626511 |
| H | 10.096783 | 16.321677 | 4.417565 |
| H | 10.751144 | 16.968636 | 5.927151 |

**$Ho_2$(1,5-COT)(1,4-$COT)_2$:**

| | | | |
|---|---|---|---|
| C | 3.820212 | 17.577663 | 8.994600 |
| Si | 4.935486 | 18.152070 | 7.568924 |
| C | 4.034101 | 19.518098 | 6.607487 |
| C | 5.327816 | 16.728434 | 6.363443 |
| C | 4.422396 | 15.633419 | 6.412695 |
| C | 4.253291 | 14.425231 | 5.696705 |
| C | 4.929048 | 13.771995 | 4.641003 |
| C | 6.065937 | 14.047658 | 3.848771 |
| C | 6.999742 | 15.115750 | 3.737360 |
| Si | 8.236954 | 14.850038 | 2.312341 |
| C | 9.607029 | 16.163587 | 2.307984 |

| | | | |
|---|---|---|---|
| C | 6.515413 | 18.887147 | 8.327191 |
| Ho | 6.782750 | 14.562705 | 6.291753 |
| C | 6.373469 | 13.318078 | 8.861711 |
| C | 7.185257 | 14.466422 | 9.071863 |
| C | 8.383405 | 15.013369 | 8.537706 |
| C | 9.329447 | 14.643452 | 7.540798 |
| C | 9.358403 | 13.502102 | 6.690646 |
| Ho | 8.949111 | 12.257468 | 9.260597 |
| C | 11.478571 | 12.394934 | 9.855647 |
| C | 11.309457 | 11.186735 | 9.139677 |
| C | 10.404026 | 10.091729 | 9.188944 |
| C | 9.289127 | 9.827665 | 10.036608 |
| C | 8.615993 | 10.477340 | 11.103996 |
| C | 8.732114 | 11.704468 | 11.815002 |
| Si | 7.494911 | 11.970209 | 13.240021 |
| C | 6.124817 | 10.656681 | 13.244396 |
| C | 6.442713 | 16.992522 | 5.515784 |
| C | 7.115854 | 16.342869 | 4.448386 |
| C | 6.402422 | 12.176732 | 8.011557 |
| C | 7.348459 | 11.806817 | 7.014644 |
| C | 8.546611 | 12.353761 | 6.480491 |
| C | 9.062449 | 13.140564 | 2.418378 |
| C | 7.284646 | 14.959033 | 0.674202 |
| Si | 4.948829 | 10.936343 | 8.203983 |
| C | 3.607052 | 11.659311 | 9.330257 |
| C | 4.178157 | 10.539595 | 6.517639 |
| C | 5.568429 | 9.302803 | 8.936215 |
| C | 9.665924 | 12.772554 | 11.703572 |
| C | 10.802817 | 13.048195 | 10.911336 |
| Si | 10.796345 | 8.668073 | 7.983483 |
| C | 11.697721 | 7.302052 | 8.944937 |
| C | 11.911621 | 9.242450 | 6.557796 |

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|---|---|---|---|
| C | 9.216410 | 7.932999 | 7.225228 |
| C | 6.669437 | 13.679694 | 13.133974 |
| C | 8.447224 | 11.861217 | 14.878158 |
| Si | 10.783041 | 15.883841 | 7.348376 |
| C | 12.124792 | 15.160902 | 6.222052 |
| C | 11.553754 | 16.280543 | 9.034713 |
| C | 10.163428 | 17.517404 | 6.616204 |
| H | 6.978696 | 17.896208 | 5.799580 |
| H | 7.997654 | 16.908653 | 4.158738 |
| H | 6.303916 | 13.200936 | 3.206734 |
| H | 4.534256 | 12.776986 | 4.453895 |
| H | 3.463514 | 13.809160 | 6.120457 |
| H | 3.723600 | 15.693109 | 7.242962 |
| H | 4.262140 | 16.746437 | 9.553506 |
| H | 2.828838 | 17.267527 | 8.649647 |
| H | 3.674979 | 18.408723 | 9.693645 |
| H | 7.184502 | 19.310514 | 7.571692 |
| H | 7.071843 | 18.130148 | 8.889042 |
| H | 6.254722 | 19.695343 | 9.019538 |
| H | 3.792366 | 20.369122 | 7.253733 |
| H | 3.099829 | 19.137304 | 6.182512 |
| H | 4.648086 | 19.885443 | 5.778876 |
| H | 5.513711 | 13.336458 | 9.523838 |
| H | 7.105512 | 10.871388 | 6.516186 |
| H | 8.957191 | 11.718718 | 5.700915 |
| H | 3.418263 | 9.759522 | 6.638424 |
| H | 4.916718 | 10.169607 | 5.799687 |
| H | 3.694060 | 11.417214 | 6.082453 |
| H | 4.745352 | 8.584018 | 9.015215 |
| H | 5.991033 | 9.448119 | 9.933964 |
| H | 6.342882 | 8.857038 | 8.304419 |
| H | 3.224977 | 12.613639 | 8.954076 |

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|---|---|---|---|
| H | 3.956857 | 11.810278 | 10.356347 |
| H | 2.764962 | 10.959934 | 9.373827 |
| H | 8.753136 | 8.923978 | 9.752829 |
| H | 7.734190 | 9.911567 | 11.393655 |
| H | 9.427949 | 13.619290 | 12.345593 |
| H | 11.197615 | 14.043206 | 11.098423 |
| H | 12.268353 | 13.010991 | 9.431884 |
| H | 12.008253 | 11.127027 | 8.309411 |
| H | 11.469692 | 10.073659 | 5.998868 |
| H | 12.902992 | 9.552599 | 6.902744 |
| H | 12.056861 | 8.411371 | 5.858774 |
| H | 8.547312 | 7.509662 | 7.980734 |
| H | 8.659995 | 8.689992 | 6.663354 |
| H | 9.477093 | 7.124782 | 6.532903 |
| H | 11.939448 | 6.451017 | 8.298703 |
| H | 12.631996 | 7.682844 | 9.369906 |
| H | 11.083735 | 6.934723 | 9.773554 |
| H | 10.218167 | 13.483718 | 6.028525 |
| H | 8.626348 | 15.948804 | 9.036158 |
| H | 6.774677 | 15.101466 | 9.851437 |
| H | 12.313631 | 17.060633 | 8.913935 |
| H | 10.815205 | 16.650493 | 9.752698 |
| H | 12.037878 | 15.402917 | 9.469857 |
| H | 10.986506 | 18.236188 | 6.537206 |
| H | 9.740799 | 17.372117 | 5.618462 |
| H | 9.388991 | 17.963155 | 7.248032 |
| H | 12.506881 | 14.206567 | 6.598203 |
| H | 11.774963 | 15.009956 | 5.195968 |
| H | 12.966880 | 15.860283 | 6.178477 |
| H | 6.007541 | 13.835756 | 13.993040 |
| H | 7.400262 | 14.494579 | 13.130205 |
| H | 6.066414 | 13.765513 | 12.224356 |

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|---|---|---|---|
| H | 5.447095 | 10.849173 | 14.083455 |
| H | 5.528082 | 10.679145 | 12.327010 |
| H | 6.520927 | 9.644052 | 13.370202 |
| H | 7.786967 | 12.037002 | 15.734553 |
| H | 8.903098 | 10.872965 | 14.995751 |
| H | 9.251934 | 12.602438 | 14.913528 |
| H | 7.944910 | 14.783265 | -0.182191 |
| H | 6.479946 | 14.217801 | 0.638821 |
| H | 6.828760 | 15.947280 | 0.556615 |
| H | 10.284758 | 15.971111 | 1.468928 |
| H | 9.210904 | 17.176211 | 2.182185 |
| H | 10.203759 | 16.141124 | 3.225374 |
| H | 9.724359 | 12.984522 | 1.559319 |
| H | 9.665461 | 13.054741 | 3.328003 |
| H | 8.331636 | 12.325668 | 2.422125 |

**$Tm_2$(1,4-COT)$_3$:**

| | | | |
|---|---|---|---|
| C | 6.044716 | 19.269986 | 9.054023 |
| Si | 6.790724 | 19.088382 | 7.319246 |
| C | 6.177505 | 17.499920 | 6.454866 |
| C | 5.113974 | 16.810982 | 7.104631 |
| C | 4.351434 | 15.646172 | 6.848270 |
| C | 4.347141 | 14.642703 | 5.851979 |
| C | 5.088620 | 14.391249 | 4.673140 |
| C | 6.116664 | 15.058972 | 3.945733 |
| Si | 6.508559 | 14.202450 | 2.284336 |
| C | 6.791561 | 12.339240 | 2.514166 |
| C | 8.683278 | 19.093813 | 7.488936 |
| C | 6.268342 | 20.574964 | 6.262753 |
| C | 6.857850 | 17.248949 | 5.225509 |
| Tm | 6.813843 | 15.048612 | 6.452251 |
| C | 8.246908 | 14.742419 | 8.596089 |

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|---|---|---|---|
| C | 9.157864 | 14.692864 | 7.515032 |
| C | 9.431392 | 13.738307 | 6.495637 |
| Si | 10.941611 | 14.217442 | 5.427100 |
| C | 12.510677 | 14.110963 | 6.493222 |
| C | 6.821842 | 16.268191 | 4.200652 |
| C | 8.980617 | 12.402653 | 6.353879 |
| C | 7.979961 | 11.562276 | 6.895262 |
| Tm | 8.538455 | 11.863091 | 9.585429 |
| C | 10.489801 | 10.163677 | 9.803069 |
| C | 9.331957 | 9.582150 | 10.395082 |
| C | 8.287039 | 9.997421 | 11.262363 |
| C | 7.938855 | 11.184551 | 11.972604 |
| Si | 6.383069 | 11.077107 | 13.072299 |
| C | 5.183250 | 12.507326 | 12.714871 |
| C | 6.790720 | 11.735526 | 7.667283 |
| C | 6.397132 | 12.849064 | 8.460896 |
| C | 7.053068 | 14.031079 | 8.931547 |
| Si | 5.513055 | 10.327591 | 7.468521 |
| C | 4.875387 | 10.299548 | 5.682456 |
| C | 6.289625 | 8.637618 | 7.841791 |
| C | 4.036855 | 10.588424 | 8.632102 |
| C | 5.016929 | 14.449782 | 1.137175 |
| C | 8.038306 | 14.954687 | 1.452735 |
| C | 8.584494 | 12.451364 | 12.072023 |
| C | 9.740337 | 13.052617 | 11.522881 |
| C | 10.744943 | 12.655465 | 10.610034 |
| C | 11.048756 | 11.468455 | 9.898314 |
| Si | 11.480496 | 8.916974 | 8.750067 |
| C | 12.895609 | 9.764218 | 7.813557 |
| C | 10.386614 | 8.034293 | 7.472497 |
| C | 12.209078 | 7.616469 | 9.924793 |
| C | 6.932474 | 11.186278 | 14.885160 |

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|---|---|---|---|
| C | 5.457707 | 9.440861 | 12.816055 |
| C | 11.137784 | 13.058362 | 3.937616 |
| C | 10.791800 | 16.000947 | 4.795657 |
| H | 7.678724 | 17.943129 | 5.052459 |
| H | 7.606891 | 16.454635 | 3.472585 |
| H | 4.818831 | 13.428149 | 4.243954 |
| H | 3.672545 | 13.825823 | 6.096716 |
| H | 3.682247 | 15.407800 | 7.671622 |
| H | 4.866193 | 17.230999 | 8.075590 |
| H | 6.297609 | 18.425054 | 9.703000 |
| H | 4.954899 | 19.367906 | 9.028731 |
| H | 6.442923 | 20.176657 | 9.522752 |
| H | 9.187587 | 18.995808 | 6.522682 |
| H | 9.022914 | 18.274239 | 8.130876 |
| H | 9.019835 | 20.033676 | 7.940574 |
| H | 6.612427 | 21.516557 | 6.704317 |
| H | 5.178459 | 20.619646 | 6.170965 |
| H | 6.682906 | 20.504578 | 5.252118 |
| H | 5.420166 | 12.740899 | 8.924460 |
| H | 8.062842 | 10.555767 | 6.485780 |
| H | 9.559387 | 11.850545 | 5.614587 |
| H | 4.169677 | 9.474669 | 5.535031 |
| H | 5.697334 | 10.172256 | 4.971475 |
| H | 4.360598 | 11.233343 | 5.436662 |
| H | 5.556685 | 7.843646 | 7.659926 |
| H | 6.611258 | 8.567221 | 8.885420 |
| H | 7.157582 | 8.435525 | 7.207246 |
| H | 3.481856 | 11.502945 | 8.399109 |
| H | 4.338986 | 10.630430 | 9.683333 |
| H | 3.341050 | 9.749315 | 8.522807 |
| H | 9.133968 | 8.576007 | 10.027865 |
| H | 7.531991 | 9.220370 | 11.350604 |

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|---|---|---|---|
| H | 8.014277 | 13.175076 | 12.652934 |
| H | 9.816090 | 14.106341 | 11.780554 |
| H | 11.398804 | 13.478599 | 10.333446 |
| H | 11.890904 | 11.622493 | 9.229938 |
| H | 12.522638 | 10.521832 | 7.116971 |
| H | 13.615542 | 10.239053 | 8.487344 |
| H | 13.439130 | 9.014840 | 7.227649 |
| H | 9.532855 | 7.526733 | 7.931265 |
| H | 10.002800 | 8.746449 | 6.735180 |
| H | 10.971793 | 7.277817 | 6.937771 |
| H | 12.773633 | 6.856109 | 9.374086 |
| H | 12.883292 | 8.083199 | 10.649991 |
| H | 11.418301 | 7.109422 | 10.486729 |
| H | 8.407456 | 15.593008 | 9.254107 |
| H | 6.495299 | 14.517994 | 9.727816 |
| H | 4.333032 | 12.470729 | 13.404951 |
| H | 5.660162 | 13.485428 | 12.833796 |
| H | 4.789264 | 12.446923 | 11.695126 |
| H | 4.565127 | 9.429502 | 13.451286 |
| H | 5.126742 | 9.304588 | 11.781572 |
| H | 6.068861 | 8.576636 | 13.095013 |
| H | 6.072315 | 11.144006 | 15.562252 |
| H | 7.603878 | 10.358589 | 15.134991 |
| H | 7.470640 | 12.118953 | 15.081457 |
| H | 5.179785 | 13.968076 | 0.166751 |
| H | 4.108593 | 14.025387 | 1.576646 |
| H | 4.833929 | 15.514763 | 0.962249 |
| H | 8.241360 | 14.413505 | 0.521982 |
| H | 7.888910 | 16.007035 | 1.191067 |
| H | 8.932693 | 14.881382 | 2.078943 |
| H | 7.054090 | 11.879378 | 1.554773 |
| H | 7.603531 | 12.141542 | 3.220775 |

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|---|---|---|---|
| H | 5.895802 | 11.831444 | 2.884566 |
| H | 9.820641 | 15.557933 | 7.516264 |
| H | 11.947403 | 13.425218 | 3.297073 |
| H | 11.398434 | 12.037831 | 4.235746 |
| H | 10.227823 | 13.012213 | 3.331880 |
| H | 13.396626 | 14.401876 | 5.918025 |
| H | 12.442513 | 14.774555 | 7.361419 |
| H | 12.668119 | 13.093010 | 6.862735 |
| H | 11.672126 | 16.263970 | 4.198771 |
| H | 9.905775 | 16.126678 | 4.166669 |
| H | 10.725144 | 16.722917 | 5.615678 |

**$Tm_2$(1,5-COT)(1,4-COT)$_2$:**

| | | | |
|---|---|---|---|
| C | 4.123214 | 17.899850 | 9.161303 |
| Si | 5.340956 | 18.432667 | 7.807649 |
| C | 6.988575 | 18.880692 | 8.642499 |
| C | 4.658209 | 19.975590 | 6.939290 |
| C | 5.576620 | 17.065359 | 6.498574 |
| C | 6.591879 | 17.389150 | 5.548153 |
| C | 7.139701 | 16.806703 | 4.373363 |
| Tm | 7.050966 | 14.996534 | 6.161990 |
| C | 9.256852 | 13.250332 | 6.119894 |
| C | 8.632004 | 11.992968 | 6.246365 |
| C | 7.663373 | 11.387797 | 7.072450 |
| C | 6.642403 | 11.874075 | 7.940992 |
| Si | 5.149924 | 10.692595 | 8.112918 |
| C | 5.708653 | 8.976361 | 8.695627 |
| C | 4.705454 | 15.946601 | 6.601971 |
| C | 4.513180 | 14.738375 | 5.890678 |
| C | 5.104178 | 14.123687 | 4.761727 |
| C | 6.114605 | 14.480671 | 3.837481 |
| C | 6.965475 | 15.603957 | 3.633241 |

| | | | |
|---|---|---|---|
| Si | 7.956823 | 15.469082 | 2.007493 |
| C | 6.726156 | 15.620402 | 0.570627 |
| C | 9.235636 | 16.861174 | 1.837442 |
| C | 8.850192 | 13.799082 | 1.862430 |
| C | 7.453429 | 14.257747 | 8.724094 |
| Tm | 8.585372 | 11.986639 | 9.647582 |
| C | 8.147767 | 11.428890 | 12.101789 |
| C | 8.886450 | 12.648144 | 12.090935 |
| C | 10.042482 | 13.128176 | 11.434088 |
| C | 10.934214 | 12.613626 | 10.465235 |
| C | 11.063737 | 11.397284 | 9.750813 |
| C | 10.386948 | 10.145210 | 9.731242 |
| Si | 11.162249 | 8.828910 | 8.586015 |
| C | 9.836793 | 7.809147 | 7.686034 |
| C | 8.696909 | 14.695211 | 8.155509 |
| C | 9.430583 | 14.372497 | 6.980158 |
| Si | 10.933505 | 15.506212 | 6.639356 |
| C | 10.430800 | 17.335629 | 6.688085 |
| C | 6.545894 | 13.160209 | 8.540068 |
| C | 9.260521 | 9.671410 | 10.462975 |
| C | 8.349606 | 10.192611 | 11.419003 |
| Si | 6.716870 | 11.461672 | 13.363961 |
| C | 7.471754 | 11.459687 | 15.104798 |
| C | 5.586753 | 9.947357 | 13.194772 |
| C | 5.657452 | 13.027817 | 13.167382 |
| C | 3.879736 | 11.378270 | 9.342972 |
| C | 4.307396 | 10.495319 | 6.424066 |
| C | 12.201975 | 7.660384 | 9.661119 |
| C | 12.281814 | 9.622409 | 7.274430 |
| C | 11.708237 | 15.124613 | 4.953457 |
| C | 12.255901 | 15.234760 | 7.973223 |
| H | 7.133650 | 18.298687 | 5.804330 |

| | | | |
|---|---|---|---|
| H | 7.958392 | 17.413941 | 3.994955 |
| H | 6.311653 | 13.663331 | 3.146475 |
| H | 4.740770 | 13.111991 | 4.603198 |
| H | 3.804397 | 14.080966 | 6.388120 |
| H | 4.088010 | 15.970813 | 7.495823 |
| H | 4.467502 | 17.010461 | 9.699217 |
| H | 3.124552 | 17.694374 | 8.763196 |
| H | 4.024450 | 18.709650 | 9.892545 |
| H | 7.754476 | 19.175893 | 7.918708 |
| H | 7.378260 | 18.034500 | 9.218362 |
| H | 6.847971 | 19.718722 | 9.334222 |
| H | 4.519839 | 20.800199 | 7.647128 |
| H | 3.691262 | 19.760120 | 6.473553 |
| H | 5.335607 | 20.318474 | 6.150765 |
| H | 5.632785 | 13.318910 | 9.108963 |
| H | 7.555146 | 10.328487 | 6.840960 |
| H | 8.994971 | 11.296508 | 5.490468 |
| H | 3.506552 | 9.749418 | 6.474937 |
| H | 5.021796 | 10.171057 | 5.660890 |
| H | 3.865281 | 11.439496 | 6.091734 |
| H | 4.853448 | 8.291852 | 8.720235 |
| H | 6.135952 | 9.022770 | 9.701583 |
| H | 6.461552 | 8.540075 | 8.032124 |
| H | 3.456102 | 12.330743 | 9.008205 |
| H | 4.306129 | 11.525405 | 10.339970 |
| H | 3.049935 | 10.669678 | 9.440289 |
| H | 8.944815 | 8.678101 | 10.150157 |
| H | 7.557731 | 9.475255 | 11.618304 |
| H | 8.425200 | 13.432847 | 12.688084 |
| H | 10.232796 | 14.176878 | 11.650505 |
| H | 11.638286 | 13.364642 | 10.120229 |
| H | 11.848379 | 11.470172 | 9.002728 |

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|---|---|---|---|
| H | 11.743271 | 10.366905 | 6.679551 |
| H | 13.161525 | 10.103893 | 7.713128 |
| H | 12.644232 | 8.845866 | 6.591583 |
| H | 9.171556 | 7.278547 | 8.374133 |
| H | 9.222819 | 8.446557 | 7.042285 |
| H | 10.317994 | 7.055637 | 7.052532 |
| H | 12.678155 | 6.879275 | 9.058411 |
| H | 12.988503 | 8.214335 | 10.183514 |
| H | 11.581298 | 7.172352 | 10.419523 |
| H | 9.889662 | 13.289303 | 5.236708 |
| H | 9.078601 | 15.561118 | 8.695069 |
| H | 7.096963 | 14.946165 | 9.488383 |
| H | 13.124148 | 15.876334 | 7.785990 |
| H | 11.873061 | 15.475948 | 8.969801 |
| H | 12.599131 | 14.195760 | 7.981308 |
| H | 11.311492 | 17.974275 | 6.557952 |
| H | 9.721488 | 17.570858 | 5.888427 |
| H | 9.964647 | 17.608016 | 7.640235 |
| H | 12.122997 | 14.112655 | 4.912394 |
| H | 10.991730 | 15.234915 | 4.134283 |
| H | 12.531142 | 15.824284 | 4.770301 |
| H | 4.873162 | 13.047784 | 13.932241 |
| H | 6.246241 | 13.943685 | 13.280092 |
| H | 5.169741 | 13.061385 | 12.187804 |
| H | 4.772697 | 10.026232 | 13.923831 |
| H | 5.133008 | 9.871285 | 12.201783 |
| H | 6.117862 | 9.012517 | 13.400259 |
| H | 6.692988 | 11.495205 | 15.874508 |
| H | 8.068796 | 10.556390 | 15.265742 |
| H | 8.130447 | 12.321747 | 15.249969 |
| H | 7.235652 | 15.543865 | -0.396291 |
| H | 5.965843 | 14.834191 | 0.614894 |

| | | | |
|---|---|---|---|
| H | 6.207681 | 16.583901 | 0.606814 |
| H | 9.782719 | 16.728359 | 0.897481 |
| H | 8.761814 | 17.847368 | 1.802075 |
| H | 9.971750 | 16.865226 | 2.647342 |
| H | 9.341632 | 13.721203 | 0.886189 |
| H | 9.617136 | 13.687383 | 2.634743 |
| H | 8.161751 | 12.952879 | 1.951448 |

**$Lu_2$(1,4-COT)$_3$:**

| | | | |
|---|---|---|---|
| C | 5.475596 | 1.410550 | 4.313876 |
| C | 6.795614 | 1.022961 | 4.687510 |
| H | 7.129474 | 0.129327 | 4.167111 |
| C | 7.836803 | 1.539423 | 5.503418 |
| H | 8.723540 | 0.914094 | 5.412545 |
| C | 8.061754 | 2.697517 | 6.301765 |
| C | 7.238470 | 3.819079 | 6.590784 |
| H | 7.752672 | 4.596846 | 7.147577 |
| C | 5.919674 | 4.219542 | 6.263353 |
| H | 5.692817 | 5.216825 | 6.630100 |
| C | 4.860493 | 3.675914 | 5.499472 |
| H | 4.013090 | 4.353124 | 5.435512 |
| C | 4.682827 | 2.531429 | 4.689107 |
| H | 3.725038 | 2.569583 | 4.172743 |
| C | 3.170975 | -0.633358 | 4.228265 |
| H | 2.584803 | -1.334783 | 3.624519 |
| H | 2.484260 | 0.110949 | 4.643804 |
| H | 3.606273 | -1.186556 | 5.066548 |
| C | 5.670344 | -1.163425 | 2.505632 |
| H | 6.479235 | -0.756506 | 1.890630 |
| H | 5.081908 | -1.836214 | 1.871836 |
| H | 6.116077 | -1.771958 | 3.298863 |
| C | 3.720008 | 1.083066 | 1.724390 |

| | | | |
|---|---|---|---|
| H | 4.470199 | 1.558293 | 1.084071 |
| H | 3.015358 | 1.856380 | 2.045361 |
| H | 3.161585 | 0.367260 | 1.110896 |
| C | 10.141688 | 4.345886 | 7.993240 |
| H | 11.137947 | 4.303759 | 8.447171 |
| H | 9.428284 | 4.573982 | 8.791409 |
| H | 10.136681 | 5.177407 | 7.281258 |
| C | 9.751309 | 1.321319 | 8.473056 |
| H | 10.713010 | 1.259183 | 8.994034 |
| H | 9.545305 | 0.343106 | 8.026809 |
| H | 8.972359 | 1.515885 | 9.217172 |
| C | 11.173020 | 2.320410 | 5.925668 |
| H | 12.127594 | 2.249547 | 6.459010 |
| H | 11.263889 | 3.119605 | 5.183155 |
| H | 11.026846 | 1.376349 | 5.391630 |
| C | 8.245370 | 3.936890 | 1.957526 |
| C | 6.896999 | 4.339120 | 1.667313 |
| H | 6.416744 | 3.703849 | 0.925506 |
| C | 5.929827 | 5.250828 | 2.235925 |
| H | 4.929907 | 4.986792 | 1.897543 |
| C | 5.965907 | 6.501149 | 2.941444 |
| C | 7.103369 | 7.209349 | 3.420539 |
| H | 6.882404 | 8.227335 | 3.742732 |
| C | 8.424365 | 6.831387 | 3.733005 |
| H | 8.972246 | 7.637095 | 4.218219 |
| C | 9.169092 | 5.640136 | 3.697528 |
| H | 10.073285 | 5.705949 | 4.300765 |
| C | 9.118871 | 4.439815 | 2.960003 |
| H | 10.007539 | 3.827282 | 3.112326 |
| C | 10.635739 | 3.177075 | 0.093900 |
| H | 10.453756 | 3.978215 | -0.626810 |
| H | 11.137035 | 2.357540 | -0.433006 |

| | | | |
|---|---|---|---|
| H | 11.328237 | 3.560206 | 0.850032 |
| C | 9.516893 | 1.065746 | 1.971377 |
| H | 8.642277 | 0.602879 | 2.436555 |
| H | 10.208368 | 1.352730 | 2.769916 |
| H | 10.017440 | 0.308014 | 1.357959 |
| C | 7.835754 | 1.971895 | -0.455445 |
| H | 7.541257 | 2.791638 | -1.118133 |
| H | 6.926249 | 1.525616 | -0.040537 |
| H | 8.323221 | 1.207657 | -1.070532 |
| C | 2.844275 | 6.339625 | 2.674030 |
| H | 1.904756 | 6.837562 | 2.937549 |
| H | 2.812505 | 5.330694 | 3.097438 |
| H | 2.872990 | 6.251124 | 1.583138 |
| C | 4.217875 | 9.101136 | 2.628285 |
| H | 5.055135 | 9.720291 | 2.965699 |
| H | 3.294280 | 9.591257 | 2.956499 |
| H | 4.224778 | 9.091822 | 1.534939 |
| C | 4.111150 | 7.539135 | 5.231426 |
| H | 4.989949 | 8.027722 | 5.664115 |
| H | 3.982105 | 6.576696 | 5.733118 |
| H | 3.236407 | 8.157004 | 5.462775 |
| C | 6.053713 | 7.163476 | -1.433516 |
| C | 6.021740 | 8.438208 | -0.795824 |
| H | 5.021169 | 8.861179 | -0.755904 |
| C | 6.944738 | 9.284252 | -0.124336 |
| H | 6.433876 | 10.160095 | 0.266049 |
| C | 8.312444 | 9.234008 | 0.264226 |
| C | 9.309260 | 8.232803 | 0.097016 |
| H | 10.233569 | 8.452204 | 0.628443 |
| C | 9.383294 | 6.969727 | -0.539314 |
| H | 10.334521 | 6.473630 | -0.364799 |
| C | 8.483311 | 6.164350 | -1.275760 |

| | | | |
|---|---|---|---|
| H | 8.919424 | 5.207350 | -1.547701 |
| C | 7.117582 | 6.240769 | -1.635157 |
| H | 6.795010 | 5.317594 | -2.114103 |
| C | 2.975905 | 7.726982 | -1.788243 |
| H | 2.801127 | 7.765286 | -0.708336 |
| H | 2.061216 | 7.347433 | -2.256796 |
| H | 3.125542 | 8.750424 | -2.146593 |
| C | 3.985601 | 4.817415 | -1.736666 |
| H | 3.793557 | 4.752122 | -0.660714 |
| H | 4.782567 | 4.107379 | -1.978685 |
| H | 3.081337 | 4.484291 | -2.258075 |
| C | 4.660446 | 6.646130 | -4.131250 |
| H | 4.888584 | 7.664784 | -4.460873 |
| H | 3.757347 | 6.312670 | -4.654002 |
| H | 5.489358 | 6.003823 | -4.444974 |
| C | 7.600794 | 12.036898 | 1.515449 |
| H | 8.034494 | 12.914003 | 2.008575 |
| H | 6.850366 | 11.616337 | 2.192584 |
| H | 7.088898 | 12.388313 | 0.614085 |
| C | 10.210513 | 11.627879 | -0.073941 |
| H | 10.637728 | 12.536710 | 0.363796 |
| H | 9.712815 | 11.901476 | -1.009771 |
| H | 11.035374 | 10.952774 | -0.323168 |
| C | 9.892339 | 10.397767 | 2.737894 |
| H | 10.362068 | 11.302165 | 3.140534 |
| H | 10.678570 | 9.648864 | 2.603432 |
| H | 9.193176 | 10.018789 | 3.489567 |
| Si | 4.531075 | 0.189524 | 3.192267 |
| Si | 9.769752 | 2.686062 | 7.154029 |
| Si | 9.032861 | 2.552518 | 0.894861 |
| Si | 4.299707 | 7.347648 | 3.352579 |
| Si | 4.425395 | 6.593440 | -2.249465 |

| | | | |
|---|---|---|---|
| Si | 8.986583 | 10.802606 | 1.118932 |
| Lu | 6.977309 | 3.448929 | 4.110635 |
| Lu | 7.244757 | 6.961472 | 0.795388 |

**$Lu_2$(1,5-COT)(1,4-COT)$_2$:**

| | | | |
|---|---|---|---|
| C | 4.065714 | -1.394045 | 3.668222 |
| Si | 5.432290 | -0.359908 | 2.853459 |
| C | 4.781604 | 0.307192 | 1.196871 |
| C | 5.885613 | 1.065331 | 4.037981 |
| Lu | 6.912746 | 3.370188 | 3.925844 |
| C | 7.301889 | 4.031334 | 1.471969 |
| Lu | 6.990832 | 6.905965 | 0.685826 |
| C | 8.358398 | 6.208389 | -1.338183 |
| C | 7.009364 | 5.972778 | -1.686991 |
| C | 5.792727 | 6.673092 | -1.523362 |
| C | 5.400601 | 7.933803 | -0.987182 |
| Si | 3.530865 | 8.254846 | -1.197797 |
| C | 3.178534 | 8.460729 | -3.050520 |
| C | 7.171114 | 0.989982 | 4.650411 |
| C | 7.926024 | 1.758168 | 5.575700 |
| C | 7.759213 | 2.971425 | 6.302098 |
| Si | 9.230916 | 3.405490 | 7.438093 |
| C | 10.897836 | 2.972366 | 6.638133 |
| C | 4.814631 | 1.991951 | 4.196543 |
| C | 4.589785 | 3.163605 | 4.953598 |
| C | 5.357307 | 3.946689 | 5.845556 |
| C | 6.666044 | 3.879643 | 6.383319 |
| C | 8.585355 | 3.954856 | 2.076352 |
| Si | 9.853302 | 2.739253 | 1.325316 |
| C | 9.038773 | 1.634375 | 0.016519 |
| C | 9.135531 | 4.817112 | 3.073052 |
| C | 8.875108 | 6.143142 | 3.468606 |

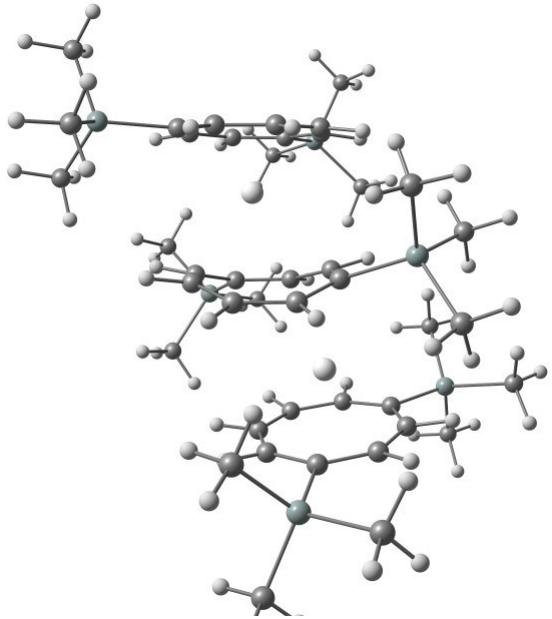
| | | | |
|---|---|---|---|
| C | 7.810038 | 7.058082 | 3.367035 |
| C | 6.400308 | 6.922016 | 3.186071 |
| C | 5.696735 | 5.824859 | 2.622868 |
| C | 6.076599 | 4.705490 | 1.805704 |
| C | 6.158759 | 8.995891 | -0.412254 |
| C | 7.519397 | 9.244591 | -0.092286 |
| C | 8.752740 | 8.539008 | -0.176641 |
| Si | 10.273752 | 9.509993 | 0.447830 |
| C | 11.602453 | 8.339383 | 1.130539 |
| C | 9.070418 | 7.252615 | -0.698950 |
| C | 6.916955 | -1.488855 | 2.507058 |
| C | 9.257992 | 5.255114 | 7.863326 |
| C | 9.044789 | 2.404348 | 9.039772 |
| C | 11.250767 | 3.726277 | 0.503957 |
| C | 10.630843 | 1.636346 | 2.658312 |
| C | 2.982696 | 9.830849 | -0.295047 |
| C | 2.504659 | 6.796520 | -0.540473 |
| C | 9.811203 | 10.735523 | 1.822342 |
| C | 10.996400 | 10.480178 | -1.015018 |
| H | 7.770988 | 0.173567 | 4.256562 |
| H | 8.930561 | 1.351017 | 5.666380 |
| H | 6.892927 | 4.772923 | 6.958670 |
| H | 4.851191 | 4.869849 | 6.114919 |
| H | 3.641219 | 3.635190 | 4.708048 |
| H | 3.981630 | 1.802738 | 3.521285 |
| H | 3.757904 | -2.221705 | 3.019880 |
| H | 3.181183 | -0.785778 | 3.882087 |
| H | 4.413821 | -1.815724 | 4.616554 |
| H | 7.752905 | -0.955339 | 2.043801 |
| H | 6.608648 | -2.281481 | 1.816351 |
| H | 7.284085 | -1.973754 | 3.417245 |
| H | 5.552008 | 0.880359 | 0.670885 |

| | | | |
|---|---|---|---|
| H | 3.910228 | 0.956800 | 1.327172 |
| H | 4.478561 | -0.521462 | 0.547314 |
| H | 10.164879 | 5.479867 | 8.435710 |
| H | 8.404602 | 5.558108 | 8.477783 |
| H | 9.268234 | 5.874528 | 6.960948 |
| H | 9.870353 | 2.601707 | 9.732298 |
| H | 9.027889 | 1.330358 | 8.828408 |
| H | 8.107639 | 2.656771 | 9.546152 |
| H | 11.710115 | 3.214379 | 7.332619 |
| H | 11.056382 | 3.552008 | 5.723455 |
| H | 10.989654 | 1.910872 | 6.389208 |
| H | 7.138597 | 3.311438 | 0.673746 |
| H | 5.218678 | 4.259032 | 1.305940 |
| H | 8.100063 | 8.047418 | 3.720721 |
| H | 9.728981 | 6.580143 | 3.987147 |
| H | 10.094663 | 4.468697 | 3.455716 |
| H | 10.874108 | 4.341888 | -0.318326 |
| H | 12.012737 | 3.050987 | 0.099290 |
| H | 11.739570 | 4.392273 | 1.221563 |
| H | 9.889384 | 0.967495 | 3.104828 |
| H | 11.084142 | 2.220220 | 3.465088 |
| H | 11.420329 | 1.018785 | 2.215471 |
| H | 8.643233 | 2.213254 | -0.824335 |
| H | 8.224413 | 1.031528 | 0.430466 |
| H | 9.786676 | 0.943184 | -0.387210 |
| H | 5.529791 | 9.803478 | -0.046815 |
| H | 7.610942 | 10.183492 | 0.447991 |
| H | 10.104476 | 6.965346 | -0.526410 |
| H | 8.984591 | 5.339887 | -1.524853 |
| H | 6.855579 | 4.967892 | -2.073214 |
| H | 4.948535 | 6.056794 | -1.827895 |
| H | 3.181985 | 9.787576 | 0.780326 |

| | | | |
|---|---|---|---|
| H | 1.902678 | 9.961638 | -0.424923 |
| H | 3.470108 | 10.724773 | -0.697005 |
| H | 2.657758 | 6.655798 | 0.534422 |
| H | 2.753698 | 5.855312 | -1.040668 |
| H | 1.437272 | 6.981370 | -0.704770 |
| H | 3.723788 | 9.320552 | -3.452707 |
| H | 2.110390 | 8.616722 | -3.237089 |
| H | 3.494358 | 7.576417 | -3.613002 |
| H | 10.713566 | 11.255181 | 2.163389 |
| H | 9.376207 | 10.221500 | 2.685081 |
| H | 9.103926 | 11.501356 | 1.489441 |
| H | 11.887962 | 11.043623 | -0.718588 |
| H | 10.263312 | 11.188809 | -1.413568 |
| H | 11.277780 | 9.802669 | -1.827637 |
| H | 12.401579 | 8.926352 | 1.596791 |
| H | 12.064119 | 7.726572 | 0.350192 |
| H | 11.185372 | 7.669476 | 1.888807 |
| H | 4.614085 | 5.907821 | 2.681910 |
| Si | 5.376927 | 8.273752 | 4.066358 |
| C | 5.709558 | 8.177072 | 5.932218 |
| C | 5.863627 | 10.009792 | 3.478096 |
| C | 3.521599 | 8.025232 | 3.760177 |
| H | 5.322360 | 10.764601 | 4.059577 |
| H | 6.932946 | 10.203426 | 3.604552 |
| H | 5.618934 | 10.156858 | 2.422245 |
| H | 5.170836 | 8.968891 | 6.464166 |
| H | 5.387833 | 7.215347 | 6.342844 |
| H | 6.776295 | 8.291330 | 6.148515 |
| H | 2.963759 | 8.831628 | 4.248711 |
| H | 3.273666 | 8.052296 | 2.694581 |
| H | 3.155994 | 7.079591 | 4.173233 |

**Scandium complex (4Sc)**

1,4 isomer



1,5 isomer

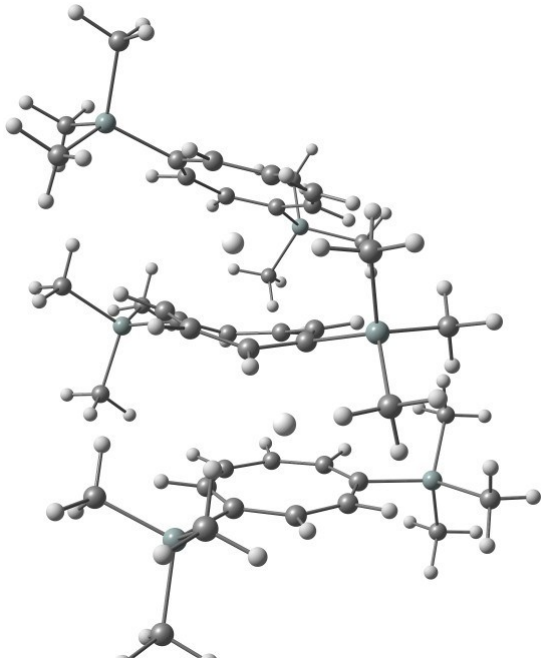


**Figure S19.** Optimized structures

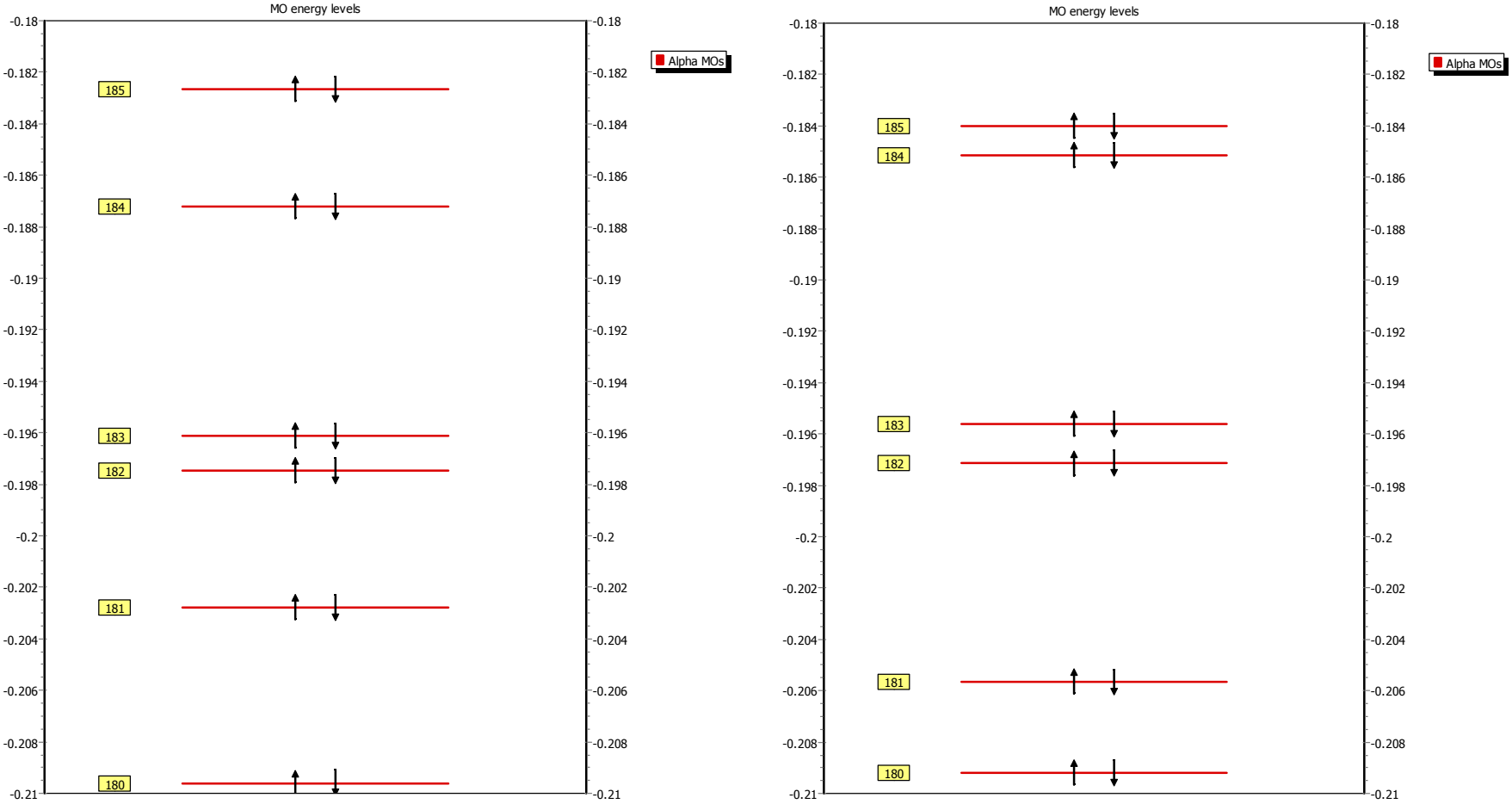
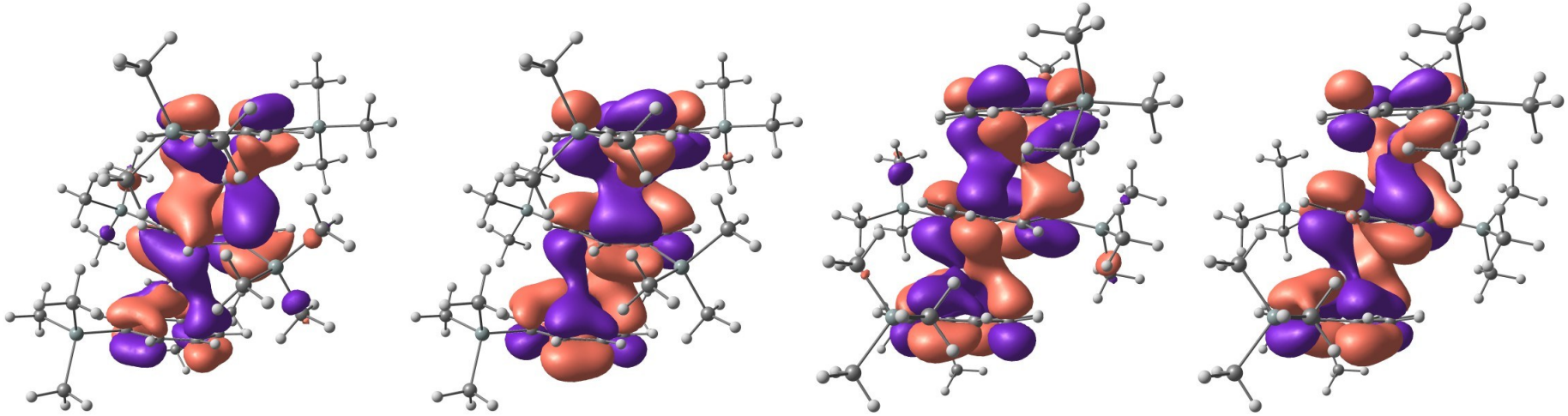



**Figure S20.** Associated MO diagrams focusing on the frontier orbitals (MO 185 being the HOMO)



(a) (b) (c) (d)

**Figure S21.** δ-bonding orbitals: HOMO (a,c) and HOMO-1 (b,d)

The two δ-bonds are overall slightly more stable for the 1,4-COT'' complex than for the 1,5-COT'' one, as the two formally degenerated orbitals are strongly energetically splitted in the 1,4 isomer in line with a first order Jahn-Teller effect associated with the strongly distorted COT ring in between the two metal centers. The same holds true for the Lutetium complex.

**Lanthanum complex (4La)**

1,4 isomer

1,5 isomer

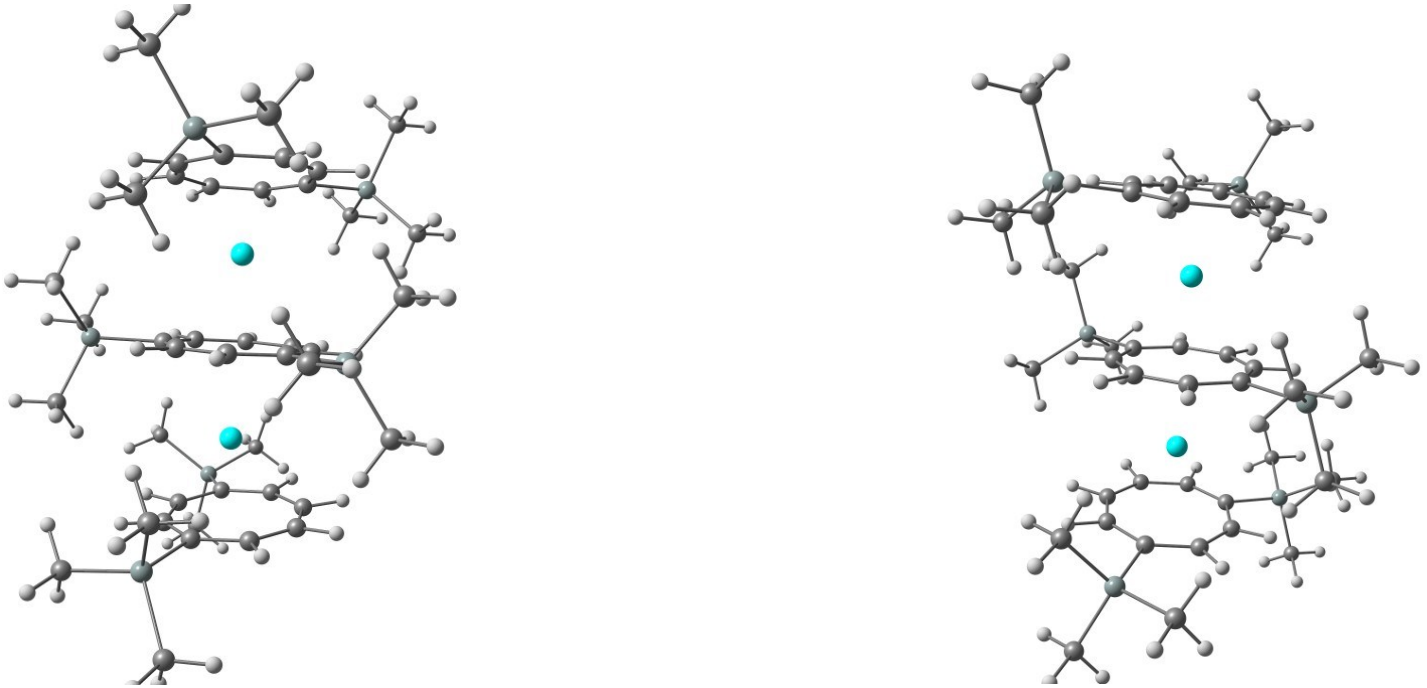


**Figure S22.** Optimized structures

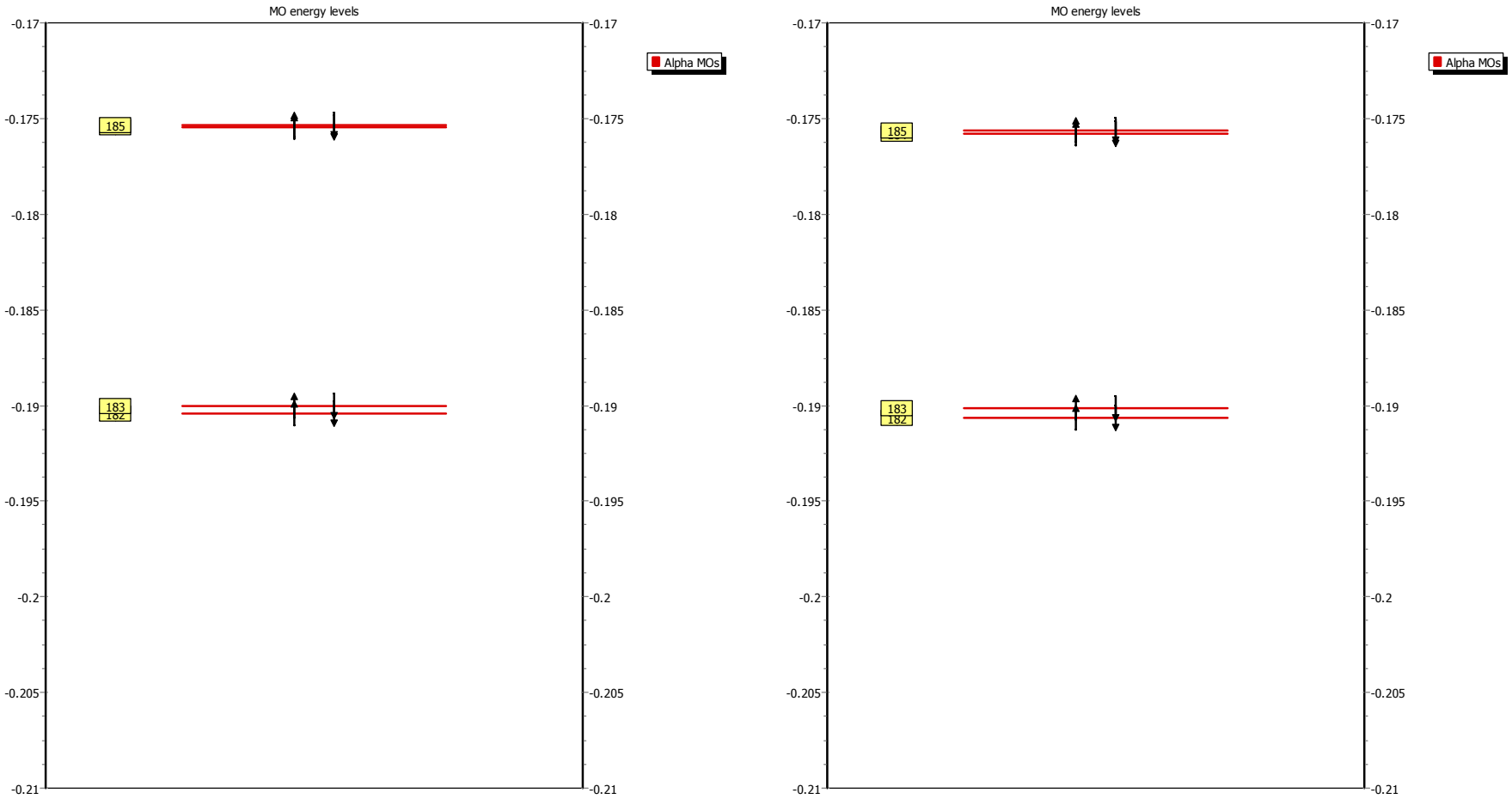
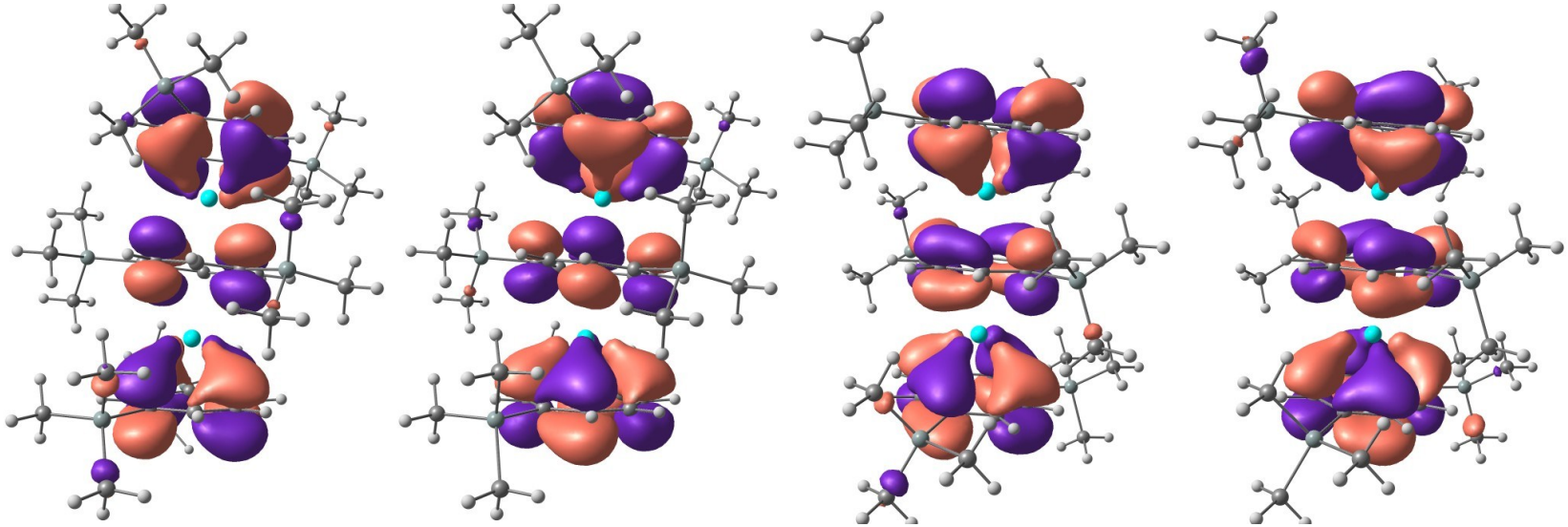



**Figure S23.** Associated MO diagrams focusing on the frontier orbitals (MO 185 being the HOMO)



(a) (b) (c) (d)

**Figure S24.** δ-bonding orbitals: HOMO (a,c) and HOMO-1 (b,d)

The two δ-bonds are overall slightly more stable for the 1,5-COT'' isomer than for the 1,4-COT'' one, as the two formally degenerated orbitals are energetically splitted in the 1,5 isomer in line with a first order Jahn-Teller effect. This is the same effect as for **4Sc** and **4Lu**, but in the opposite direction as there is no distortion of the ring. Therefore, it is the steric repulsion between the silyl groups inducing the first order Jahn teller effect. The same holds true for **4Y**.

**Yttrium complex (4Y)**

1,4 isomer

1,5 isomer

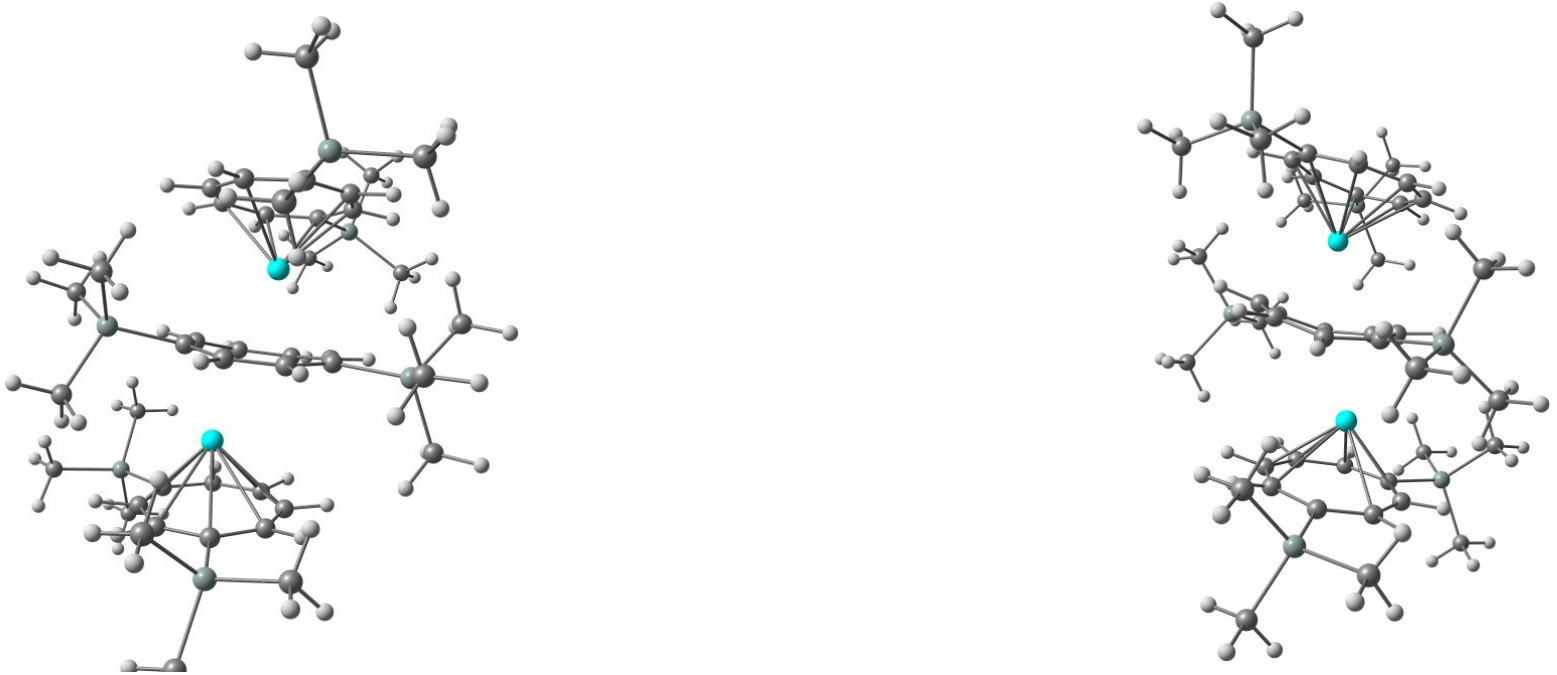


**Figure S25.** Optimized structures

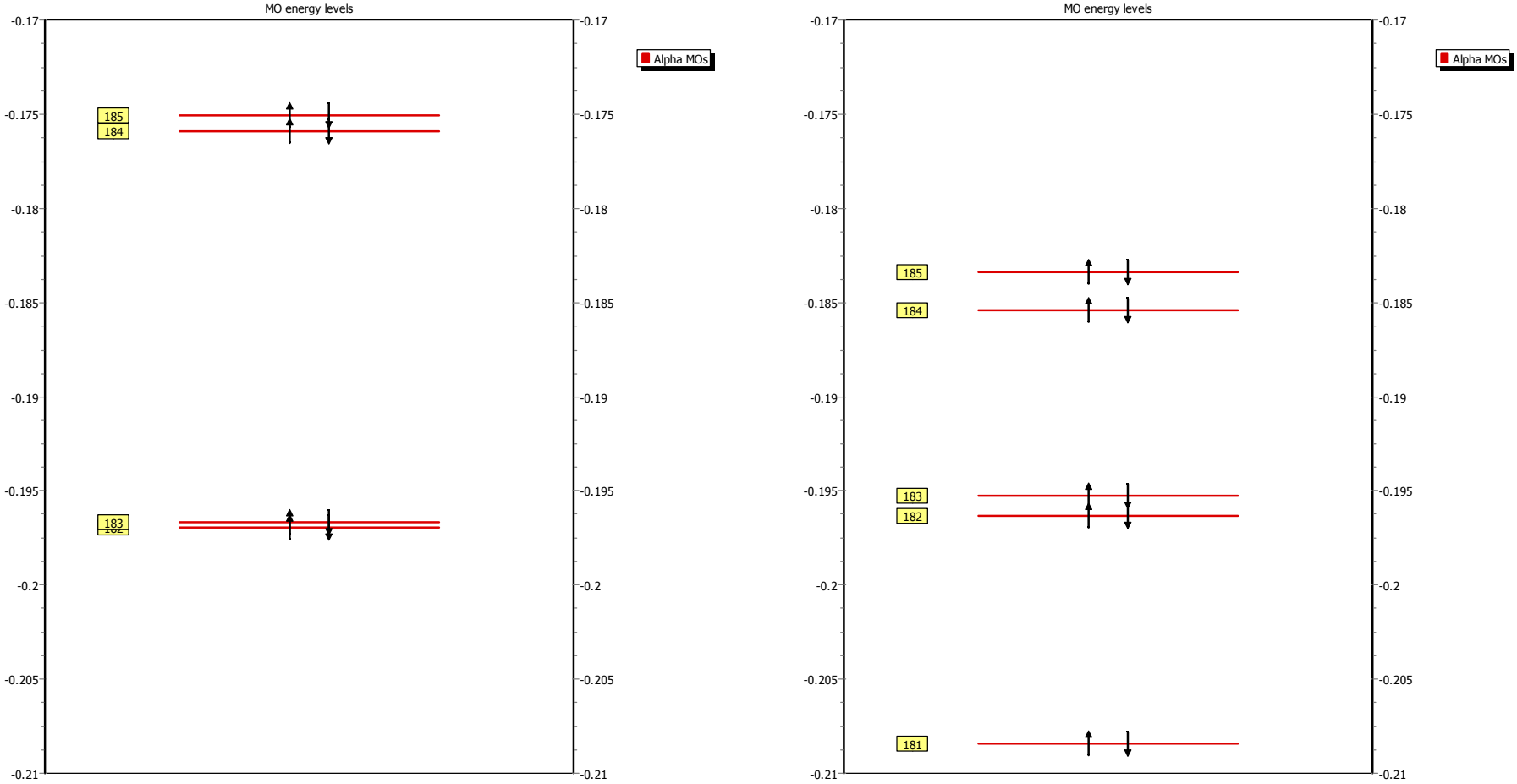
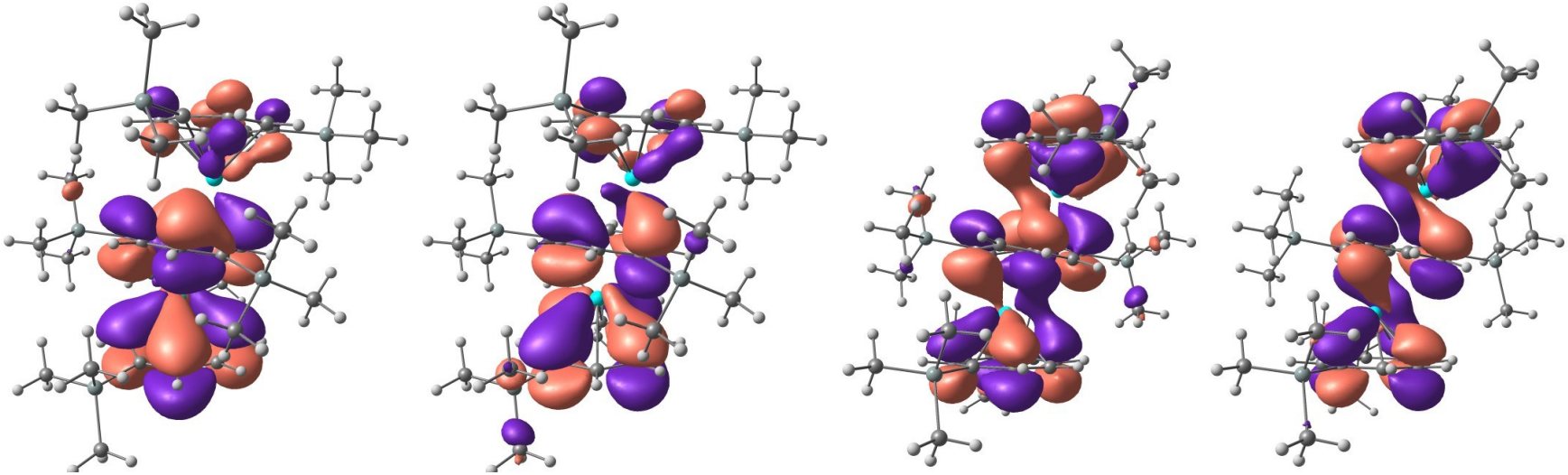



**Figure S26.** Associated MO diagrams focusing on the frontier orbitals (MO 185 being the HOMO)



(a) (b) (c) (d)

**Figure S27.** δ-bonding orbitals: HOMO (a,c) and HOMO-1 (b,d)

**Neodymium complex (4Nd)**

1,4 isomer

1,5 isomer

**Figure S28.** Optimized structures

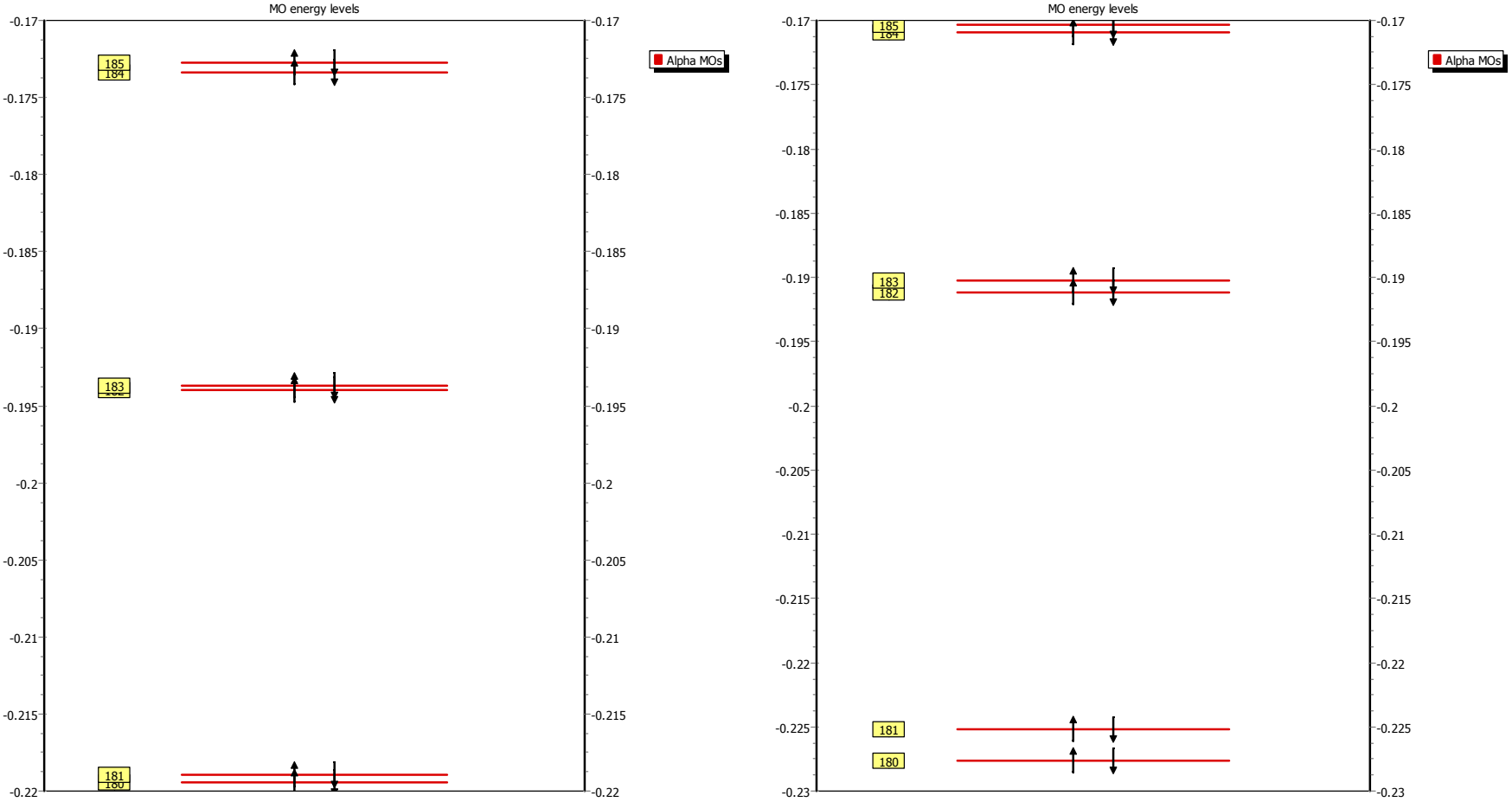
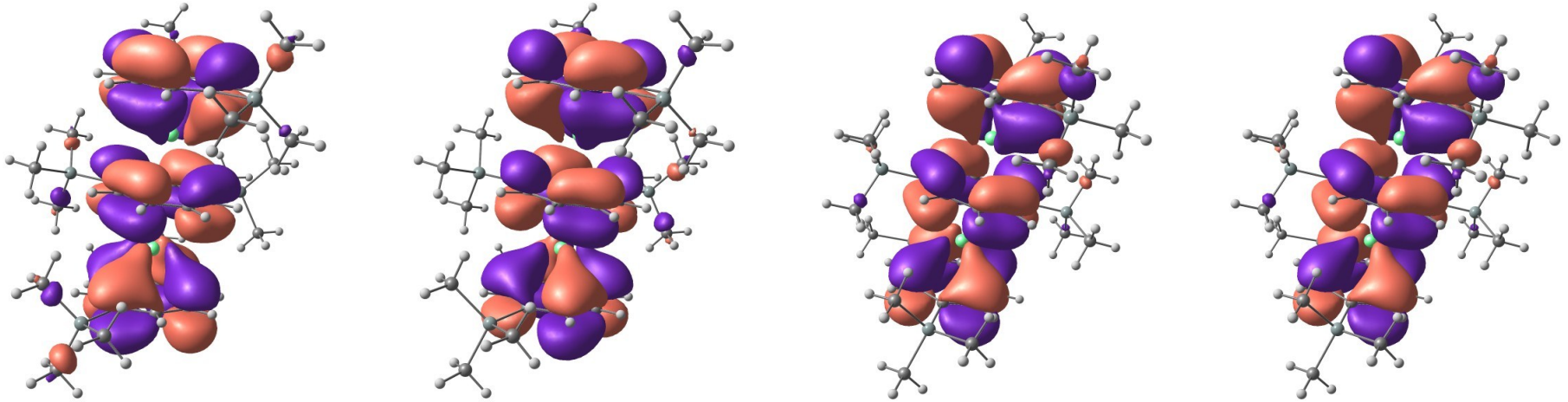



**Figure S29.** Associated MO diagrams focusing on the frontier orbitals (MO 185 being the HOMO)



(a) (b) (c) (d)

**Figure S20.** δ-bonding orbitals: HOMO (a,c) and HOMO-1 (b,d)

**Holmium complex (4Ho)**

1,4 isomer

1,5 isomer

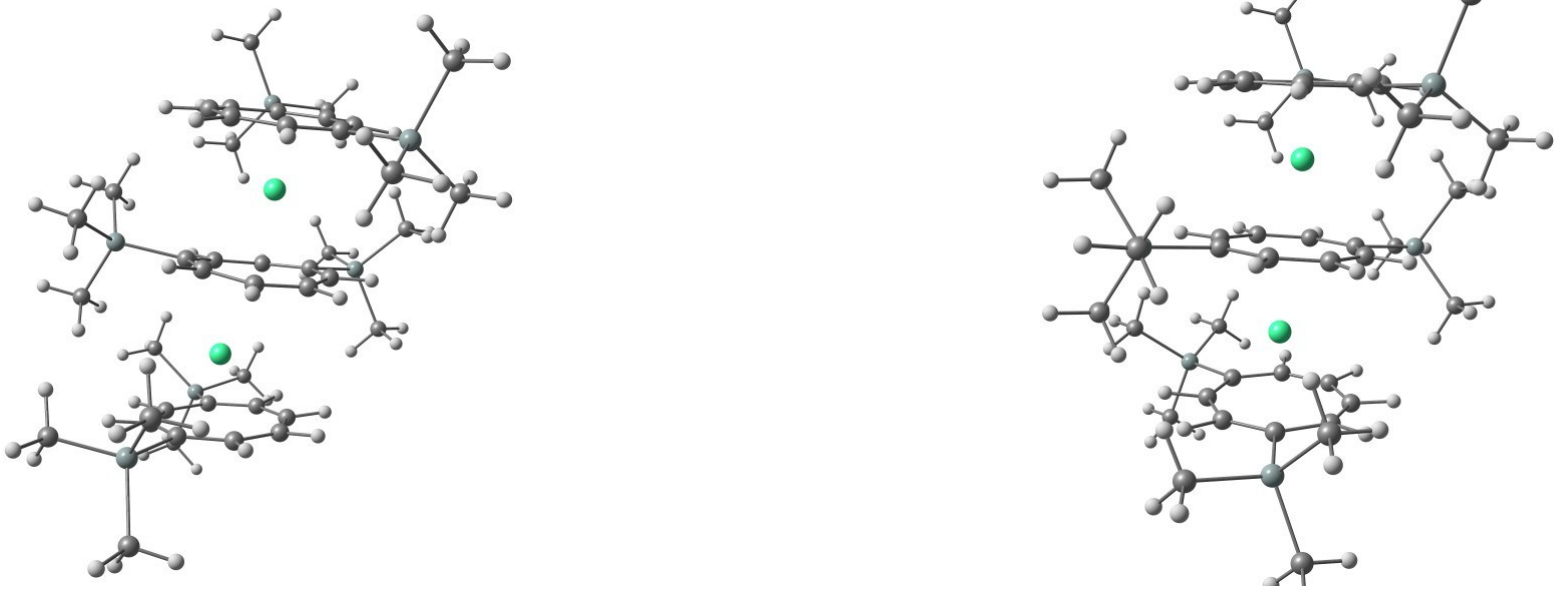


**Figure S31.** Optimized structures

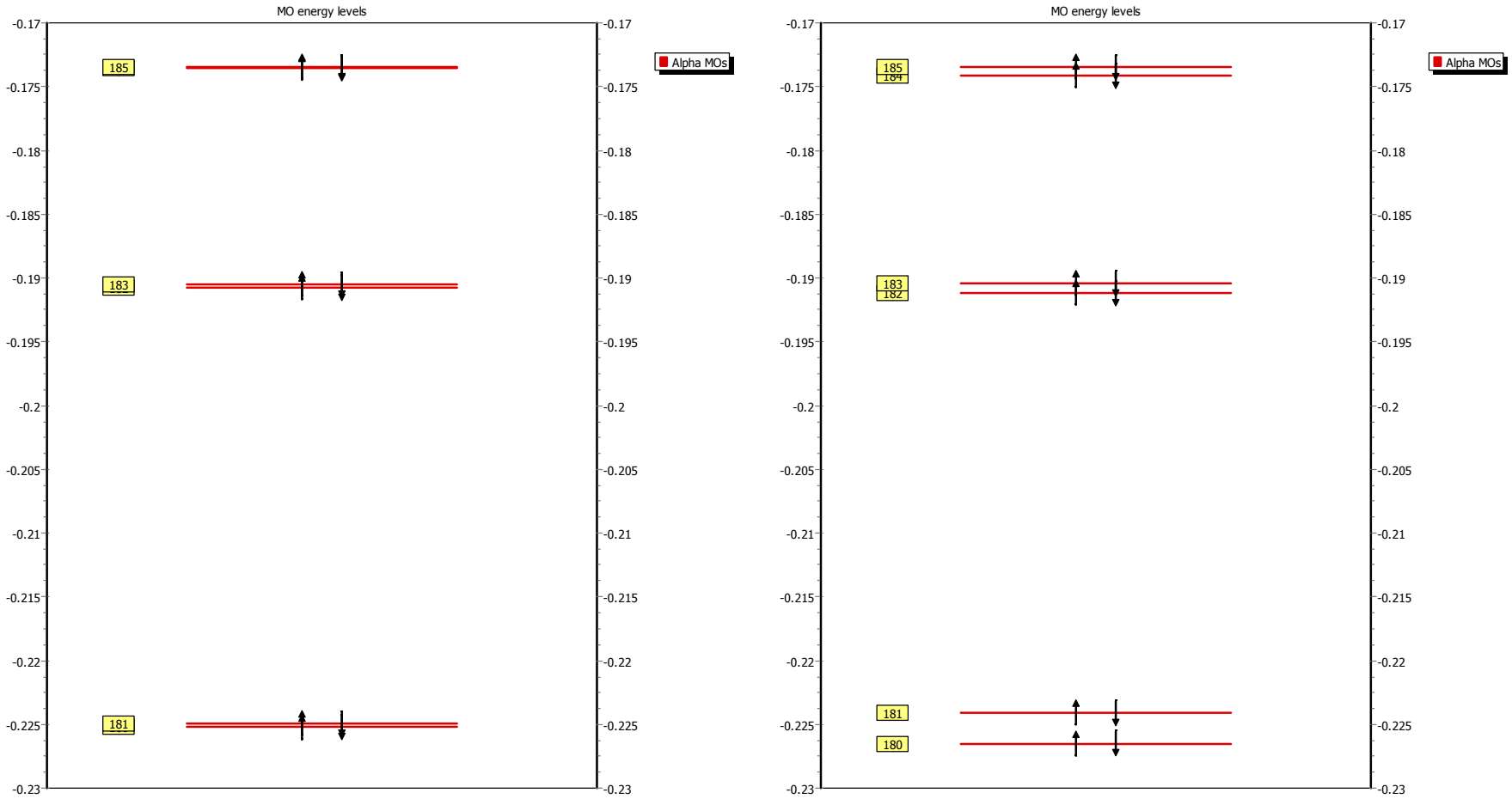
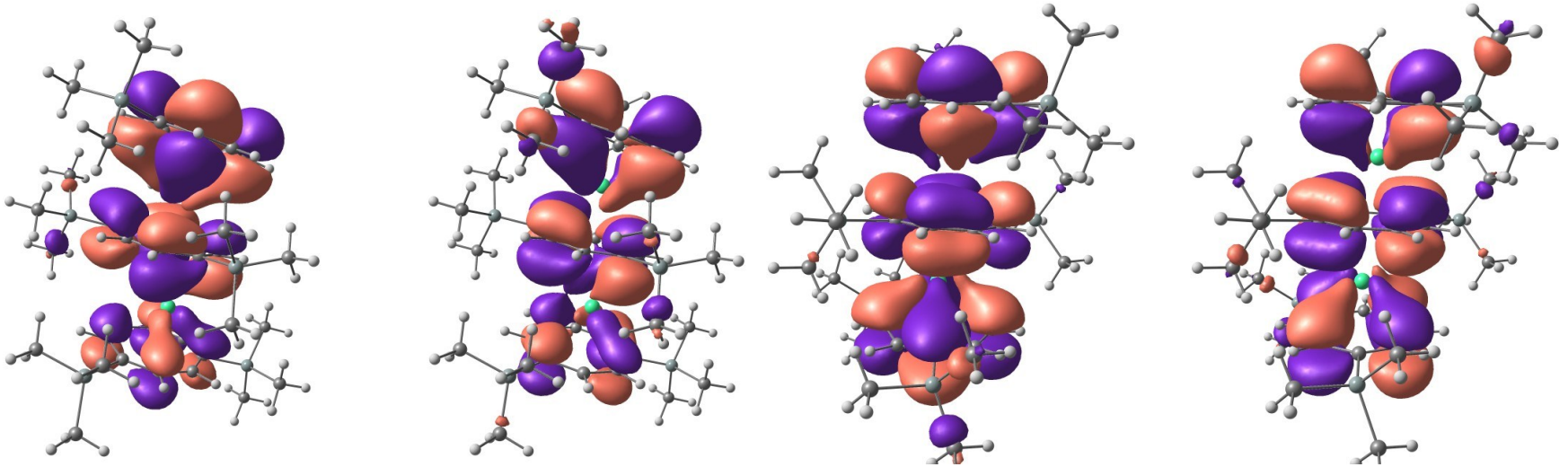



**Figure S32.** Associated MO diagrams focusing on the frontier orbitals (MO 185 being the HOMO)



(a) (b) (c) (d)

**Figure S33.** δ-bonding orbitals: HOMO (a,c) and HOMO-1 (b,d)

**Lutetium complex (4Lu)**

1,4 isomer

1,5 isomer

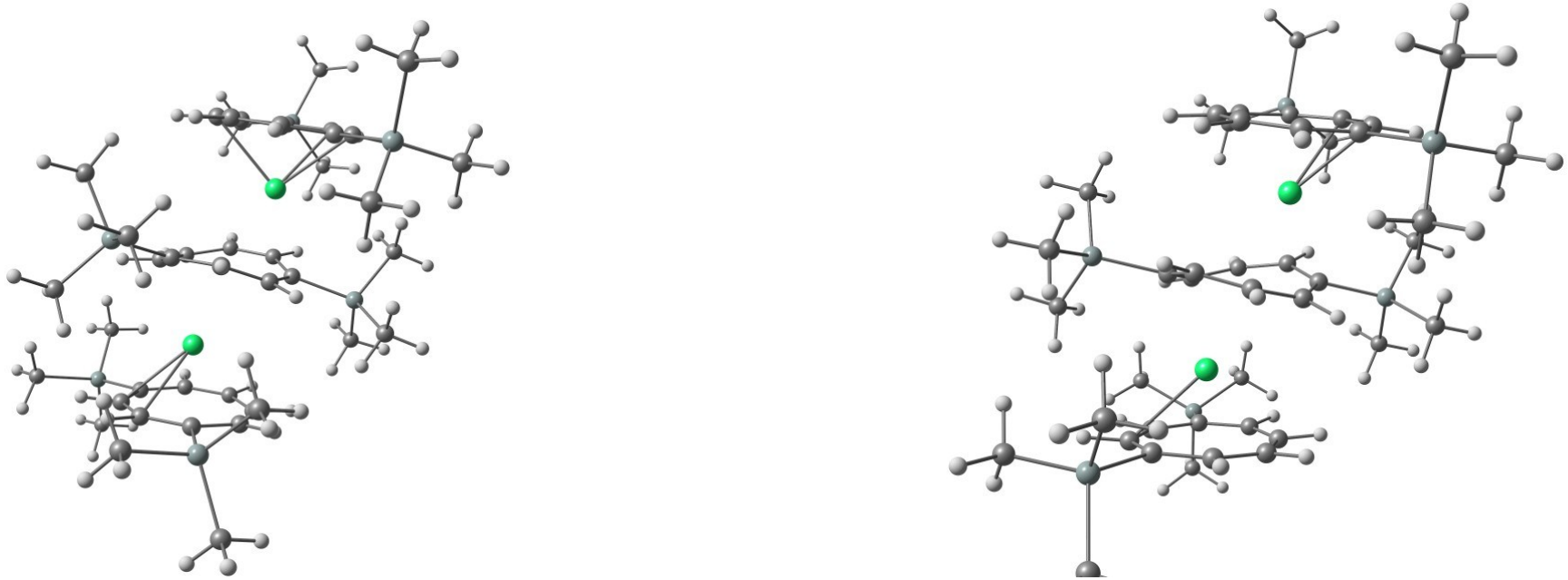


**Figure S34.** Optimized structures

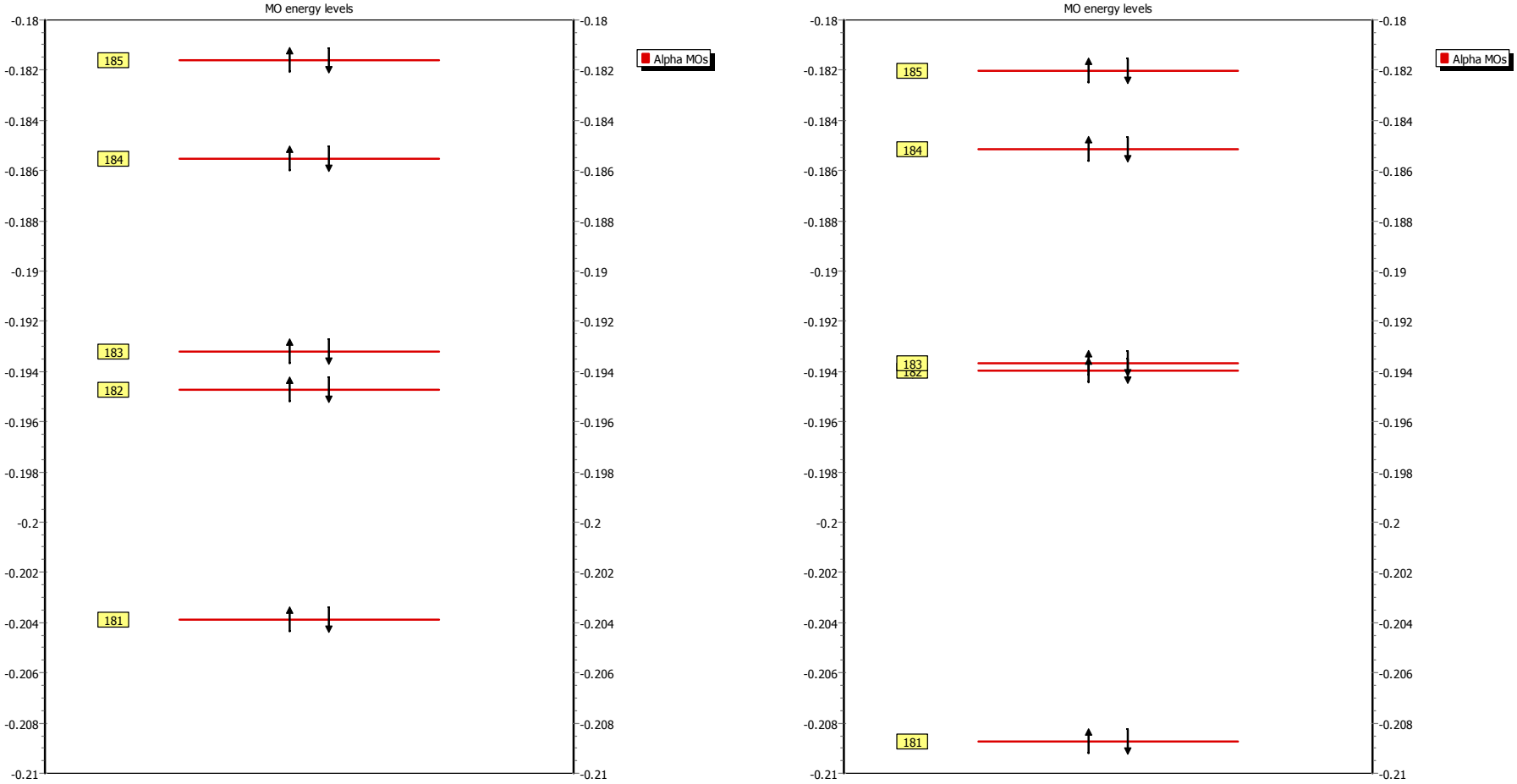
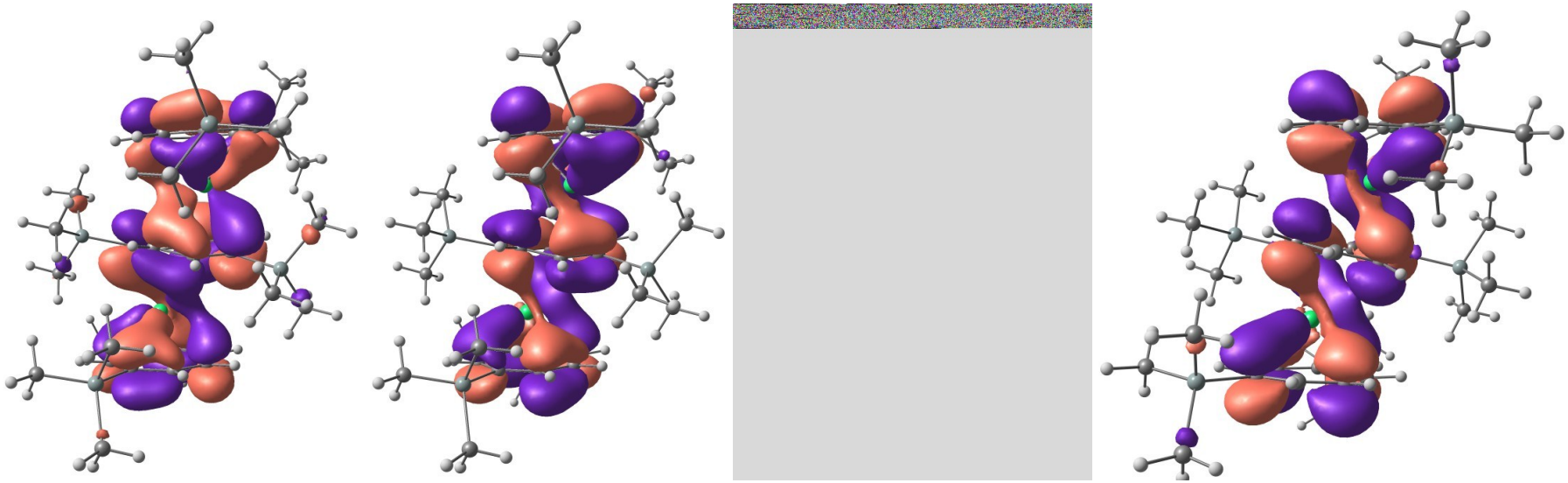



**Figure S35.** Associated MO diagrams focusing on the frontier orbitals (MO 185 being the HOMO)



(a) (b) (c) (d)

**Figure S36.** δ-bonding orbitals: HOMO (a,c) and HOMO-1 (b,d)

The situation is different for **4Y** and **4La**. The Frontier orbitals are also δ-bonding orbitals, but the overall stabilization is greater in the 1,5 isomer than in the 1,4 isomer.

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