SUPPORTING INFORMATION

Methyl and Arylchalcogenolate Complexes of Cadmium in a Sulfur Rich Coordination Environment: Syntheses and Structural Characterization of the *Tris*(2-mercapto-1-t-butylimidazolyl)hydroborato Cadmium Complexes $[Tm^{But}]CdMe$, and $[Tm^{But}]CdAr$ (E = O, S, Se, Te) and Analysis of the Bonding in Chalcogenolate Compounds

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EXPERIMENTAL SECTION

General Considerations

All manipulations were performed using a combination of glovebox, high-vacuum and Schlenk techniques under a nitrogen or argon atmosphere, except where otherwise stated. Solvents were purified and degassed by standard procedures. ^{1}H and ^{13}C NMR spectra were measured on Bruker 300 DRX and Bruker 400 DRX spectrometers. ^{1}H Chemical shifts are reported in ppm relative to $SiMe_4$ ($\delta = 0$) and were referenced internally with respect to the protio solvent impurity (δ 7.16 for C_6D_5H and δ 1.94 for CD_2HCN). ^{13}C NMR spectra are reported in ppm relative to $SiMe_4$ ($\delta = 0$) and were referenced internally with respect to the solvent (δ 128.06 for C_6D_5H). ^{113}Cd chemical shifts are reported relative to $CdMe_2$ ($\delta = 0$) and were referenced externally with respect to $CdCl_2$ (1 M in D_2O, δ -545.1). Coupling constants are given in hertz. IR spectra were recorded as KBr pellets on a Nicolet Avatar DTGS spectrometer, and the data are reported in reciprocal centimeters.

X-ray structure determinations

X-ray diffraction data were collected on a Bruker P4 diffractometer equipped with a SMART CCD detector and crystal data, data collection and refinement parameters are summarized in Table 3. The structures were solved using direct methods and standard difference map techniques, and were refined by full-matrix least-squares procedures on F^2 with SHELXTL (Version 5.10).[i]

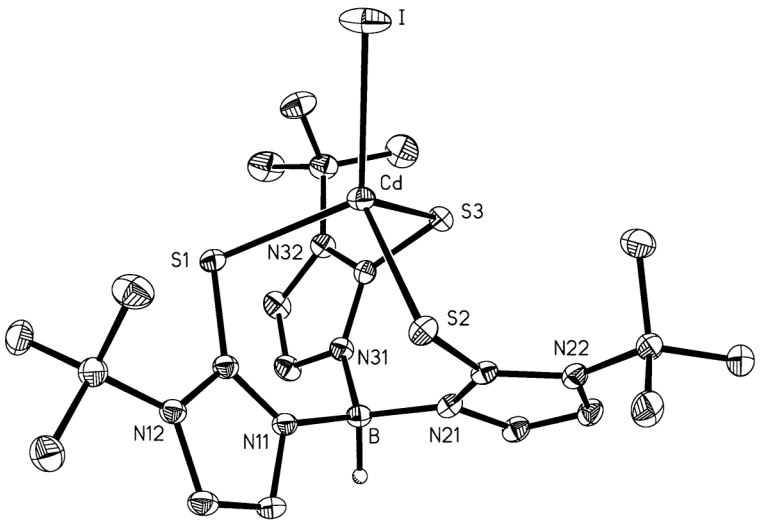
Computational Details

All calculations were initially carried out using DFT as implemented in the Jaguar 6.0 suite of *ab initio* quantum chemistry programs.[ii] Geometry optimizations were performed with the B3LYP density functional[iii] and the 6-31G** (C, H, N, B, O, S), LAV3P (Se, Te, Zn, Cd), LACVP (Zr, La) and CSDZ (Lu) basis sets. NBO charges for $[Tm^{But}]ZnEPh$, $[Tm^{But}]CdEPh$, $Cp_2Zr(EH)_2$ and $Cp^*_2Zr(EPh)_2$ were determined using the

same basis sets employed for geometry optimization, while the NBO charges for $[Tp]_2LnEPh$ (Ln = La, Lu) were determined using the SDDAll basis set employing Gaussian 03.[iv] Molecular orbital analyses were performed with the aid of Jimp 2,[v] which employs Fenske-Hall calculations[vi] and visualization using MOPLOT.[vii]

Synthesis of $[Tm^{But}]CdI$

A solution of $[Tm^{But}]Tl$ (0.200 g, 0.293 mmol) in CH_2Cl_2 (20 mL) was added to a suspension of CdI_2 (0.106 g, 0.289 mmol) in CH_2Cl_2 (20 mL) resulting in the immediate formation of a yellow precipitate. The solution was stirred for 3 hours and allowed to settle for 30 minutes. The mixture was filtered and volatile components were removed from the filtrate under vacuum to give $[Tm^{But}]CdI$ as a white powder (0.080 mg, 38% yield). Crystals of the composition $[Tm^{But}]CdI$ suitable for X-ray diffraction were obtained from CH_3CN. Analysis calcd. for $[Tm^{But}]CdI$: C, 35.2%; H, 4.8%; N, 11.7%. Found: C, 35.0%; H, 4.1%; N, 11.3%. ^1H NMR (C_6D_6): 1.44 [s, 27H, $HB\{C_3N_2H_2[C(C\underline{H}_3)_3]S\}_3$], 6.36 [d, 3H, $^3J_{H-H}$ = 2, $HB\{C_3N_2\underline{H}_2[C(CH_3)_3]S\}_3$], 6.62 [d, 3H, $^3J_{H-H}$ = 2, $HB\{C_3N_2\underline{H}_2[C(CH_3)_3]S\}_3$]. $^{13}C\{^1H\}$ NMR (C_6D_6): 28.8 [9C, $HB\{C_3N_2H_2[C(\underline{C}H_3)_3]S\}_3$], 59.6 [3C, $HB\{C_3N_2H_2[\underline{C}(CH_3)_3]S\}_3$], 117.2 [3C, $HB\{\underline{C}_2N_2H_2[C(CH_3)_3]CS\}_3$], 123.0 [3C, $HB\{\underline{C}_2N_2H_2[C(CH_3)_3]CS\}_3$], 157.0 [3C, $HB\{C_2N_2H_2[C(CH_3)_3]\underline{C}S\}_3$]. IR Data (KBr pellet, cm^{-1}): 3176 (w), 3148 (m), 3106 (w), 2978 (m), 2924 (m), 2663 (w), 2466 (w), 2304 (w), 2253 (w), 1678 (w), 1568 (m), 1481 (m), 1420 (s), 1396 (m), 1362 (vs), 1307 (m), 1259 (w), 1228 (m), 1196 (vs), 1175 (s), 1137 (m), 1070 (m), 1028 (w), 981 (w), 928 (w), 819 (m), 759 (m), 732 (s), 685 (s), 587 (m), 550 (m), 493 (w), 454 (w). Mass spectrum: m/z = 717.2 $\{M - 1\}^+$, 591.2 $\{M - I\}^+$.

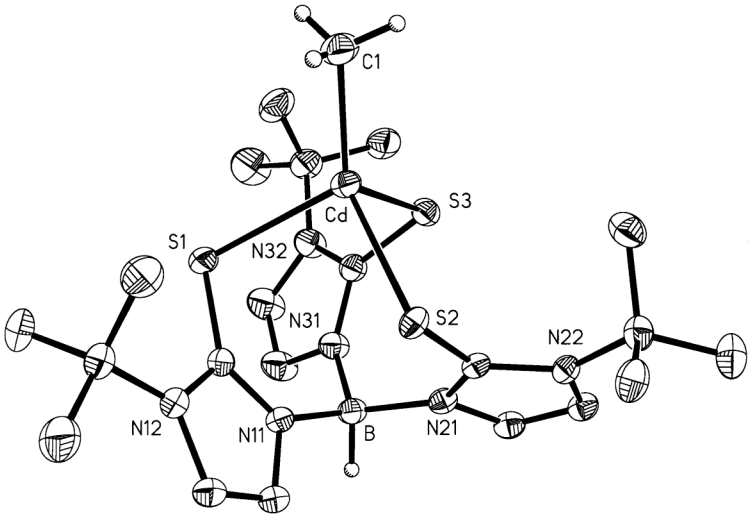


Molecular structure of [Tm^{But}]CdI

Synthesis of [Tm^{But}]CdMe

A suspension of [Tm^{But}]Tl (2.350 g, 3.446 mmol) in C_6H_6 (20 mL) was added to a solution of Me_2Cd (0.6 mL, 8.359 mmol) in C_6H_6 (20 mL) resulting in the immediate deposition of a black precipitate. The mixture was stirred for 1 hour, allowed to settle for an additional 30 minutes, and filtered. The volatile components were removed from the filtrate by lyophilization and the resulting solid was washed with pentane and dried *in vacuo* to give [Tm^{But}]CdMe as a white powder (1.735 g, 83 % yield). Colorless crystals of composition [Tm^{But}]CdMe•0.5(Et_2O) suitable for X-ray diffraction were obtained from Et_2O. ^{1}H NMR (C_6D_6): 0.37 [s, $^2J_{Cd^{111}\text{-}H}$ = 67.1, $^2J_{Cd^{113}\text{-}H}$ = 70.0, 3H of CdC$\underline{H}_3$], 1.55 [s, 27 H of HB{$C_3N_2H_2$[C(C$\underline{H}_3$)$_3$]S}$_3$], 6.43 [d, $^3J_{H\text{-}H}$= 2, 3 H of HB{$C_3N_2\underline{H}_2$[C(CH_3)$_3$]S}$_3$], 6.73 [d, $^3J_{H\text{-}H}$= 2, 3 H of HB{$C_3N_2\underline{H}_2$[C(CH_3)$_3$]S}$_3$]. ^{13}C{^{1}H} NMR (C_6D_6): –10.4 [1 C, Cd$\underline{C}H_3$], 28.8 [9 C, HB{$C_3N_2H_2$[C($\underline{C}H_3$)$_3$]S}$_3$], 59.0 [3 C, HB{$C_3N_2H_2$[$\underline{C}$(CH_3)$_3$]CS}$_3$], 116.4 [3 C of HB{$\underline{C}_2N_2H_2$[C(CH_3)$_3$]CS}$_3$], 122.5 [3 C of HB{$\underline{C}_2N_2H_2$[C(CH_3)$_3$]S}$_3$], 159.3 [3 C, HB{$C_2N_2H_2$[C(CH_3)$_3$]$\underline{C}$S}$_3$]. ^{113}Cd NMR (C_6D_6): 48.6. IR Data (KBr pellet, cm^{-1}): 3182(w), 3161(m), 3131(s), 3099(w), 2962(s), 2898(s), 2821(m), 2653(w), 2497(w), 2449(m), 2423(m), 2302(w), 2248(w), 2178(w), 1688(w), 1660(w), 1583(m), 1565(m), 1518(w), 1484(m), 1455(m), 1418(s), 1396(s), 1359(vs), 1299(vs), 1254(m), 1228(s), 1195(vs), 1136(m),

1070(m), 1029(m), 978(w), 927(w), 821(m), 771(w), 757(m), 740(s), 725(s), 687(s), 639(s), 586(m), 550(m), 494(m), 456(m). Mass spectrum: $m/z = 591.2$ $\{M\text{-}CH_3\}^+$.

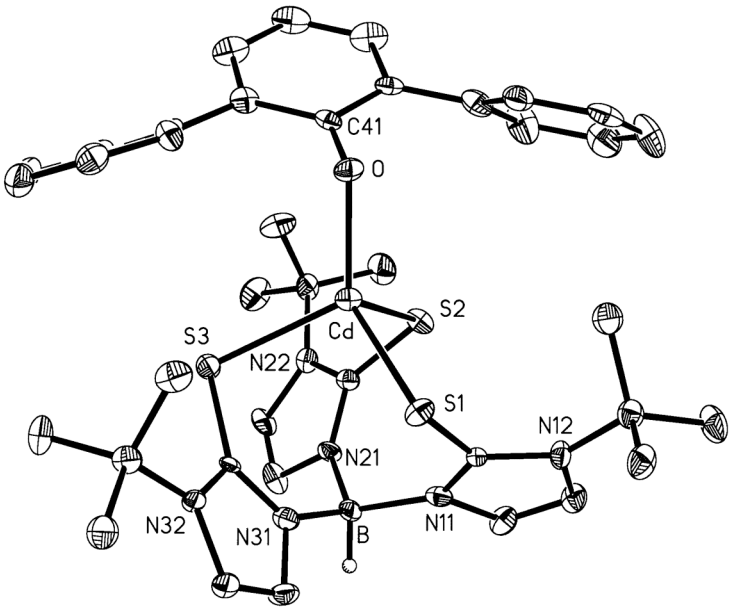


Molecular structure of [Tm^{But}]CdMe

Synthesis of [Tm^{But}]CdOAr (Ar = 2,6-Ph$_2$C$_6$H$_3$)

A mixture of [Tm^{But}]CdMe (195 mg, 0.322 mmol) and 2,6-diphenylphenol (80 mg, 0.325 mmol) was treated with C_6H_6 (20 mL). The solution was stirred for 1 day leading to the formation of a white precipitate. The volatile components were removed by lyophilization to give [Tm^{But}]CdOAr (Ar = 2,6-Ph$_2$C$_6$H$_3$) as a white solid (173 mg, 64% yield). Crystals of composition [Tm^{But}]CdOAr•C_7H_8 suitable for X-ray diffraction were obtained from toluene. Analysis calcd. for [Tm^{But}]CdOAr•0.5(C_7H_8): C, 57.9%; H, 5.8%; N, 9.5%. Found: C, 57.9%; H, 5.6%; N, 9.2%. ^{1}H NMR (C_6D_6): 1.31 [s, 27H, HB{$C_3N_2H_2$[C(C$\underline{H}_3$)$_3$]S}$_3$], 6.22 [d, 3H, $^3J_{H\text{-}H}$ = 2, HB{$C_3N_2\underline{H}_2$[C(CH_3)$_3$]S}$_3$], 6.44 [d, 3H, $^3J_{H\text{-}H}$ = 2, HB{$C_3N_2\underline{H}_2$[C(CH_3)$_3$]S}$_3$], 6.91 [t, 1H, $^3J_{H\text{-}H}$ = 7, CdOC$_6\underline{H}_3$(Ph)$_2$], 7.16 [obscured by solvent, 2H, OC$_6$H$_3$(C$_6\underline{H}_5$)$_2$], 7.38 [t, 4H, $^3J_{H\text{-}H}$ = 7, CdOC$_6$H$_3$(C$_6\underline{H}_5$)$_2$], 7.53 [d, 2H, $^3J_{H\text{-}H}$ = 7, CdOC$_6\underline{H}_3$(Ph)$_2$], 8.29 [d, 4H, $^3J_{H\text{-}H}$ = 7, CdOC$_6$H$_3$($\underline{Ph}$)$_2$]. IR Data (KBr pellet, cm^{-1}): 3518 (w), 3189 (w), 3170 (m), 3140 (m), 3031 (w), 2999 (w), 2970 (m), 2912 (m), 2653 (w), 2415 (w), 2267 (w), 2238 (w), 1595 (w), 1568 (w), 1480 (w), 1454 (m), 1400 (s), 1357 (vs), 1301 (m), 1282 (m), 1263 (m), 1227 (w), 1193 (s), 1173 (s), 1134 (m), 1089 (w), 1067 (m), 1028

(w), 1010 (w), 927 (w), 842 (w), 819 (w), 751 (m), 732 (w), 722 (m), 697 (m), 684 (m), 585 (m), 550 (s), 496 (m), 458 (w), 427(w). Mass spectrum: m/z = 591.3 $\{M - OAr\}^+$.

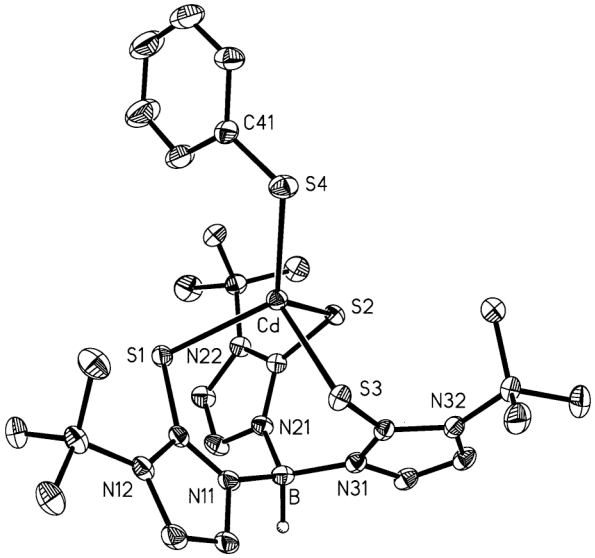


Molecular structure of [Tm^{But}]CdOC$_6$H$_3$Ph$_2$

Synthesis of [Tm^{But}]CdSPh

A solution of [Tm^{But}]CdMe (120 mg, 0.198 mmol) in C_6H_6 (20 mL) was treated with PhSH (50 μL, 0.487 mmol) and stirred for 2h. The volatile components were removed by lyophilization to give [Tm^{But}]CdSPh as a white solid (79 mg, 57% yield). Crystals of composition [Tm^{But}]CdSPh•(C_6H_6) suitable for X-ray diffraction were obtained from C_6H_6. Analysis calcd. for [Tm^{But}]CdSPh: C, 46.4%; H, 5.6%; N, 12.0%. Found: C, 46.0%; H, 4.9%; N, 11.0%. ^{1}H NMR (C_6D_6): 1.43 [s, 27H, HB{$C_3N_2H_2$[C(C$\underline{H}_3$)$_3$]S}$_3$], 6.37 [d, 3H, $^3J_{H\text{-}H}$ = 2, HB{$C_3N_2\underline{H}_2$[C(CH$_3$)$_3$]S}$_3$], 6.63[d, 3H, $^3J_{H\text{-}H}$ = 2, HB{$C_3N_2\underline{H}_2$[C(CH$_3$)$_3$]S}$_3$], 6.90 [br, 1H, *p*-CdS$\underline{Ph}$], 7.00 [br m, 2H, *m*-CdS$\underline{Ph}$], 7.90 [br, 2H, *o*-CdS$\underline{Ph}$]. ^{13}C{^{1}H} NMR (C_6D_6): 28.8 [9C, HB{$C_3N_2H_2$[C($\underline{C}$H$_3$)$_3$]S}$_3$], 59.4 [3C, HB{$C_3N_2H_2$[$\underline{C}$(CH$_3$)$_3$]S}$_3$], 117.0 [3C, HB{$\underline{C}_2N_2H_2$[C(CH$_3$)$_3$]CS}$_3$], 122.9 [3C, HB{$\underline{C}_2N_2H_2$[C(CH$_3$)$_3$]CS}$_3$], 134.6 CdS$\underline{Ph}$], 157.4 [3C, HB{$C_2N_2H_2$[C(CH$_3$)$_3$]$\underline{C}$S}$_3$]. IR Data (KBr pellet, cm^{-1}): 3179 (w), 3146 (w), 3064 (w), 2976 (m), 2925 (w), 2655 (w), 2486 (w), 2404 (w), 2293 (w), 2227 (w), 1567 (m), 1473 (m), 1416

(m), 1397 (w), 1359 (vs), 1303 (m), 1261 (w), 1227 (w), 1194 (s), 1172 (s), 1129 (w), 1085 (w), 1069 (w), 1025 (w), 928 (w), 820 (w), 757 (w), 731 (m), 687 (m), 588 (w), 551 (w), 493 (w), 475 (w), 421 (m). Mass spectrum: m/z = 699.3 $\{M - 1\}^+$, 591.2 $\{M - SPh\}^+$.



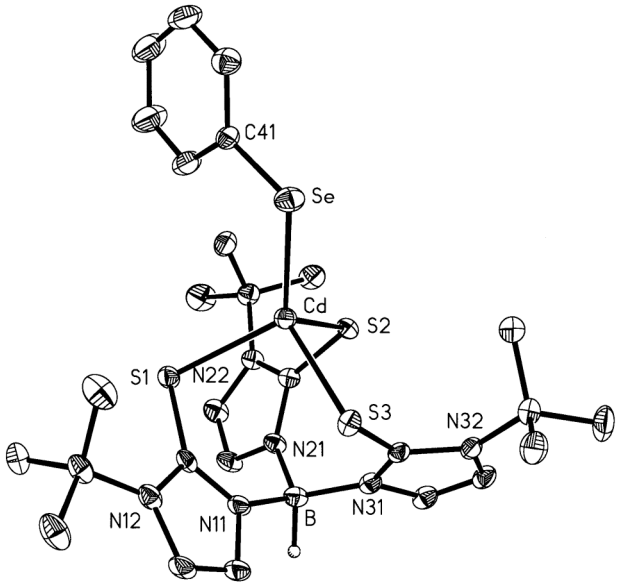
Molecular structure of [Tm^{But}]CdSPh

Synthesis of [Tm^{But}]CdSePh

A solution of [Tm^{But}]CdMe (90 mg, 0.149 mmol) in C_6H_6 (15 mL) was treated with PhSeH (50 μL, 0.471 mmol) and stirred for 3 hours. The volatile components were removed by lyophilization and the resulting solid was extracted into C_6H_6 and filtered. The volatile components were removed from the filtrate by lyophilization to give [Tm^{But}]CdSePh as a white solid (57 mg, 51 % yield). Crystals of composition [Tm^{But}]CdSePh•(C_6H_6) suitable for X-ray diffraction were obtained from C_6H_6. Analysis calcd. for [Tm^{But}]CdSePh: C, 43.5%; H, 5.3%; N, 11.3%. Found: C, 41.7%; H, 4.8%; N, 10.3%. ^{1}H NMR (C_6D_6): 1.45 [s, 27H, HB{$C_3N_2H_2$[C(C$\underline{H}_3$)$_3$]S}$_3$], 6.37 [d, 3H, $^3J_{H\text{-}H}$ = 2, HB{$C_3N_2\underline{H}_2$[C(CH$_3$)$_3$]S}$_3$], 6.64 [d, 3H, $^3J_{H\text{-}H}$ = 2, HB{$C_3N_2\underline{H}_2$[C(CH$_3$)$_3$]S}$_3$], 6.95-7.05 [m, 3H, *p,m*-CdSe$\underline{Ph}$], 8.18 [d, 2H, $^3J_{H\text{-}H}$ = 6, *o*-CdSe$\underline{Ph}$]. $^{13}C\{^1H\}$ NMR (C_6D_6): 28.7 [9C, HB{$C_3N_2H_2$[C($\underline{C}$H$_3$)$_3$]S}$_3$], 59.4 [3C, HB{$C_3N_2H_2$[$\underline{C}$(CH$_3$)$_3$]S}$_3$], 117.0 [3C, HB{$\underline{C}_2N_2H_2$[C(CH$_3$)$_3$]CS}$_3$], 122.8[3C, HB{$\underline{C}_2N_2H_2$[C(CH$_3$)$_3$]CS}$_3$], 137.2 [3C, HB{$C_2N_2H_2$[C(CH$_3$)$_3$]$\underline{C}$S}$_3$]. IR Data (KBr pellet, cm^{-1}): 3448(br), 3180(w), 3144(w),

3060(w), 2975(m), 2924(w), 2412(w), 1572(m), 1471(m), 1418(m), 1397(w), 1359(vs), 1303(w), 1260(w), 1227(w), 1195(s), 1174(s), 1132(w), 1106(s), 1069(m), 1022(w), 821(w), 760(w), 729(m), 686(m), 667(w), 552(w), 494(m), 464(m).

Mass spectrum: m/z= 591.3 $\{M\text{-}SePh\}^+$.

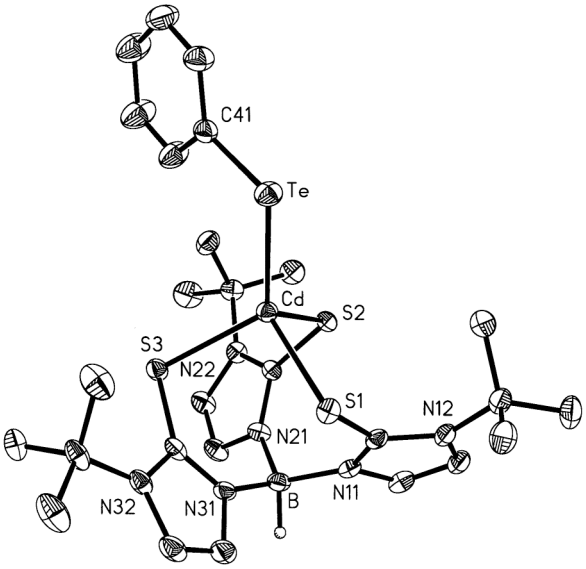


Molecular structure of [Tm^{But}]CdSePh

Synthesis of [Tm^{But}]CdTePh

A mixture of [Tm^{But}]CdMe (100 mg, 0.165 mmol) and Ph_2Te_2 (68 mg, 0.166 mmol) was treated with C_6H_6 (20 mL) resulting in the immediate deposition of a dark precipitate. The solution was stirred for 1 hr. and allowed to settle for 30 minutes. The mixture was filtered and the volatile components were removed from the filtrate by lyophilization. The resulting solid was washed twice with pentane and residual solvent removed under vacuum to give [Tm^{But}]CdTePh as a white powder (84 mg, 64% yield). Crystals suitable for X-ray diffraction were obtained from Et_2O. Analysis calcd. for [Tm^{But}]CdTePh: C, 40.8%; H, 4.9%; N, 10.6%. Found: C, 40.3%; H, 4.0%; N, 10.1%. ^{1}H NMR (C_6D_6): 1.45 [s, 27H, HB{$C_3N_2H_2$[C(C$\underline{H}_3$)$_3$]S}$_3$], 6.38 [d, 3H, $^3J_{H\text{-}H}$ = 2, HB{$C_3N_2\underline{H}_2$[C(CH$_3$)$_3$]S}$_3$], 6.65 [d, 3H, $^3J_{H\text{-}H}$ = 2, HB{$C_3N_2\underline{H}_2$[C(CH$_3$)$_3$]S}$_3$], 6.90 [t, 2H, $^3J_{H\text{-}H}$ = 7, *m*-CdTe$\underline{Ph}$], 7.03 [t, 1H, $^3J_{H\text{-}H}$ = 7, *m*-CdTe$\underline{Ph}$], 8.35[d, 2H, $^3J_{H\text{-}H}$ = 7, *o*-CdTe$\underline{Ph}$].

$^{13}C\{^1H\}$ NMR (C_6D_6): 28.8 [9C, HB{$C_3N_2H_2[C(\underline{C}H_3)_3]S\}_3$], 59.4 [3C, HB{$C_3N_2H_2[\underline{C}(CH_3)_3]S\}_3$], 116.9 [3C, HB{$\underline{C}_2N_2H_2[C(CH_3)_3]CS\}_3$], 122.8 [3C, HB{$\underline{C}_2N_2H_2[C(CH_3)_3]CS\}_3$], 142.5 [3C, HB{$C_2N_2H_2[C(CH_3)_3]\underline{C}S\}_3$]. IR Data (KBr pellet, cm^{-1}): 3425 (br), 3179 (w), 3146 (w), 3064 (w), 2969 (m), 2924 (m), 2407 (w), 2374 (m), 2225 (m), 1563 (m), 1545 (w), 1525 (w), 1510 (w), 1476 (m), 1416 (m), 1398 (w), 1358 (s), 1302 (m), 1260 (m), 1226 (m), 1192 (vs), 1170 (s), 1098 (s), 1065 (s), 1019 (s), 818 (m), 799 (m), 775 (w), 756 (w), 729 (m), 687 (m), 672 (w), 651 (w), 629 (w), 606 (w), 586 (w), 544 (w), 512 (m), 491 (m), 467 (s), 452 (s), 421 (w). Mass spectrum: m/z = 795.3 $\{M - 1\}^+$, 591.3 $\{M - TePh\}^+$.

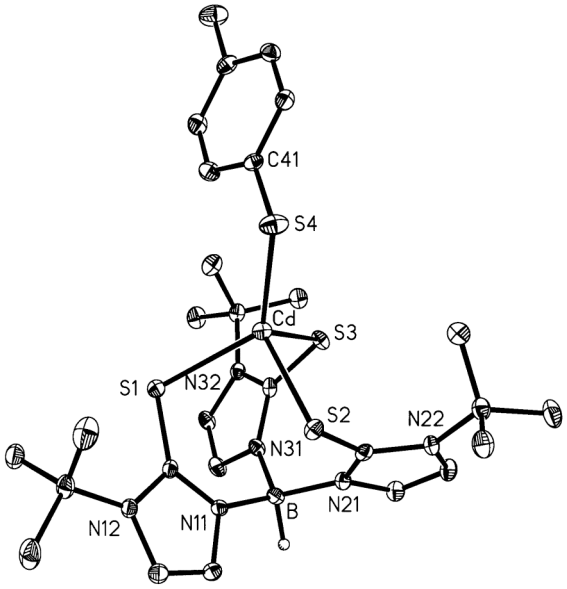


Molecular structure of [Tm^{But}]CdTePh

Synthesis of [Tm^{But}]CdSC$_6$H$_4$Me

A solution of [Tm^{But}]CdMe (ca. 5 mg) in C_6D_6 was treated with *p*-TolSH (ca. 2 mg) in C_6D_6 and was monitored by ^1H NMR spectroscopy, thereby demonstrating the immediate formation of [Tm^{But}]CdSC$_6$H$_4$Me in quantitative yield. The volatile components were removed by lyophilization to give [Tm^{But}]CdSC$_6$H$_4$Me as a white solid. Crystals of composition [Tm^{But}]CdSC$_6$H$_4$Me•2(C_6H_6) suitable for X-ray diffraction were obtained from C_6H_6. ^1H NMR (C_6D_6): 1.44 [s, 27H, HB{$C_3N_2H_2[C(C\underline{H}_3)_3]S\}_3$], 2.15 [s,

3H, $CdSC_6H_4C\underline{H}_3$], 6.37 [d, 3H, $^3J_{H\text{-}H}$ = 2, $HB\{C_3N_2\underline{H}_2[C(CH_3)_3]S\}_3$], 6.64 [d, 3H, $^3J_{H\text{-}H}$ = 2, $HB\{C_3N_2\underline{H}_2[C(CH_3)_3]S\}_3$], 6.91 [d, 2H, $^3J_{H\text{-}H}$ = 8, $CdSC_6\underline{H}_4Me$], 7.96 [d, 2H, $^3J_{H\text{-}H}$ = 8, $CdSC_6\underline{H}_4Me$].



Molecular structure of [Tm^{But}]CdSTol

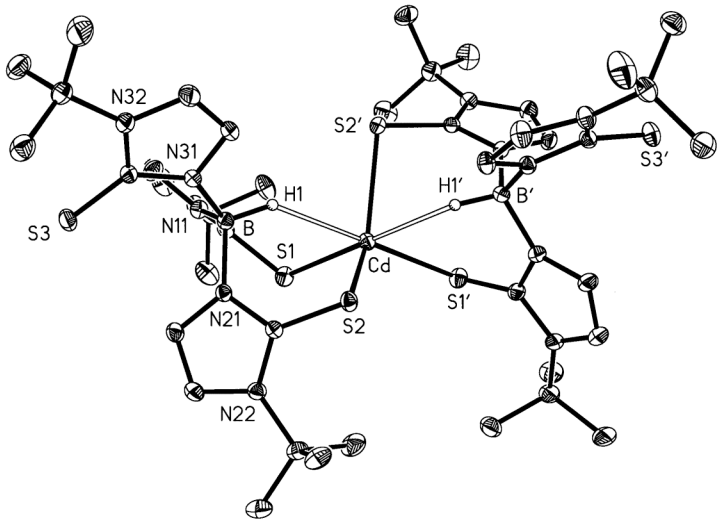
Synthesis of [Tm^{But}]CdSC$_6$H$_4$NO$_2$

A mixture of [Tm^{But}]CdMe (100 mg, 0.165 mmol) and *p*-$NO_2C_6H_4SH$ (26 mg, 0.168 mmol) were treated with C_6H_6 (20 mL) resulting in a yellow solution. The mixture was stirred for 2 hours and the volatile components were removed by lyophilization to give [Tm^{But}]$CdSC_6H_4NO_2$ as a yellow solid (65 mg, 53 % yield). ^{1}H NMR (C_6H_6): 1.40 [s, 27H, $HB\{C_3N_2H_2[C(C\underline{H}_3)_3]S\}_3$], 6.36 [d, 3H, $^3J_{H\text{-}H}$ = 2.4, $HB\{C_3N_2\underline{H}_2[C(CH_3)_3]S\}_3$], 6.60 [d, 3H, $^3J_{H\text{-}H}$ = 2.4, $HB\{C_3N_2\underline{H}_2[C(CH_3)_3]S\}_3$], 7.76 [A part of "AB" quartet, 2H, $^3J_{H\text{-}H}$ = 9, $CdSC_6\underline{H}_4NO_2$], 7.87 [B part of "AB" quartet, d, 2H, $^3J_{H\text{-}H}$ = 9, $CdSC_6\underline{H}_4NO_2$].

Synthesis of [Tm^{But}]$_2$Cd

A mixture of [Tm^{But}]Tl (220 mg, 0.323 mmol) and CdI_2 (59 mg, 0.161 mmol) was treated with CH_2Cl_2 (30 mL) resulting in the immediate deposition of a yellow precipitate. The solution was stirred for 3 hours and allowed to settle for 1 hour. The mixture was

filtered and the volatile components were removed *in vacuo* from the filtrate to give $[Tm^{But}]_2Cd$ as a white powder (112 mg, 65% yield). Crystals of the composition $[Tm^{But}]_2Cd$ suitable for X-ray diffraction were obtained from CH_2Cl_2. ^1H NMR (CD_3CN): 1.75 [s, 54H, $[HB\{C_3N_2H_2[C(C\underline{H}_3)_3]S\}_3]_2Cd$], 6.51 [d, 6H, $^3J_{H\text{-}H} = 2$, $[HB\{C_3N_2\underline{H}_2[C(CH_3)_3]S\}_3]_2Cd$], 7.03 [d, 6H, $^3J_{H\text{-}H} = 2$, $[HB\{C_3N_2\underline{H}_2[C(CH_3)_3]S\}_3]_2Cd$]. $^{13}C\{^1H\}$ NMR (C_6D_6): 28.6 [18C, $[HB\{C_3N_2H_2[C(\underline{C}H_3)_3]S\}_3]_2Cd$], 58.5 [6C, $[HB\{C_3N_2H_2[\underline{C}(CH_3)_3]S\}_3]_2Cd$], 114.7 [6C, $[HB\{\underline{C}_2N_2H_2[C(CH_3)_3]CS\}_3]_2Cd$], 125.0 [6C, $[HB\{\underline{C}_2N_2H_2[C(CH_3)_3]CS\}_3]_2Cd$], not observed [6C, $HB(C_2N_2H_2(C(CH_3)_3)\underline{C}S)_3$]. IR Data (KBr pellet, cm^{-1}): 3433 (br), 3144 (w), 2973 (m), 2923 (w), 2462 (w), 2361 (w), 2340 (w), 1656 (w), 1564 (w), 1481 (w), 1400 (m), 1358 (vs), 1295 (m), 1261 (m), 1199 (s), 1162 (m), 1101 (m), 1057 (w), 983 (w), 928 (w), 821 (w), 771 (w), 713 (m), 680 (m), 595 (w), 547 (w), 495 (w), 467 (w). Mass spectrum: $m/z = 1068.6$ $\{M\}^+$.



Molecular structure of $[Tm^{But}]_2Cd$

Table 1. Calculated *d*(M–E) bond length and NBO charges for [Tm^{But}]ZnEPh, [Tm^{But}]CdEPh, Cp*$_2$Zr(EPh)$_2$, and [Tp]$_2$LaEPh.

	***d*(M–E)/Å**	q_M	q_E	$[q_M q_E/d^2]/Å^{-2}$
[Tm^{But}]ZnOPh	1.917	1.465	–0.929	–0.370
[Tm^{But}]ZnSPh	2.336	1.370	–0.527	–0.132
[Tm^{But}]ZnSePh	2.493	1.326	–0.447	–0.095
[Tm^{But}]ZnTePh	2.678	1.280	–0.316	–0.056
[Tm^{But}]CdOPh	2.109	1.481	–0.909	–0.303
[Tm^{But}]CdSPh	2.517	1.394	–0.518	–0.114
[Tm^{But}]CdSePh	2.651	1.344	–0.437	–0.084
[Tm^{But}]CdTePh	2.832	1.297	–0.312	–0.050
Cp*$_2$Zr(OPh)$_2$	2.105	1.933	–0.796	–0.347
Cp*$_2$Zr(SPh)$_2$	2.560	1.149	–0.170	–0.030
Cp*$_2$Zr(SePh)$_2$	2.722	0.981	–0.051	–0.007
Cp*$_2$Zr(TePh)$_2$	2.939	0.761	0.152	0.013
[Tp]$_2$LaOPh	2.280	2.794	–1.066	–0.573
[Tp]$_2$LaSPh	2.894	2.713	–0.614	–0.199
[Tp]$_2$LaSePh	3.061	2.728	–0.584	–0.170
[Tp]$_2$LaTePh	3.314	2.698	–0.485	–0.119
[Tp]$_2$LuOPh	2.068	2.025	–0.943	–0.446
[Tp]$_2$LuSPh	2.726	1.852	–0.412	–0.103
[Tp]$_2$LuSePh	2.957	1.824	–0.335	–0.070
[Tp]$_2$LuTePh	3.130	1.764	–0.185	–0.033

Table 2. Comparison of DFT calculated in-plane and out-of-plane Zr–E bond lengths in $Cp_2Zr(EH)_2$. The calculations were performed with idealized Zr–O–H and Zr–E–H (E = S, Se, Te) bond angles of 120˚ and 90˚, respectively.

	***d*(Zr–E)/Å for E–Zr–E–H = 90˚**	***d*(Zr–E)/Å for E–Zr–E–H = 0˚**	***d*(Zr–E)/Å for E–Zr–E–H = 180˚**	**Δ*d*/Å**	**Δd_{av}/Å**
O	2.013	2.013		0.000	0.004
	2.010		2.018	0.008	
S	2.536	2.599		0.063	0.065
	2.522		2.589	0.067	
Se	2.704	2.793		0.089	0.084
	2.693		2.771	0.078	
Te	2.905	3.034		0.129	0.118
	2.892		2.998	0.106	

Table 3. Crystal, intensity collection and refinement data.

	[Tm^{But}]CdMe	[Tm^{But}]CdI
lattice	Triclinic	Monoclinic
formula	$C_{24}H_{42}BCdN_6O_{0.50}S_3$	$C_{21}H_{34}BCdIN_6S_3$
formula weight	642.03	716.83
space group	P–1	$P2_1/n$
a/Å	10.8046(7)	10.7361(6)
b/Å	12.3830(8)	16.8058(9)
c/Å	14.3266(9)	16.252(1)
α/°	89.976(1)	90.00
β/°	69.697(1)	90.286(1)
γ/°	64.505(1)	90.00
V/Å^3	1597.35(18)	2932.3(3)
Z	2	4
temperature (K)	243	243
radiation (λ, Å)	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.335	1.624
μ (Mo Kα), mm^{-1}	0.904	2.032
θ max, deg.	28.12	28.31
no. of data	6931	6673
no. of parameters	360	303
R_1	0.0322	0.0270
wR_2	0.0839	0.0635
GOF	1.017	1.042

Table 3. Crystal, intensity collection and refinement data (continued).

	$[Tm^{But}]CdOC_6H_3Ph_2$	$[Tm^{But}]CdSPh$
lattice	Monoclinic	Monoclinic
formula	$C_{46}H_{55}BCdN_6OS_3$	$C_{27}H_{39}BCdN_6S_4$
formula weight	927.35	699.09
space group	$P2_1/c$	$P2_1/c$
a/Å	22.379(3)	10.2408(7)
b/Å	10.827(1)	32.833(2)
c/Å	21.656(3)	10.4732(7)
α/°	90.00	90.00
β/°	118.560(3)	112.149(1)
γ/°	90.00	90.00
V/Å^3	4608.8(10)	3261.6(4)
Z	4	4
temperature (K)	243	243
radiation (λ, Å)	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.336	1.424
μ (Mo Kα), mm^{-1}	0.651	0.953
θ max, deg.	23.26	28.31
no. of data	5652	7468
no. of parameters	515	357
R_1	0.0588	0.0312
wR_2	0.0804	0.0721
GOF	1.017	1.002

Table 3. Crystal, intensity collection and refinement data (continued).

	$[Tm^{But}]CdSC_6H_4Me$	$[Tm^{But}]CdSePh$
lattice	Monoclinic	Monoclinic
formula	$C_{37}H_{50}BCdN_6S_4$	$C_{27}H_{39}BCdN_6S_3Se$
formula weight	830.28	745.99
space group	$P2_1/n$	$P2_1/c$
a/Å	15.0659(9)	10.4001(6)
b/Å	10.9688(6)	32.699(2)
c/Å	25.434(2)	10.6389(7)
α/°	90.00	90.00
β/°	104.608(1)	113.717(1)
γ/°	90.00	90.00
V/Å^3	4067.3(4)	3312.4(4)
Z	4	4
temperature (K)	243	243
radiation (λ, Å)	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.356	1.496
μ (Mo Kα), mm^{-1}	0.776	1.974
θ max, deg.	28.28	28.29
no. of data	9449	7646
no. of parameters	447	357
R_1	0.0480	0.0419
wR_2	0.0538	0.0620
GOF	1.002	1.007

Table 3. Crystal, intensity collection and refinement data (continued).

	$[Tm^{But}]CdTePh$	$[Tm^{But}]_2Cd$
lattice	Monoclinic	Tetragonal
formula	$C_{27}H_{39}BCdN_6S_3Te$	$C_{42}H_{68}B_2CdN_{12}S_6$
formula weight	794.63	1067.46
space group	$P2_1/c$	$I4_1/a$
a/Å	10.6859(6)	19.7140(8)
b/Å	32.577(2)	19.7140(8)
c/Å	10.8236(5)	30.131(2)
α/°	90.00	90.00
β/°	115.5480(10)	90.00
γ/°	90.00	90.00
V/Å^3	3399.5(3)	11710.2(9)
Z	4	8
temperature (K)	243	243
radiation (λ, Å)	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.553	1.211
μ (Mo Kα), mm^{-1}	1.694	0.625
θ max, deg.	28.29	28.25
no. of data	7931	6946
no. of parameters	357	290
R_1	0.0459	0.0566
wR_2	0.0940	0.1937
GOF	1.020	1.065

Table 4. Cartesian Coordinated for Geometry Optimized Structures

[Tm$^{Bu^t}$]ZnOPh

atom	x	y	z
Zn1	-0.122191601	0.373557464	-0.993570064
S2	0.06501335	-1.945644743	-0.18344879
S3	1.316516277	1.679927772	0.545823737
S4	1.169706904	0.390313119	-3.109457903
O5	-1.983334349	0.854136485	-1.00899432
C6	-2.551103741	1.949149829	-1.504821369
C7	-1.853431011	2.90633556	-2.277885451
C8	-2.495980771	4.037947901	-2.77702503
C9	-3.851282873	4.260171773	-2.528233941
C10	-4.55504826	3.320495632	-1.767864771
C11	-3.924168758	2.187480262	-1.264847223
B12	3.335426761	-0.877205751	-0.698392639
N13	2.629932834	-1.311670567	0.625106413
N14	1.323923669	-1.936061631	2.289169572
N15	3.496159263	0.671321884	-0.830454902
N16	3.450668544	2.876594356	-0.757996266
N17	2.769104253	-1.562720764	-1.981394928
N18	1.783371831	-2.212656569	-3.844841507
C19	1.368371601	-1.718338581	0.934161754
C20	3.374290752	-1.278909923	1.791928394

C21	2.579354044	-1.657718562	2.816679406
C22	0.128809273	-2.338235337	3.119655961
C23	0.550810797	-2.422202831	4.597243628
C24	-0.360466784	-3.728250252	2.675323091
C25	-0.969497164	-1.266198605	2.987472377
C26	2.785094038	1.738530312	-0.369899435
C27	4.603334496	1.148062234	-1.510999284
C28	4.581305742	2.498264422	-1.472425393
C29	3.062450437	4.31120521	-0.491529705
C30	1.719221509	4.617913511	-1.17887785
C31	4.135682586	5.239834639	-1.087189764
C32	3.00485298	4.550590441	1.028264898
C33	1.919811868	-1.164490433	-2.968774402
C34	3.154611204	-2.866750935	-2.240260854
C35	2.55405995	-3.271952049	-3.380875581
C36	0.943898905	-2.264756377	-5.098575257
C37	1.106865605	-3.648056993	-5.752667251
C38	-0.53970991	-2.070803907	-4.733081543
C39	1.440350595	-1.19723418	-6.090609562
H40	-0.79641151	2.748052267	-2.486510671
H41	-1.928257852	4.75328557	-3.369864968
H42	-4.34944526	5.143492835	-2.918915688
H43	-5.613061737	3.474567067	-1.562818227

H44	-4.471293913	1.456744964	-0.674849433
H45	4.462587562	-1.296381738	-0.598529054
H46	4.412262821	-0.98830005	1.787310878
H47	2.806482828	-1.755604632	3.862258566
H48	0.886128214	-1.456419116	4.988087367
H49	1.331994074	-3.170722006	4.765667049
H50	-0.32352715	-2.724243677	5.179955878
H51	-0.69278146	-3.723828791	1.637154961
H52	-1.201828455	-4.030958728	3.307029745
H53	0.436574094	-4.471129785	2.788772225
H54	-1.339625421	-1.187903779	1.965276548
H55	-0.588332928	-0.287904701	3.297724575
H56	-1.808163631	-1.530369469	3.639949868
H57	5.315656102	0.477251043	-1.962975115
H58	5.274615142	3.208323667	-1.88413903
H59	0.907166155	4.01033136	-0.780174872
H60	1.793108638	4.440368721	-2.256798303
H61	1.469495223	5.672417046	-1.022832871
H62	5.118997144	5.087767284	-0.63023011
H63	3.836805319	6.271805481	-0.885042683
H64	4.221877659	5.131258079	-2.172915712
H65	3.974728192	4.333186626	1.488932262
H66	2.242594663	3.933502233	1.504403726

H67	2.765667625	5.602127718	1.216705885
H68	3.832904087	-3.391373008	-1.587168642
H69	2.61670228	-4.214710154	-3.892358026
H70	0.756986186	-4.457124507	-5.103928372
H71	2.140442856	-3.847945647	-6.053599791
H72	0.493311068	-3.666086855	-6.657323431
H73	-0.723889903	-1.088178462	-4.299332663
H74	-0.862004008	-2.835191504	-4.018649565
H75	-1.147348579	-2.169020396	-5.638559318
H76	1.331941603	-0.190671557	-5.686183988
H77	0.85417135	-1.264172022	-7.01279849
H78	2.493126474	-1.365651772	-6.342182719

$[Tm^{But}]ZnSPh$

atom	x	y	z
Zn1	-0.326672378	-0.119784929	0.476361907
S2	0.727645766	0.413032999	2.670588355
S3	-0.351955079	2.096272853	-0.672437925
S4	1.480740157	-1.303722343	-0.763153066
S5	-2.392638896	-1.182176177	0.78637734
C6	-2.873620991	-1.495497443	-0.91270779
C7	-3.966810815	-0.812470825	-1.472317676
C8	-4.377543629	-1.07083213	-2.780424026
C9	-3.705165887	-2.01354786	-3.560864603
C10	-2.619473502	-2.700446187	-3.014060243
C11	-2.210810669	-2.45021496	-1.703477589
B12	2.962859269	1.651185262	0.311963985
N13	2.156908463	2.412134565	1.410672774
N14	0.826193379	3.171187897	2.996928755
N15	2.365248458	1.822972326	-1.119729924
N16	1.201274979	2.117629598	-2.970714517
N17	3.311282117	0.175697469	0.682082486
N18	3.513049711	-1.998746604	0.993334519
C19	1.238751354	2.03566538	2.342796525
C20	2.313353418	3.785380539	1.482407439

C21	1.49922682	4.258114912	2.451182626
C22	-0.212000664	3.285635898	4.086414508
C23	-0.354012221	4.764710786	4.487375639
C24	-1.570548755	2.794675469	3.552228441
C25	0.249299491	2.490090661	5.320863041
C26	1.104300135	2.000892804	-1.604960144
C27	3.245076512	1.811604799	-2.188442146
C28	2.538784479	1.99029956	-3.326168686
C29	0.083336664	2.336906747	-3.961630435
C30	-0.599763249	3.684758137	-3.664666384
C31	-0.904578239	1.158205069	-3.896608327
C32	0.676145876	2.397917502	-5.381034528
C33	2.78895858	-1.033602989	0.337425223
C34	4.355776149	-0.037601333	1.564928668
C35	4.484266173	-1.368021416	1.762454985
C36	3.30099695	-3.492515814	0.960844626
C37	1.896243518	-3.825535253	1.497622054
C38	4.341494179	-4.166188005	1.872800318
C39	3.509110778	-4.006434953	-0.475762889
H40	-4.489482871	-0.075282132	-0.870207656
H41	-5.226879582	-0.529916227	-3.191704069
H42	-4.025495737	-2.212984702	-4.580217207
H43	-2.08978502	-3.442520694	-3.607188655

H44	-1.37523045	-2.999792526	-1.279556483
H45	4.029258431	2.215183384	0.268402136
H46	2.998114476	4.306727133	0.833692189
H47	1.353725518	5.265641418	2.794619567
H48	0.577530185	5.179870328	4.885532998
H49	-1.105573894	4.828075599	5.278599313
H50	-0.699989416	5.387496671	3.656666932
H51	-1.543241671	1.738720985	3.284864169
H52	-1.86541614	3.371184077	2.669717583
H53	-2.332534087	2.936411756	4.325417899
H54	0.352958775	1.42832094	5.097385756
H55	-0.490287178	2.605912047	6.119558694
H56	1.20936688	2.870004329	5.686489724
H57	4.305090479	1.684986843	-2.040898774
H58	2.879446288	2.047180783	-4.343336812
H59	-1.054679975	3.694435521	-2.674025987
H60	-1.384132432	3.861758377	-4.407492182
H61	0.123483321	4.504920334	-3.729821064
H62	-1.3894963	1.084125024	-2.923948055
H63	-0.391327068	0.213799083	-4.101967424
H64	-1.679254905	1.297764707	-4.6572206
H65	1.384142417	3.224246685	-5.502328991
H66	-0.145906371	2.565948196	-6.081686268

H67	1.163479891	1.460800616	-5.667320833
H68	4.924508649	0.783560794	1.969560977
H69	5.186486648	-1.906719321	2.371213041
H70	1.111986416	-3.403536733	0.869866567
H71	1.773062106	-3.440715176	2.514935154
H72	1.772202355	-4.912923429	1.524717679
H73	5.368447238	-3.979008743	1.542938975
H74	4.176147985	-5.245898986	1.83113839
H75	4.23685042	-3.85872962	2.917750142
H76	4.518171556	-3.766514491	-0.827725479
H77	2.78458426	-3.573378979	-1.165587746
H78	3.392627158	-5.094820337	-0.48894475

[Tm^{But}]ZnSePh

atom	x	y	z
Zn1	2.928583214	4.219128674	9.007346527
Se2	0.884398615	5.171041497	10.093938
S3	4.111783519	2.604266264	10.49424583
S4	4.748121813	5.783894749	8.349244771
S5	2.600628182	2.892730201	6.914481524
N6	6.410141692	3.048001287	9.024174553
N7	6.647257954	3.507768573	11.16911429
N8	5.713132355	3.842370621	6.632314335
N9	5.205999962	5.732125029	5.61342051
N10	4.917250058	1.514409949	7.524212257
N11	3.143787379	0.210220798	7.37571159
B12	6.005055204	2.632874462	7.574039273
H13	6.995822828	2.118258713	7.115084117
C14	5.756478353	3.069188241	10.218761
C15	7.708539713	3.480830874	9.231224079
H16	8.415080753	3.542864712	8.419833312
C17	7.860740694	3.766817281	10.54285638
H18	8.725914307	4.120572432	11.07234783
C19	6.399985484	3.710260591	12.64400994
C20	7.69640036	4.210972725	13.30546998

H21	8.018525183	5.177824325	12.90665098
H22	8.516214752	3.491434567	13.21228098
H23	7.499344776	4.346646496	14.37206526
C24	5.309721748	4.779751925	12.84075628
H25	5.607188154	5.721168505	12.36804426
H26	5.174397371	4.96087659	13.91190949
H27	4.355213044	4.464832886	12.41993443
C28	6.016225629	2.365095212	13.28793912
H29	5.091334444	1.968389574	12.86905367
H30	5.875481794	2.508922034	14.3639864
H31	6.814072789	1.628730235	13.14341854
C32	5.227688176	5.099273055	6.832531755
C33	5.984160542	3.690358916	5.283514679
H34	6.380664407	2.768196652	4.891250991
C35	5.673497004	4.843876659	4.652290468
H36	5.755399673	5.100520774	3.61241853
C37	4.743859083	7.137204134	5.310513915
C38	4.906669357	7.403862765	3.803392754
H39	4.576508214	8.426922235	3.605475592
H40	4.287229081	6.737114244	3.195707689
H41	5.948644675	7.326290449	3.476260154
C42	5.625791249	8.139200679	6.078136208
H43	5.316811205	9.158073036	5.82353964

H44	6.677553965	8.020618614	5.796015076
H45	5.534061576	8.010865881	7.156829796
C46	3.254523158	7.280967867	5.671253574
H47	2.913725088	8.28271291	5.390872479
H48	3.078403934	7.145753384	6.737623566
H49	2.651369651	6.550096666	5.12396356
C50	3.575456035	1.512128851	7.288862858
C51	5.319463221	0.211613388	7.762157449
H52	6.349350564	-0.028029475	7.970525288
C53	4.237684336	-0.593085891	7.67512933
H54	4.163158857	-1.658265096	7.793157341
C55	1.735033935	-0.307887342	7.218317133
C56	0.835788796	0.313491577	8.303329497
H57	1.216897255	0.07200301	9.300612636
H58	-0.174348938	-0.099012755	8.212756302
H59	0.777066571	1.397377333	8.208243741
C60	1.738420655	-1.835086504	7.407844677
H61	2.356280258	-2.345623461	6.662115561
H62	0.712771291	-2.192275961	7.283582942
H63	2.067602706	-2.12726417	8.409746447
C64	1.229765676	0.001310679	5.796995869
H65	1.87954117	-0.464513722	5.048283774
H66	1.190493668	1.074285059	5.609309884

H67	0.222037865	-0.409277555	5.676969208
C68	0.101826265	6.043646968	8.51059344
C69	-0.011212105	7.440117985	8.467666026
H70	0.36876868	8.030333359	9.296127402
C71	-0.606572014	8.072162294	7.373717859
H72	-0.688605255	9.156763736	7.36197411
C73	-1.092498535	7.322091721	6.300732058
H74	-1.555053664	7.81511321	5.449771149
C75	-0.983784431	5.930632431	6.338142153
H76	-1.362911657	5.331673934	5.513259956
C77	-0.398193231	5.295208968	7.435457134
H78	-0.331609155	4.211868163	7.460912183

[Tm^{But}]ZnTePh

atom	x	y	z
Zn1	-1.539424641	-0.815322979	-0.343698353
Te2	-4.188981724	-1.129950703	-0.660794575
S3	-0.222672046	-2.886920215	-0.842504696
S4	-0.769232998	-0.21545896	1.961398018
S5	-0.350267204	0.866536063	-1.744184048
B6	2.177025538	-0.569193496	0.159564772
N7	2.02315104	-1.313288564	-1.205468342
N8	1.551607339	-2.572605606	-2.954845342
N9	1.660638184	-1.392655697	1.379906788
N10	0.627506962	-2.334389687	3.086403942
N11	1.673593072	0.906838298	0.13601019
N12	0.738257399	2.880240599	-0.179232662
C13	1.144234401	-2.237145096	-1.684895599
C14	2.970500289	-1.06407141	-2.18315024
C15	2.687427779	-1.830618151	-3.258942951
C16	0.919522989	-3.568700766	-3.896064463
C17	1.73274236	-3.61448676	-5.202052414
C18	0.954673584	-4.968725751	-3.255820615
C19	-0.51447437	-3.120680111	-4.232911342
C20	0.529977221	-1.345052107	2.13753677

C21	2.461023691	-2.416746345	1.855482018
C22	1.832905833	-3.000943678	2.899258817
C23	-0.385865442	-2.703496391	4.141815304
C24	0.158811093	-3.881180184	4.969773951
C25	-1.693378082	-3.151322595	3.463093842
C26	-0.602440354	-1.506101802	5.085878844
C27	0.709326683	1.562890499	-0.567562085
C28	2.302030472	1.818695711	0.966012213
C29	1.732649987	3.030096678	0.780146818
C30	-0.140976575	4.006493372	-0.667062775
C31	0.074327328	4.199612943	-2.179556728
C32	0.266227034	5.305039048	0.051230111
C33	-1.611333191	3.703977267	-0.324599223
C34	-4.721209844	0.78460767	0.184170211
C35	-5.316103807	1.768542345	-0.618577654
C36	-5.704052321	2.996099362	-0.074680757
C37	-5.500068097	3.265318854	1.279796805
C38	-4.909786956	2.291135661	2.087350905
C39	-4.530038118	1.059382906	1.547296368
H40	3.369085551	-0.484831709	0.329194458
H41	3.771152477	-0.360895197	-2.02221331
H42	3.202089172	-1.910556453	-4.19846051
H43	1.72809108	-2.654504135	-5.727464968

H44	1.267296209	-4.350620082	-5.862800833
H45	2.767954452	-3.930137697	-5.036935675
H46	0.375787172	-5.00306251	-2.332668206
H47	1.98636084	-5.264721269	-3.036927854
H48	0.532663744	-5.695774631	-3.957088774
H49	-0.507342038	-2.124527324	-4.686619402
H50	-1.146257467	-3.094811998	-3.345422003
H51	-0.950909098	-3.822482127	-4.95105542
H52	3.415476088	-2.637784677	1.406188448
H53	2.147556011	-3.820630908	3.518423973
H54	1.090877151	-3.630842798	5.486696677
H55	0.31326488	-4.778481923	4.362515042
H56	-0.583455157	-4.127635814	5.733556797
H57	-2.14489373	-2.348024953	2.881548028
H58	-2.406304585	-3.466394157	4.231909965
H59	-1.507685086	-4.001157455	2.798552615
H60	-1.006464924	-0.644153208	4.554746191
H61	0.340518334	-1.217013042	5.562427419
H62	-1.30882011	-1.791594153	5.872113373
H63	3.106179939	1.521371577	1.61908346
H64	1.959284717	3.973124625	1.24234502
H65	-0.214342027	3.311535088	-2.742313339
H66	1.12416714	4.428203766	-2.393422153

H67	-0.535362177	5.040878262	-2.524417179
H68	1.302974119	5.589566657	-0.156208504
H69	0.118898384	5.242768576	1.133945798
H70	-0.374741681	6.109046552	-0.319904741
H71	-1.975421962	2.816150585	-0.839598081
H72	-2.231111423	4.554486089	-0.625939611
H73	-1.736477167	3.556451012	0.752436764
H74	-5.476203036	1.574732854	-1.675510574
H75	-6.166061116	3.744009032	-0.715474764
H76	-5.802478411	4.22038104	1.70191215
H77	-4.749209283	2.484605592	3.145610854
H78	-4.085025399	0.306617564	2.191393773

[Tm^{But}]CdOPh

atom	x	y	z
Cd1	-0.403479631	0.900894059	0.077116197
S2	-0.473097617	-0.581645805	-2.139720326
S3	1.65220483	2.465838313	-0.605386749
S4	0.806621226	-0.770817331	1.74912776
O5	-2.102695051	1.729671758	1.012897837
B6	2.851678096	-0.786494172	-1.085932366
N7	1.757432236	-1.899252837	-1.164322008
N8	0.008534638	-3.220042273	-1.421455645
N9	2.652535254	0.370730313	-2.117016749
N10	2.25800234	2.190992079	-3.300730955
N11	3.149910967	-0.280838469	0.360997912
N12	3.221584514	0.403560779	2.456738986
C13	0.451870375	-1.925448283	-1.55373121
C14	2.124823796	-3.179769315	-0.788468698
C15	1.058233244	-3.994423993	-0.941489298
C16	-1.364434643	-3.764305851	-1.734557584
C17	-2.410150426	-3.070355335	-0.842163597
C18	-1.388987029	-5.27164341	-1.424431338
C19	-1.660789525	-3.571220196	-3.233075662
C20	2.186132606	1.649574527	-2.038253601

C21	3.002088943	0.114806792	-3.431639322
C22	2.761481233	1.224371118	-4.163115102
C23	1.863611893	3.581631391	-3.738419621
C24	2.130669596	3.728787203	-5.247573391
C25	2.725890931	4.617237567	-2.99336216
C26	0.358950621	3.791442485	-3.490246633
C27	2.422453368	-0.190744501	1.509418754
C28	4.40239349	0.260297155	0.595092985
C29	4.45259107	0.68539276	1.876165355
C30	2.860121141	0.762212352	3.878158816
C31	4.069439307	1.4403999	4.546533987
C32	1.68703443	1.760145691	3.872449306
C33	2.526967312	-0.519921928	4.662095141
C34	-2.952824381	2.580407232	0.44463272
C35	-3.04816531	2.769599838	-0.954967485
C36	-3.957180042	3.671059001	-1.505339314
C37	-4.807951897	4.41678886	-0.687336745
C38	-4.731074213	4.237620987	0.697905805
C39	-3.827189171	3.340436982	1.257784641
H40	3.868689046	-1.334958242	-1.435652481
H41	3.121922703	-3.398049894	-0.442742189
H42	0.965984544	-5.047769596	-0.751809953
H43	-2.46777741	-2.00141019	-1.044844898

H44	-2.168080088	-3.215393146	0.215486187
H45	-3.39354281	-3.512049606	-1.032228195
H46	-0.677308163	-5.834932572	-2.036439378
H47	-2.388941217	-5.646466089	-1.657914516
H48	-1.199825987	-5.480279551	-0.366950002
H49	-0.911624713	-4.087688708	-3.842760556
H50	-1.671355277	-2.51625502	-3.507558412
H51	-2.641697099	-3.999063173	-3.463471742
H52	3.400247222	-0.841266749	-3.729737437
H53	2.915313502	1.401443221	-5.211291233
H54	3.189475635	3.606401464	-5.497508177
H55	1.840119188	4.74027045	-5.543231385
H56	1.536166246	3.030493083	-5.844650116
H57	3.789085915	4.446241428	-3.193771905
H58	2.560290473	4.579104025	-1.916702256
H59	2.468945855	5.620325181	-3.348500569
H60	0.108609692	3.729651686	-2.431551851
H61	-0.225233746	3.042387569	-4.034411284
H62	0.069803293	4.78196147	-3.855474241
H63	5.152002071	0.294398918	-0.178550192
H64	5.257418215	1.151536541	2.413752955
H65	4.348322177	2.374307311	4.04893208
H66	4.942960987	0.782257855	4.594847837

H67	3.789921464	1.68842696	5.573773264
H68	1.943846912	2.649276428	3.287802774
H69	1.478737306	2.074542244	4.900072678
H70	0.781160587	1.317989537	3.45869727
H71	1.665361659	-1.03590739	4.238329999
H72	2.298086764	-0.256682293	5.699733482
H73	3.383056703	-1.203143072	4.663746126
H74	-2.403621361	2.183342806	-1.610961387
H75	-4.002174384	3.788024137	-2.586683142
H76	-5.51618815	5.119287558	-1.117995426
H77	-5.385860411	4.809225553	1.353141952
H78	-3.768630114	3.20262207	2.334061734

[Tm^{But}]CdSPh

atom	x	y	z
Cd1	1.56534257	4.274383908	-0.562210003
S2	1.370268832	2.792675104	-2.797614336
S3	3.598181655	5.869776507	-1.266776363
S4	2.987661459	2.535200233	0.91789902
S5	-0.584599615	5.257737259	0.311853828
B6	4.783033712	2.68925573	-2.079758252
H7	5.77921814	2.207105943	-2.561908188
N8	3.734004668	1.53446835	-2.110585501
N9	2.021564634	0.150470066	-2.244440679
N10	4.436746492	3.892944777	-3.011147084
N11	3.91617249	5.784035508	-4.023355321
N12	5.210344302	3.102867959	-0.635131955
N13	5.528493221	3.483129101	1.514538497
C14	2.396859096	1.469128923	-2.362960188
C15	4.188866888	0.257408461	-1.830183042
H16	5.225021732	0.068649178	-1.600951472
C17	3.144869772	-0.595794918	-1.906938335
H18	3.115891236	-1.659322826	-1.758278818
C19	0.642232755	-0.437042921	-2.411314602
C20	-0.304480042	0.171556223	-1.360273449

H21	-0.418425747	1.246910781	-1.495495071
H22	0.073994345	-0.016750367	-0.350308067
H23	-1.290228771	-0.296391298	-1.450086281
C24	0.710485667	-1.957358001	-2.178874563
H25	1.360043147	-2.460624791	-2.902271462
H26	-0.296640071	-2.363194605	-2.306156019
H27	1.038459064	-2.207561608	-1.165130154
C28	0.150060015	-0.18886882	-3.849037631
H29	0.833570924	-0.645796445	-4.572810482
H30	0.06868882	0.876231683	-4.066662028
H31	-0.836551961	-0.646395424	-3.975337497
C32	3.986024682	5.161780442	-2.798620531
C33	4.641435734	3.725644388	-4.369749974
H34	4.999052326	2.792053587	-4.772243712
C35	4.322255844	4.878742362	-4.996692847
H36	4.355320873	5.123143406	-6.042318764
C37	3.48953554	7.202277596	-4.318608905
C38	3.580505726	7.446879747	-5.835583653
H39	4.600958774	7.334095008	-6.216092654
H40	3.271003868	8.477310379	-6.029092291
H41	2.910186969	6.792339982	-6.40133253
C42	4.449263755	8.178329785	-3.612551996
H43	5.478403266	8.019436219	-3.952892566

H44	4.415000366	8.061432968	-2.529086566
H45	4.163084876	9.205822303	-3.859456658
C46	2.027964029	7.408233462	-3.881610629
H47	1.904455152	7.289459228	-2.806076951
H48	1.366462695	6.698893964	-4.388241456
H49	1.712238425	8.420459137	-4.153541857
C50	4.60596107	3.057518605	0.585809185
C51	6.502041564	3.570274981	-0.466302732
H52	7.169133346	3.69012339	-1.304361723
C53	6.704173165	3.80737122	0.847484452
H54	7.579847396	4.171906025	1.351772508
C55	5.360987381	3.578215982	3.010688422
C56	6.67446599	4.085861506	3.633232548
H57	6.940762838	5.086993952	3.280421419
H58	7.512413052	3.405265506	3.45103501
H59	6.532892093	4.147520472	4.715499188
C60	4.245899212	4.586710408	3.341898795
H61	4.481866701	5.569314997	2.920993738
H62	4.165904485	4.688982828	4.428978577
H63	3.281623994	4.261186597	2.952333523
C64	5.064657693	2.178515192	3.580126594
H65	4.131131544	1.774624586	3.187375784
H66	4.984266809	2.242900331	4.670082311

H67	5.878329594	1.486105176	3.338335182
C68	-1.209950382	6.001930848	-1.199480921
C69	-1.593396626	5.222630257	-2.305836171
H70	-1.487098828	4.142738254	-2.254699471
C71	-2.107222663	5.819146396	-3.45882096
H72	-2.393218798	5.193444145	-4.301265725
C73	-2.263664283	7.205338749	-3.531608938
H74	-2.670154654	7.667959721	-4.42708418
C75	-1.897681853	7.987695398	-2.43342053
H76	-2.018029039	9.068114432	-2.470570413
C77	-1.37497029	7.395509535	-1.282601686
H78	-1.088954441	8.009289995	-0.433547427

[Tm^{But}]CdSePh

atom	x	y	z
Cd1	2.533467542	12.0988281	9.122431378
Se2	0.25644536	11.12605365	10.08324953
S3	2.438165124	13.5573217	6.86436274
S4	4.609821938	10.52005509	8.489731518
S5	3.911504367	13.85769855	10.63023426
B6	5.824214789	13.69006419	7.706449257
H7	6.833870626	14.17907014	7.260608577
N8	4.76476491	14.83679053	7.642022493
N9	3.045658485	16.20514865	7.446999789
N10	5.520691934	12.48186375	6.766764778
N11	5.033139348	10.58671817	5.746429583
N12	6.193121077	13.28036853	9.170140685
N13	6.422277451	12.90976297	11.33549331
C14	3.437213795	14.89030983	7.338662903
C15	5.197519254	16.11770016	7.938719499
H16	6.221818448	16.31588249	8.207432692
C17	4.149179215	16.96114848	7.825953058
H18	4.104302245	18.02312828	7.97935996
C19	1.667551237	16.77968408	7.231449267
C20	0.687335745	16.14614762	8.236100011

H21	1.020886525	16.32852048	9.26235973
H22	0.595468438	15.07096687	8.085480421
H23	-0.300471703	16.60014081	8.110308341
C24	1.709297896	18.29748745	7.485785461
H25	2.384127493	18.81657601	6.798112004
H26	1.990765915	18.53750908	8.515466363
H27	0.704481547	18.69422523	7.320745334
C28	1.235985844	16.54372828	5.772247963
H29	1.943574558	17.01480185	5.081917336
H30	0.251242677	16.9934486	5.611553131
H31	1.173983918	15.48060339	5.540044312
C32	5.057155276	11.21627955	6.969320093
C33	5.781478605	12.63971471	5.416626108
H34	6.160283096	13.56840387	5.0230829
C35	5.482275245	11.48401468	4.784367012
H36	5.558541253	11.23292952	3.742815861
C37	4.610229626	9.169507741	5.442737963
C38	5.533772681	8.190272166	6.191532602
H39	6.576766287	8.34219344	5.894172677
H40	5.251935109	7.164008856	5.936219604
H41	5.454939361	8.311280018	7.271856071
C42	3.130537641	8.976345071	5.822843839
H43	2.497420128	9.688207732	5.284610268

H44	2.967751667	9.105208496	6.892031591
H45	2.818617441	7.964603824	5.545535744
C46	4.75883007	8.915713242	3.931859713
H47	4.114244368	9.569866492	3.337171421
H48	4.453739737	7.88559875	3.731894985
H49	5.793493597	9.023393547	3.591504816
C50	5.540201197	13.33451084	10.36640935
C51	7.478757981	12.81965633	9.396739022
H52	8.182001908	12.70048284	8.589429467
C53	7.62650702	12.58920263	10.71931205
H54	8.482037285	12.23202946	11.26157165
C55	6.191838648	12.81491382	12.82453687
C56	7.478837238	12.30917177	13.50060588
H57	7.762064493	11.30953067	13.15761004
H58	7.291777943	12.24575705	14.57551127
H59	8.321555999	12.99191721	13.35429892
C60	5.871267624	14.21343796	13.38521023
H61	5.744798075	14.14604389	14.47026743
H62	4.955313649	14.61802688	12.95509286
H63	6.694135437	14.90617616	13.18001939
C64	5.066649007	11.80297348	13.11023313
H65	5.324302075	10.82013091	12.70323827
H66	4.120183491	12.12399175	12.67673705

H67	4.938442044	11.70332143	14.19266006
C68	-0.408848898	10.34331708	8.400836312
C69	-0.85045448	11.15136848	7.342776311
H70	-0.796379448	12.23163594	7.435244987
C71	-1.358515071	10.57758326	6.175497756
H72	-1.691398324	11.22091208	5.364791517
C73	-1.448872438	9.189743198	6.050480583
H74	-1.849293083	8.74449415	5.144120185
C75	-1.022776658	8.38095313	7.105540795
H76	-1.090480969	7.298745823	7.024440244
C77	-0.50518901	8.951015034	8.270896324
H78	-0.172036699	8.315576803	9.085623839

[Tm^{But}]CdTePh

atom	x	y	z
Cd1	-0.692373471	4.204439726	4.294931768
Te2	-3.167635663	5.265064563	5.158819623
S3	0.664071167	2.425121202	5.803474463
S4	1.401876999	5.783997268	3.703026099
S5	-0.768111097	2.777502166	2.004512772
B6	2.599967838	2.612229954	2.898382099
H7	3.612413001	2.123807161	2.457721136
N8	2.961787571	2.996646064	4.368362641
N9	3.17877642	3.348532979	6.535651301
N10	2.317933338	3.833562868	1.970662648
N11	1.868210634	5.745044311	0.965799451
N12	1.538875507	1.473290226	2.794745369
N13	-0.17551594	0.113914582	2.519784794
C14	2.298857926	2.94171304	5.558171684
C15	4.247442185	3.451118956	4.604892201
H16	4.955228817	3.574032264	3.801807103
C17	4.387501789	3.670759324	5.929843502
H18	5.241160546	4.019822393	6.480205138
C19	2.939556247	3.431366152	8.022346974
C20	4.226121902	3.921182288	8.711420814

H21	5.064737848	3.233654388	8.563407305
H22	4.033453265	3.975759479	9.785823591
H23	4.518690943	4.92187195	8.379650495
C24	2.605079085	2.029048282	8.564553031
H25	1.689986896	1.63544964	8.122151915
H26	2.470854699	2.084719222	9.649377687
H27	3.424779674	1.332996984	8.357552362
C28	1.818592897	4.446866016	8.308878752
H29	0.873561104	4.13445315	7.865849519
H30	2.084439258	5.431602543	7.912168008
H31	1.683572585	4.537429222	9.391245469
C32	1.866124237	5.101843373	2.181379509
C33	2.597033184	3.687657552	0.622855335
H34	2.971071801	2.758956405	0.224472081
C35	2.320681937	4.853656179	0.000234724
H36	2.413868881	5.115819081	-1.037114026
C37	1.472803561	7.171514038	0.672385544
C38	-0.006509014	7.387325508	1.040003203
H39	-0.649960057	6.696729948	0.486997646
H40	-0.295955299	8.408593785	0.77367547
H41	-0.183172888	7.248034542	2.10554882
C42	1.642019049	7.436142639	-0.834330259
H43	2.678279978	7.314107397	-1.165108772

H44	1.356192357	8.473025024	-1.028038468
H45	0.99263402	6.798431189	-1.441500187
C46	2.406740223	8.125115574	1.440594327
H47	3.449405387	7.958280754	1.150020009
H48	2.316541633	7.99211097	2.51874291
H49	2.145508158	9.159347272	1.195685448
C50	0.218309357	1.431022348	2.460800207
C51	1.963929341	0.184021133	3.065376337
H52	2.982283229	-0.023025373	3.35053573
C53	0.918354787	-0.654292523	2.90145921
H54	0.869956203	-1.72065661	3.019236987
C55	-1.543744826	-0.454054593	2.240488038
C56	-2.55567857	0.127941689	3.244393087
H57	-2.251664573	-0.102934862	4.270130378
H58	-3.537362312	-0.322645019	3.067886488
H59	-2.647146815	1.20876634	3.142870461
C60	-1.501829747	-1.982163447	2.423887751
H61	-1.245090777	-2.269464236	3.44791587
H62	-0.807438439	-2.465644332	1.729627723
H63	-2.500153935	-2.374407173	2.214470529
C64	-1.93363702	-0.150858817	0.782077624
H65	-1.204351135	-0.587387329	0.091540963
H66	-1.992677274	0.921852	0.59817197

H67	-2.911588784	-0.594775515	0.57132471
C68	-3.693754123	5.985415337	3.191471674
C69	-3.993137351	5.096926638	2.148008073
H70	-3.941984246	4.026505301	2.320621735
C71	-4.35605451	5.575169851	0.886254375
H72	-4.579109937	4.869010806	0.09032876
C73	-4.438534805	6.948223897	0.647796193
H74	-4.726994636	7.31931621	-0.331839414
C75	-4.152514861	7.839326461	1.683805578
H76	-4.217103205	8.911488667	1.514211521
C77	-3.780491911	7.363206171	2.944010487
H78	-3.555333824	8.067392443	3.739560912

$Cp^*_2Zr(OPh)_2$

atom	x	y	z
Zr1	-3.16074032	9.397090034	12.46335915
C2	-5.184942014	9.589927563	10.80356229
C3	-5.759868855	9.251624801	12.05784903
C4	-5.32721924	7.938526206	12.41167081
C5	-4.523945108	7.438658436	11.33105186
C6	-4.41070358	8.471266709	10.35720884
C7	-5.456058132	10.85131986	10.0307541
C8	-6.729445868	10.08575148	12.84410435
C9	-5.832427543	7.165837923	13.60223333
C10	-4.153191253	6.002725501	11.0792586
C11	-3.747498517	8.327628621	9.013814807
O12	-3.941691403	10.68511247	13.80061715
C13	-4.223847527	11.62158222	14.71068565
C14	-4.897823875	11.2882911	15.90085145
C15	-5.19650096	12.27359532	16.84031832
C16	-4.838647439	13.60416378	16.6174719
C17	-4.174894275	13.93929733	15.43505872
C18	-3.867374042	12.96497683	14.48790573
H19	-4.661357614	11.07499228	9.31751977
H20	-5.556288812	11.71934864	10.68793511

H21	-6.392776187	10.76135568	9.465590165
H22	-6.631138459	11.14898161	12.61452961
H23	-6.587231532	9.972279369	13.92022755
H24	-7.761468971	9.791560903	12.61200622
H25	-5.258691797	6.251900003	13.77028363
H26	-6.879810067	6.868729435	13.46293979
H27	-5.791422887	7.756882433	14.52324592
H28	-4.165042446	5.404676577	11.99017478
H29	-3.170587347	5.89486688	10.61239763
H30	-4.88058231	5.553524412	10.38989273
H31	-2.83475773	7.725958526	9.068152899
H32	-3.478645611	9.297181703	8.590544786
H33	-4.416959116	7.830224229	8.299372527
H34	-5.174776363	10.25285976	16.07338315
H35	-5.715125697	11.99656465	17.75474589
H36	-5.071270166	14.36771586	17.3532128
H37	-3.890192911	14.96948542	15.24704836
H38	-3.341719579	13.22144416	13.57450196
C39	-1.140984978	9.575478362	14.12794942
C40	-0.564289116	9.247345372	12.87201932
C41	-0.993328974	7.935395472	12.50885019
C42	0.402889906	10.09257565	12.09496736
H43	0.244756376	11.15913889	12.2692159

H44	0.31756496	9.92488365	11.01996957
H45	1.435024879	9.858948233	12.38733002
C46	-1.798167326	7.427185824	13.58451147
C47	-1.914776903	8.453266722	14.56492718
C48	-0.869801799	10.8285217	14.91332527
H49	-1.694441944	11.08309238	15.58082522
H50	-0.701390312	11.68873623	14.26011422
H51	0.030184066	10.70766729	15.53020768
C52	-2.167189866	5.988980717	13.82695271
H53	-2.165593374	5.396663153	12.91200259
H54	-3.145139565	5.878741979	14.30300142
H55	-1.433395509	5.534130384	14.50586391
C56	-2.578849415	8.303703989	15.90707117
H57	-3.494623408	7.707091121	15.84952108
H58	-2.841851804	9.27269654	16.33560723
H59	-1.911722394	7.798877921	16.61854852
O60	-2.376704885	10.68551027	11.12841805
C61	-2.099859661	11.61548896	10.21009097
C62	-1.418099425	11.27631651	9.026069112
C63	-1.125679377	12.25444257	8.077063314
C64	-1.496797934	13.58392372	8.284806049
C65	-2.167446475	13.9250522	9.461693787
C66	-2.469367967	12.95766227	10.41780406

H67	-2.999833393	13.21892055	11.32706156
H68	-2.462223313	14.95444287	9.638128157
H69	-1.268953817	14.34187384	7.541776425
H70	-0.601269002	11.97289128	7.167284825
H71	-1.130418909	10.24193671	8.865803512
C72	-0.486730229	7.169699221	11.3142348
H73	-1.057414198	6.254276595	11.14396673
H74	0.561836724	6.875666959	11.45065438
H75	-0.531586411	7.763429221	10.39517146

$Cp^*_2Zr(SPh)_2$

atom	x	y	z
Zr1	6.165036357	1.065937447	4.442951231
S2	7.87140301	2.683032404	5.458239671
C3	7.321538188	3.996474778	6.537886544
C4	6.146467355	4.730591093	6.312400358
C5	5.825548092	5.816081775	7.130155911
C6	6.666332267	6.188964384	8.17972226
C7	7.840069205	5.46644127	8.40467475
C8	8.167136261	4.381605975	7.592519989
C9	3.855493119	0.219707931	5.379913238
C10	4.264390722	1.251127767	6.291979003
C11	5.443819285	0.810658075	6.950410431
C12	5.775857407	-0.489678333	6.448996564
C13	4.760737167	-0.87177153	5.512828252
C14	2.547470938	0.18113252	4.63721235
C15	3.43316819	2.446944819	6.665004029
C16	6.090331249	1.428685076	8.156436297
C17	6.81966614	-1.37370628	7.079256154
C18	4.467495979	-2.268050874	5.035329081
H19	5.488589885	4.453220493	5.495390545
H20	4.912769757	6.374798253	6.938044894

H21	6.413228171	7.035567114	8.812105939
H22	8.506638244	5.747584518	9.21630948
H23	9.08470207	3.82700939	7.766719761
H24	1.747389148	-0.186836136	5.2946587
H25	2.255286703	1.170391243	4.278255112
H26	2.58933941	-0.486097173	3.77119788
H27	2.638793998	2.139735974	7.359021226
H28	4.026802758	3.217068504	7.1612698
H29	2.9596316	2.901565441	5.791922782
H30	5.749994962	0.906135433	9.061229673
H31	7.180229753	1.355065889	8.120168211
H32	5.836808064	2.482986178	8.267115346
H33	6.552036073	-1.586568641	8.122583444
H34	6.908990792	-2.333367739	6.568083292
H35	7.809559931	-0.904697199	7.096550831
H36	3.713520143	-2.721635205	5.693794073
H37	4.058465974	-2.294675456	4.023060414
H38	5.345714619	-2.91376972	5.067074927
S39	4.459504641	2.688194533	3.434487946
C40	5.010062017	3.997389694	2.35052823
C41	6.183350716	4.734702415	2.573504457
C42	6.504957772	5.814151359	1.748092012
C43	5.665929683	6.178396743	0.69402055

C44	4.493041269	5.453346483	0.472380927
C45	4.165622188	4.374284616	1.292037314
H46	3.248882736	3.817446247	1.120266784
H47	3.827772208	5.727479618	-0.342714327
H48	5.919693163	7.020254686	0.055573542
H49	7.417588876	6.374243533	1.937105541
H50	6.841281933	4.46257743	3.392215618
C51	8.473499875	0.223136883	3.506502047
C52	8.066074615	1.256967378	2.596410845
C53	6.887104256	0.818881716	1.935602501
C54	8.900713718	2.452006543	2.227653704
H55	9.703029358	2.142017196	1.544128292
H56	8.312452801	3.219510692	1.721574102
H57	9.365028055	2.910291809	3.103926573
C58	6.553711298	-0.482677962	2.433521992
C59	7.56816687	-0.867492264	3.369667276
C60	9.781587381	0.181234176	4.249361728
H61	10.58106517	-0.188064568	3.591930762
H62	10.07581026	1.16945421	4.609439882
H63	9.738016517	-0.48669644	5.114755715
C64	5.509728672	-1.365020981	1.800583597
H65	5.774010824	-1.572294503	0.754925911
H66	5.423523172	-2.327405559	2.307287395

H67	4.518907812	-0.897733387	1.788850131
C68	7.860224314	-2.26470083	3.844921035
H69	8.612964889	-2.71848469	3.185218357
H70	8.270459651	-2.292827499	4.856606333
H71	6.981023499	-2.908973333	3.81378733
C72	6.240731891	1.439910823	0.731356234
H73	6.574867557	0.914632858	-0.174113187
H74	5.150493298	1.373362084	0.771366702
H75	6.500763605	2.49245616	0.619097897

$Cp^*_2Zr(SePh)_2$

atom	x	y	z
Zr1	0.097078462	7.821968778	7.984375077
Se2	1.013177883	5.687298691	9.403229714
Se3	2.208495779	8.154161286	6.290712468
C4	-1.049923712	9.387358879	9.746413862
C5	-0.282530179	10.21045717	8.859528793
C6	1.103955246	9.95907531	9.11567292
C7	1.194684957	8.956248951	10.11924895
C8	-0.140997655	8.587641691	10.49687691
C9	-2.257198404	7.016059774	7.358215991
C10	-2.068026851	8.18973863	6.559751588
C11	-1.040863538	7.913686608	5.611970275
C12	-0.642696735	6.542946143	5.773948172
C13	-1.396148735	5.992211259	6.846439202
C14	-2.498291178	9.570764693	10.11308044
C15	-0.773121904	11.3877457	8.057436989
C16	2.22188035	10.82044045	8.603051704
C17	2.44658391	8.559327618	10.85305836
C18	-0.515509047	7.733195554	11.6782489
C19	-3.378593916	6.748092726	8.326304836
C20	-3.007455579	9.36100783	6.461350678

C21	-0.655281178	8.81004765	4.465092068
C22	0.19747112	5.759534385	4.802631258
C23	-1.513426927	4.539345517	7.208447956
C24	1.629145085	4.139024286	8.371424625
C25	2.399907813	4.267141143	7.209278558
C26	2.910719574	3.129771836	6.578222457
C27	2.660496495	1.858432394	7.09628876
C28	1.89694727	1.729990251	8.257937419
C29	1.383335198	2.861516493	8.893101425
C30	3.986939497	8.32787378	7.098861651
C31	4.451752521	7.445221002	8.081262877
C32	5.769961785	7.533863384	8.535932199
C33	6.636499119	8.496357099	8.01613115
C34	6.176237318	9.374115438	7.03316
C35	4.860540546	9.291261196	6.574649513
H36	-2.569419167	10.25226196	10.9721559
H37	-3.087131797	10.01455857	9.309131721
H38	-2.977541649	8.635886101	10.41046315
H39	-0.456924887	12.32429637	8.535060276
H40	-0.369973716	11.40000646	7.039472321
H41	-1.861154777	11.41119249	7.990714936
H42	2.275274593	11.74601258	9.193245837
H43	3.188831088	10.32355286	8.674076437

H44	2.074165604	11.09898312	7.556763869
H45	2.576879276	9.203235796	11.73375128
H46	2.409267355	7.523707003	11.19645673
H47	3.335023839	8.667793799	10.22885837
H48	-0.574008027	8.349781276	12.58571456
H49	-1.489626369	7.254390118	11.54553054
H50	0.215684461	6.943650993	11.86046402
H51	-4.116202526	6.074840847	7.870751708
H52	-3.030053856	6.263466952	9.244197292
H53	-3.904230273	7.662198989	8.603690436
H54	-3.776598165	9.141331368	5.707944145
H55	-3.530848881	9.567119137	7.395862887
H56	-2.504555715	10.27583083	6.142709682
H57	-1.328839942	8.64685877	3.612768447
H58	-0.719742531	9.86831491	4.733291686
H59	0.364005512	8.620824551	4.123323757
H60	-0.434257316	5.401800842	3.977840356
H61	0.999104742	6.362982564	4.373265069
H62	0.656054864	4.887426072	5.272073261
H63	-2.402893517	4.111189187	6.725394703
H64	-0.647935927	3.962957197	6.882005657
H65	-1.615921597	4.394095162	8.286783499
H66	2.601224378	5.251210273	6.797675826

H67	3.508471129	3.24412011	5.677518924
H68	3.061931926	0.977059199	6.604188532
H69	1.696606085	0.745648048	8.673357226
H70	0.794621377	2.755966379	9.799505348
H71	3.786746607	6.692980999	8.493107588
H72	6.117566503	6.841889592	9.298829352
H73	7.661173319	8.560661612	8.371493523
H74	6.842485804	10.12583705	6.617566498
H75	4.509765626	9.971569494	5.80439543

$Cp^*_2Zr(TePh)_2$

atom	x	y	z
Zr1	-0.738574375	-1.218091639	0.808227398
Te2	0.219136686	-2.714987146	-1.526375437
Te3	-0.318718267	1.485952331	-0.265213901
C4	1.036744578	-2.863525012	1.851558163
C5	1.797586696	-1.718461835	1.436316841
C6	1.381922404	-0.608398304	2.223182278
C7	0.361511763	-1.055151332	3.123054025
C8	0.176939118	-2.45990872	2.915344172
C9	-3.080413302	-0.083569386	1.214591238
C10	-3.136003534	-0.573901387	-0.134412201
C11	-3.075310997	-1.994602377	-0.085908208
C12	-2.979407573	-2.390952948	1.286600945
C13	-3.022433513	-1.207428797	2.090172835
C14	1.310197896	-4.296670818	1.47725918
C15	3.016912458	-1.733239028	0.553644332
C16	2.098413104	0.705685131	2.349274807
C17	-0.133669831	-0.229652149	4.281662272
C18	-0.487194238	-3.427555689	3.857512083
C19	-3.360651208	1.328031145	1.65829467
C20	-3.507359766	0.225932452	-1.354530186

C21	-3.404845399	-2.934170533	-1.210536745
C22	-3.157096608	-3.814154998	1.746493336
C23	-3.343118825	-1.13475552	3.558689356
C24	-0.775374379	-2.179623619	-3.353963529
C25	-1.219605108	-3.200238073	-4.207862301
C26	-1.750020227	-2.895315356	-5.463550039
C27	-1.845326518	-1.568119765	-5.883820223
C28	-1.40393022	-0.547774439	-5.039949544
C29	-0.869695074	-0.848778893	-3.78421996
C30	1.689715801	1.85783079	-0.938928139
C31	2.324513294	1.02595608	-1.872029915
C32	3.573197086	1.372909168	-2.395686663
C33	4.203946633	2.554539482	-2.001558047
C34	3.575037315	3.38887576	-1.07611892
C35	2.328127193	3.044501711	-0.548157924
H36	1.992563219	-4.752070216	2.208368132
H37	0.398438834	-4.900596319	1.461959999
H38	1.776671923	-4.386468794	0.494371201
H39	3.916343724	-1.846606143	1.174932507
H40	3.001477104	-2.556946994	-0.161955528
H41	3.122173423	-0.807069459	-0.014846609
H42	2.836024141	0.642390486	3.162652067
H43	2.631620566	0.975964529	1.437518566

H44	1.412330379	1.52293558	2.584203489
H45	0.703764859	0.027493493	4.943295944
H46	-0.584257162	0.71591126	3.961555616
H47	-0.867195256	-0.768086815	4.882948996
H48	0.266756353	-3.83220135	4.547235064
H49	-1.259163579	-2.960055657	4.470322757
H50	-0.931758847	-4.280231531	3.340488404
H51	-4.430546526	1.448553846	1.878295287
H52	-2.809458962	1.593473316	2.56492105
H53	-3.09944953	2.060056254	0.89213331
H54	-4.59466195	0.174496354	-1.504248086
H55	-3.235615282	1.278658606	-1.260808046
H56	-3.030047689	-0.157918039	-2.258344669
H57	-4.480473057	-3.161013494	-1.190044598
H58	-3.172767109	-2.508440648	-2.186554754
H59	-2.863473519	-3.879768552	-1.127095531
H60	-4.141167493	-4.18843112	1.435305781
H61	-2.41169827	-4.48879044	1.313018473
H62	-3.105478898	-3.904184516	2.83241958
H63	-4.431848164	-1.049041906	3.682697467
H64	-3.031128558	-2.025141036	4.106398625
H65	-2.900765549	-0.262567955	4.043562482
H66	-1.147604242	-4.2380839	-3.894392073

H67	-2.089296171	-3.69907094	-6.112433322
H68	-2.257098987	-1.33133793	-6.861218718
H69	-1.469061308	0.489961272	-5.357750796
H70	-0.530904135	-0.042616577	-3.139788967
H71	1.848965529	0.10286418	-2.190977846
H72	4.048886944	0.715401007	-3.119204061
H73	5.172511133	2.823863566	-2.4136454
H74	4.052493104	4.313901655	-0.762048026
H75	1.847875788	3.707585326	0.166239793

Tp_2LaOPh

atom	x	y	z
La1	0.206304027	-0.432911772	0.022517322
N2	0.265800872	0.44978062	-2.492618447
N3	1.367671225	1.050009638	-3.02703176
C4	-0.633899828	0.34736107	-3.48173501
C5	-0.128974202	0.888398951	-4.671129463
C6	1.145692467	1.320313766	-4.333139655
N7	2.770637704	-0.719088054	-0.755763141
N8	3.342078568	0.123375686	-1.662675726
C9	3.67173779	-1.680262351	-0.507662664
C10	4.843134385	-1.468573929	-1.246333126
C11	4.585978518	-0.310893984	-1.965732875
N12	1.424989174	1.945606888	-0.0650109
N13	2.283733003	2.338622511	-1.043163063
C14	1.312083937	2.976349697	0.784980311
C15	2.106370292	4.051664989	0.361121744
C16	2.704219618	3.601380495	-0.806693471
B17	2.646823837	1.402429399	-2.20998208
N18	0.234785906	-2.740405729	-1.448980552
N19	-0.509195659	-3.825774424	-1.102760236
C20	0.882976682	-3.070377943	-2.574799996

C21	0.563824815	-4.378063989	-2.968786178
C22	-0.32599027	-4.819239241	-2.001495726
N23	-2.265907949	-1.426624515	-0.179845489
N24	-2.531971472	-2.7527211	-0.0102079
C25	-3.451836182	-0.801660118	-0.217138293
C26	-4.502367782	-1.718744121	-0.084989492
C27	-3.868869802	-2.944555172	0.049267967
N28	0.192771287	-2.540532767	1.66032696
N29	-0.600736574	-3.624131422	1.432549863
C30	0.720018014	-2.70368674	2.883359451
C31	0.276568376	-3.899449859	3.461747916
C32	-0.562904094	-4.447880459	2.502961276
B33	-1.43087235	-3.835661908	0.132607218
O34	-0.795252869	0.798252304	1.659836054
C35	-1.757861757	1.182618656	2.501456716
C36	-2.152836336	0.369392924	3.582627542
C37	-3.170707749	0.777046249	4.441294963
C38	-3.817417311	2.00139888	4.25709743
C39	-3.426213994	2.818060017	3.195073381
C40	-2.411089653	2.420107249	2.326960721
H41	-1.594729108	-0.112573745	-3.290049778
H42	-0.615219453	0.95588033	-5.632999264
H43	1.907442585	1.802713064	-4.928057433

H44	3.430687533	-2.481705362	0.178778655
H45	5.741873313	-2.066224111	-1.256616103
H46	5.198590577	0.235151051	-2.668031257
H47	0.656704579	2.885756697	1.639538615
H48	2.224761378	5.01606075	0.83150092
H49	3.392282247	4.086282708	-1.484002668
H50	3.41456473	1.958901675	-2.947443993
H51	1.544938746	-2.355393748	-3.042816553
H52	0.925533642	-4.922621675	-3.82785703
H53	-0.840027273	-5.762727001	-1.888247151
H54	-3.49572279	0.275265988	-0.313744271
H55	-5.563050265	-1.519370332	-0.075807396
H56	-4.272874582	-3.937076662	0.18532406
H57	1.382636401	-1.952243528	3.293998961
H58	0.523069568	-4.302847238	4.432160204
H59	-1.136023038	-5.363446175	2.508208956
H60	-1.96802492	-4.907515727	0.211713407
H61	-1.654459112	-0.585561625	3.722874251
H62	-3.464790275	0.128957601	5.263451675
H63	-4.612700869	2.311817141	4.928664157
H64	-3.917865378	3.775186925	3.037927998
H65	-2.106109095	3.053705437	1.498303842

Tp_2LaSPh

atom	x	y	z
La1	-0.244925671	-0.159530159	-0.262819406
N2	-2.51457772	1.190125572	-0.045446139
N3	-3.36952027	1.346189941	-1.095223988
C4	-3.077699026	1.810424263	1.003705098
C5	-4.304643077	2.378819113	0.64360023
C6	-4.447027181	2.057606128	-0.699033405
N7	-1.925812808	-1.39504414	-1.951256538
N8	-2.948007529	-0.726187134	-2.554643766
C9	-2.112273719	-2.695867376	-2.217103754
C10	-3.256374107	-2.883964734	-3.003336464
C11	-3.755068477	-1.603792502	-3.191924427
N12	-0.579683165	1.285299041	-2.526103063
N13	-1.80696894	1.460907696	-3.096407133
C14	0.295313572	1.944169691	-3.302174396
C15	-0.358177161	2.549874637	-4.38364885
C16	-1.691776807	2.215894644	-4.21163811
B17	-3.085724043	0.817163035	-2.532812221
N18	-1.779011482	-1.829009956	1.225917926
N19	-1.250096605	-2.831518712	1.978368257
C20	-3.11052155	-1.968065504	1.292660378

C21	-3.457209569	-3.063561975	2.095742727
C22	-2.240092066	-3.582086131	2.51075031
N23	0.752370444	-0.464646774	2.18726214
N24	0.828505028	-1.674832114	2.811303403
C25	1.281260746	0.432967947	3.032242252
C26	1.695007266	-0.184751817	4.218756985
C27	1.391595738	-1.524045808	4.030645717
N28	0.929386738	-2.530621931	-0.262111903
N29	0.983739936	-3.315541651	0.850529076
C30	1.668240326	-3.144405747	-1.201306546
C31	2.207312452	-4.337034719	-0.706411812
C32	1.745742839	-4.401701979	0.600987809
B33	0.271487056	-2.976790183	2.195100317
S34	2.098281116	1.521263619	-0.506130571
C35	3.467170779	1.141504668	0.570313628
C36	4.03494883	-0.142247486	0.64002242
C37	5.120992728	-0.39708655	1.477261743
C38	5.670484916	0.621404119	2.258330898
C39	5.121231924	1.902930462	2.188376896
C40	4.033854447	2.161998523	1.354420242
H41	-2.578527866	1.815602651	1.964267334
H42	-4.986378872	2.940576466	1.263692279
H43	-5.236615292	2.287227371	-1.399382777

H44	-1.421895127	-3.428968935	-1.823118311
H45	-3.66048769	-3.811441238	-3.379639589
H46	-4.621159783	-1.255085138	-3.735154366
H47	1.34153291	1.962368136	-3.02795812
H48	0.075891377	3.147496342	-5.170677108
H49	-2.565399944	2.458322138	-4.799290486
H50	-4.020368859	1.123175984	-3.222464859
H51	-3.751546204	-1.281955318	0.757460767
H52	-4.444955046	-3.423802936	2.340428433
H53	-2.00777661	-4.424715844	3.145725388
H54	1.37203812	1.467595991	2.732083054
H55	2.162941473	0.271429831	5.077503593
H56	1.53926692	-2.379567454	4.673548122
H57	1.779821776	-2.698969422	-2.181729753
H58	2.840403356	-5.045256316	-1.218606026
H59	1.906978959	-5.143135762	1.369664741
H60	0.474237752	-3.884747531	2.954561533
H61	3.620752848	-0.941551011	0.032954067
H62	5.540872391	-1.399558164	1.516187774
H63	6.517333393	0.420339804	2.908820463
H64	5.541184665	2.709217871	2.785407842
H65	3.614411026	3.162544506	1.299114554

$Tp_2LaSePh$

atom	x	y	z
La1	0.023747784	0.16188443	-0.098185778
N2	-1.364905941	-1.975054946	0.594004952
N3	-2.570371276	-2.270480765	0.030792815
C4	-1.109253	-2.945673533	1.486161332
C5	-2.153007451	-3.877092942	1.518176415
C6	-3.057804428	-3.405742011	0.576784636
N7	-1.173694258	-0.662279157	-2.354936445
N8	-2.38289157	-1.290184587	-2.333394835
C9	-0.735680831	-0.721141241	-3.620932743
C10	-1.660354449	-1.387057236	-4.436551528
C11	-2.691080893	-1.730095775	-3.573909556
N12	-2.578476569	0.889077691	-0.141357562
N13	-3.556127245	0.013716752	-0.516286187
C14	-3.20233717	2.030620635	0.191358984
C15	-4.588897413	1.90205529	0.039279053
C16	-4.767399015	0.604599028	-0.41108774
B17	-3.259257451	-1.39609447	-1.057015521
N18	1.549161234	-1.829847668	-1.131169018
N19	2.906762406	-1.761427908	-1.178754006
C20	1.208373523	-2.995020827	-1.699752999

C21	2.347783579	-3.694745024	-2.121579206
C22	3.405926863	-2.870876275	-1.766988727
N23	2.123742453	-0.309622885	1.450507446
N24	3.377819508	-0.481909217	0.942373151
C25	2.247298011	-0.333730868	2.785935106
C26	3.581143443	-0.53722022	3.15833252
C27	4.26328408	-0.617607236	1.954414102
N28	2.035849758	1.212619962	-1.460291732
N29	3.307973434	0.741472652	-1.321577318
C30	2.121343658	2.338639853	-2.187956112
C31	3.450650544	2.608581541	-2.529989368
C32	4.166958269	1.567330348	-1.955455656
B33	3.680542507	-0.573986833	-0.571797853
Se34	-0.226451506	2.536054551	1.81826712
C35	1.523153799	3.197851551	2.394122978
C36	2.529439297	3.530277517	1.476518805
C37	3.744718999	4.059584914	1.915655249
C38	3.973634915	4.273567086	3.275727175
C39	2.973786927	3.949152614	4.19429535
C40	1.760599924	3.412991747	3.759691189
H41	-0.189205299	-2.927974793	2.055675732
H42	-2.239570382	-4.760393588	2.132559138
H43	-4.012860289	-3.796970288	0.259053499

H44	0.225478805	-0.296976948	-3.879593991
H45	-1.591311893	-1.589793931	-5.494411075
H46	-3.61943377	-2.252476665	-3.75348737
H47	-2.624237129	2.87728098	0.535879174
H48	-5.348321163	2.643764562	0.233275933
H49	-5.664659253	0.059981657	-0.666145559
H50	-4.294062174	-1.929364414	-1.350815742
H51	0.166329754	-3.268818217	-1.784186262
H52	2.39635076	-4.655543482	-2.611736963
H53	4.472085368	-2.993004753	-1.891030204
H54	1.378313566	-0.172981984	3.409347088
H55	3.992198749	-0.595442557	4.154491399
H56	5.313726914	-0.758638786	1.745801647
H57	1.22894718	2.906551757	-2.417953511
H58	3.835896705	3.437574111	-3.103465415
H59	5.226069234	1.356376053	-1.955557753
H60	4.859159469	-0.754880174	-0.713445122
H61	2.357510854	3.389614412	0.414723087
H62	4.51131316	4.31153051	1.186823377
H63	4.916410546	4.693967921	3.615438659
H64	3.135827621	4.11709639	5.256628424
H65	0.983473213	3.175085015	4.479474969

$Tp_2LaTePh$

atom	x	y	z
La1	0.362628871	0.710074564	-0.732459363
N2	2.093835548	-0.987920495	-1.831348227
N3	3.405648996	-0.65497631	-1.992736575
C4	1.988569976	-2.288104745	-2.141620038
C5	3.232524737	-2.812700226	-2.515066177
C6	4.102342042	-1.738194957	-2.404312963
N7	1.855613512	1.962315379	-2.625017633
N8	3.206595092	1.77213813	-2.68125714
C9	1.56791413	2.858039623	-3.581899608
C10	2.725436716	3.259472747	-4.260674211
C11	3.742764015	2.542787842	-3.65355461
N12	2.663934162	1.43773909	0.349585875
N13	3.848607379	1.219399238	-0.28858114
C14	2.967035821	1.832062843	1.595698739
C15	4.354336406	1.880795369	1.77742793
C16	4.872332464	1.483209075	0.553281042
B17	3.957522763	0.78035256	-1.777214345
N18	0.90715031	-1.172298996	1.152869146
N19	-0.064736154	-1.821889938	1.846497788
C20	2.071295677	-1.719296886	1.530177024

C21	1.862141258	-2.731881191	2.477153135
C22	0.485615882	-2.761752379	2.646243479
N23	-1.423042232	-1.219973356	-0.87788142
N24	-2.010543961	-1.751762913	0.230438132
C25	-2.039259714	-1.767519096	-1.937940426
C26	-3.031041643	-2.66440752	-1.526513212
C27	-2.97815469	-2.616606846	-0.140841118
N28	-1.121084362	1.067237009	1.422860284
N29	-1.74532174	0.039277717	2.064154328
C30	-1.456433696	2.185937558	2.082664387
C31	-2.292144553	1.893506157	3.166298539
C32	-2.453523775	0.518371164	3.110176988
B33	-1.552105931	-1.449008016	1.685709939
Te34	-1.758585638	2.902234104	-2.026978446
C35	-3.6591303	2.377276915	-1.156424721
C36	-4.215778546	3.165280098	-0.138318821
C37	-5.468035958	2.859420401	0.401011666
C38	-6.191733377	1.761357542	-0.06750354
C39	-5.648410785	0.97409616	-1.084266683
C40	-4.396357721	1.280218254	-1.62559966
H41	1.029358061	-2.78280462	-2.066614986
H42	3.466143139	-3.821691963	-2.819333607
H43	5.163865644	-1.666548312	-2.591161247

H44	0.544348602	3.165119035	-3.748091776
H45	2.807238756	3.964227717	-5.074005203
H46	4.805721003	2.51944052	-3.844995593
H47	2.176107386	2.051951084	2.300860045
H48	4.900662219	2.164932035	2.663897979
H49	5.894549809	1.375246274	0.221201406
H50	5.121938581	0.778108556	-2.070788562
H51	2.999076877	-1.362763297	1.105217302
H52	2.600229399	-3.348666805	2.967250393
H53	-0.138058905	-3.377775783	3.277768668
H54	-1.748187354	-1.483091941	-2.941086641
H55	-3.693229396	-3.254265835	-2.141618399
H56	-3.558002766	-3.139814644	0.605130854
H57	-1.103366463	3.145154849	1.728570556
H58	-2.731345567	2.580613277	3.873057023
H59	-3.020956944	-0.151874646	3.73901977
H60	-2.212822081	-2.119926643	2.430100378
H61	-3.669733219	4.027305644	0.232550698
H62	-5.87842508	3.485097756	1.190332117
H63	-7.166807192	1.525683516	0.350459389
H64	-6.200278568	0.117105797	-1.463580298
H65	-3.991968353	0.661024457	-2.420128429

Tp_2LuOPh

atom	x	y	z
Lu1	0.118552096	-0.436250748	0.037452623
N2	0.076913942	0.413066792	-2.255737905
N3	1.193103481	0.963775023	-2.815872579
C4	-0.832199884	0.314019586	-3.233598983
C5	-0.319980751	0.808211478	-4.439371123
C6	0.970097279	1.208568455	-4.125071055
N7	2.521093685	-0.752559077	-0.472950425
N8	3.12873905	0.020519107	-1.418490228
C9	3.391718275	-1.719748139	-0.156269177
C10	4.578590434	-1.580832081	-0.886894529
C11	4.364105108	-0.461396373	-1.677015667
N12	1.208214692	1.804013729	0.102409586
N13	2.090609321	2.227197541	-0.840620994
C14	1.060932852	2.819879058	0.964195734
C15	1.851823702	3.913408926	0.5838577
C16	2.488200177	3.490682791	-0.572503805
B17	2.474679172	1.302893015	-2.000897501
N18	0.30354127	-2.515338839	-1.488836408
N19	-0.365621101	-3.664009827	-1.20868172
C20	0.982134751	-2.741634938	-2.618853958

C21	0.754690798	-4.045699443	-3.083933497
C22	-0.11193951	-4.59713335	-2.152587284
N23	-2.131270725	-1.346041844	-0.269219747
N24	-2.398711401	-2.673084911	-0.122541683
C25	-3.31306391	-0.724378486	-0.385641726
C26	-4.363986509	-1.648374949	-0.332922846
C27	-3.734331874	-2.872306489	-0.159733628
N28	0.295958075	-2.362398287	1.509215841
N29	-0.437553948	-3.490523131	1.305755133
C30	0.916781626	-2.512927208	2.689422437
C31	0.596080912	-3.747846176	3.263979177
C32	-0.269342744	-4.331355641	2.349011552
B33	-1.282778869	-3.737933043	0.021273834
O34	-0.839809544	0.57195432	1.566697905
C35	-1.779817947	1.024220562	2.389414348
C36	-2.037870537	0.384287616	3.618676351
C37	-3.024243828	0.867858682	4.474772825
C38	-3.776726534	1.996694996	4.138656555
C39	-3.525082527	2.640755864	2.925796726
C40	-2.541280374	2.166673226	2.059509329
H41	-1.80019817	-0.119310283	-3.024076565
H42	-0.812116486	0.865271383	-5.398079549
H43	1.741903568	1.653146273	-4.736385265

H44	3.117186407	-2.474148845	0.567773579
H45	5.460641711	-2.201608087	-0.848894291
H46	5.001642043	0.028371186	-2.398661708
H47	0.389685461	2.712682423	1.802874063
H48	1.943099488	4.870088692	1.075855444
H49	3.188854355	3.995926568	-1.22151192
H50	3.259897287	1.843660425	-2.730937469
H51	1.602576673	-1.964630996	-3.042662592
H52	1.161097241	-4.517682536	-3.965467805
H53	-0.563189661	-5.576931931	-2.092804925
H54	-3.352667435	0.352809521	-0.473400832
H55	-5.423342119	-1.453379018	-0.397428975
H56	-4.14021254	-3.868023898	-0.059127467
H57	1.557853612	-1.727965522	3.068940814
H58	0.938559724	-4.153687344	4.203539686
H59	-0.774067304	-5.285782111	2.366651146
H60	-1.784570639	-4.82553835	0.102847071
H61	-1.452276585	-0.494218447	3.875358384
H62	-3.209851731	0.356507893	5.416791926
H63	-4.545855245	2.366886987	4.810568615
H64	-4.100596808	3.521672344	2.649154408
H65	-2.33409453	2.67226005	1.11940769

Tp_2LuSPh

atom	x	y	z
Lu1	0.00364643	-0.751488163	-0.490051176
N2	-1.452071712	1.105206128	0.340081772
N3	-2.465920559	1.637143872	-0.400502213
C4	-1.541997318	1.669988707	1.554731838
C5	-2.601785049	2.583143422	1.607205641
C6	-3.160583514	2.529060195	0.340359763
N7	-2.008766996	-1.165633255	-1.927910523
N8	-2.925913865	-0.180115346	-2.149155876
C9	-2.566408804	-2.30330783	-2.362482137
C10	-3.84893847	-2.06857472	-2.874723314
C11	-4.033315875	-0.704238968	-2.716386148
N12	-0.210731326	1.060778113	-2.464761263
N13	-1.390633741	1.708553907	-2.674227211
C14	0.665923092	1.617329996	-3.311916218
C15	0.061046024	2.632677391	-4.070464748
C16	-1.249164811	2.657373263	-3.62808681
B17	-2.653484011	1.327754711	-1.903313537
N18	-1.825176186	-1.858368629	0.908352799
N19	-1.55502319	-2.918328786	1.713804646
C20	-3.142796137	-1.640173331	1.000197192

C21	-3.739054395	-2.558823872	1.87509181
C22	-2.688602154	-3.354097121	2.307737113
N23	0.728633045	-0.929888079	1.817592689
N24	0.633047233	-2.090039205	2.528434083
C25	1.167552716	0.004358364	2.675341356
C26	1.348258812	-0.538361274	3.953372508
C27	0.998486864	-1.872173141	3.811255912
N28	0.682957304	-2.997418548	-0.493272654
N29	0.560245356	-3.786936173	0.613095848
C30	1.273507753	-3.743545596	-1.440876474
C31	1.531771613	-5.028398476	-0.961986171
C32	1.061361535	-5.007579973	0.345491096
B33	-0.091102878	-3.326079064	1.955597306
S34	2.340560242	0.633957481	-0.718590421
C35	3.15007259	1.597148501	0.555483158
C36	3.891825643	1.059698771	1.620042644
C37	4.450919542	1.89108792	2.596205871
C38	4.281238143	3.276038802	2.542330804
C39	3.547783452	3.824118195	1.486396391
C40	2.993202507	2.998618136	0.509655585
H41	-0.856052566	1.392415091	2.339234464
H42	-2.913896759	3.192985656	2.442070228
H43	-3.994966512	3.065866589	-0.08741245

H44	-2.027884058	-3.235690659	-2.265840723
H45	-4.541245943	-2.780110556	-3.296861629
H46	-4.866289483	-0.064714935	-2.97110975
H47	1.702407984	1.316609291	-3.284065546
H48	0.516430082	3.270496805	-4.813090452
H49	-2.08436268	3.284447797	-3.907225777
H50	-3.594967413	1.959669947	-2.302179783
H51	-3.5982562	-0.827085895	0.454022221
H52	-4.779015981	-2.625730248	2.1572305
H53	-2.663449821	-4.183786196	2.998737805
H54	1.356341602	1.011274392	2.336918912
H55	1.698123666	-0.032859154	4.840725927
H56	0.979228445	-2.677370675	4.530855203
H57	1.51257341	-3.30860488	-2.403242662
H58	1.999096972	-5.848124873	-1.484066195
H59	1.052392632	-5.774175996	1.105698831
H60	-0.030987992	-4.232897549	2.73825059
H61	4.02500971	-0.015051542	1.687183053
H62	5.014498848	1.446824773	3.413348262
H63	4.707316354	3.917236342	3.309973928
H64	3.39557376	4.900056639	1.427334527
H65	2.409699685	3.433338286	-0.296452548

$Tp_2LuSePh$

atom	x	y	z
Lu1	0.119117673	0.209727096	-0.546142181
N2	-0.966395269	-1.58233685	0.714829674
N3	-2.221339617	-2.010009122	0.39415305
C4	-0.566490794	-2.325175867	1.757724805
C5	-1.56336423	-3.233418525	2.131102474
C6	-2.596338906	-2.995982403	1.236855844
N7	-1.160313593	-0.83485196	-2.353208574
N8	-2.329503803	-1.487778476	-2.103450325
C9	-0.85782702	-1.068397257	-3.637546588
C10	-1.834165187	-1.87259565	-4.237053785
C11	-2.749042797	-2.114739011	-3.221994225
N12	-2.278666757	1.024039819	-0.474105111
N13	-3.299243091	0.116301289	-0.466613542
C14	-2.850048811	2.224291256	-0.288477794
C15	-4.238103839	2.102421818	-0.149095955
C16	-4.478179163	0.74372384	-0.267434961
B17	-3.062724175	-1.373502936	-0.739979359
N18	1.413865382	-1.774994562	-1.307581381
N19	2.769646111	-1.762402659	-1.4065342
C20	1.023769738	-3.019781074	-1.612691527

C21	2.128789368	-3.828084745	-1.908546158
C22	3.219831315	-2.984759695	-1.761127111
N23	1.998685971	-0.159634992	1.035053959
N24	3.269636712	-0.369081464	0.588465972
C25	2.066243189	-0.160322855	2.374009664
C26	3.377546182	-0.392536148	2.807704711
C27	4.108947078	-0.513396085	1.638004567
N28	1.879588166	1.173549118	-1.826698103
N29	3.16545037	0.729221348	-1.709776493
C30	1.931346456	2.33196885	-2.503808417
C31	3.249298997	2.647009196	-2.840088767
C32	3.996505963	1.602854527	-2.310237145
B33	3.574097811	-0.545693065	-0.912930033
Se34	-0.076390525	2.561333217	1.235658547
C35	1.390090826	2.956648889	2.466820087
C36	2.677900248	3.31906636	2.04853063
C37	3.668931712	3.629222745	2.983276409
C38	3.394309357	3.590906885	4.352130195
C39	2.110271832	3.243415991	4.77698831
C40	1.119907167	2.930487707	3.845242779
H41	0.41685112	-2.17787541	2.179214766
H42	-1.536552456	-3.955220552	2.933301208
H43	-3.569512322	-3.455362547	1.142858607

H44	0.052819827	-0.664871515	-4.058537315
H45	-1.871069634	-2.228251289	-5.255061822
H46	-3.667773214	-2.68292687	-3.215701135
H47	-2.238959401	3.113179142	-0.230308188
H48	-4.957027041	2.888160974	0.025033641
H49	-5.397089851	0.177181399	-0.22401939
H50	-4.112327157	-1.952736291	-0.804505243
H51	-0.025866864	-3.274918574	-1.606442845
H52	2.133162126	-4.871350724	-2.185367498
H53	4.278462142	-3.167127932	-1.874719835
H54	1.181727132	0.044160026	2.959016524
H55	3.740660528	-0.430906702	3.823188192
H56	5.162995491	-0.686292803	1.47657613
H57	1.024086432	2.887543236	-2.700532815
H58	3.608786982	3.509462889	-3.379317027
H59	5.061364922	1.423285781	-2.315375443
H60	4.748931314	-0.733844886	-1.069553481
H61	2.903556125	3.357660159	0.987133094
H62	4.663134071	3.90393644	2.638051699
H63	4.166951176	3.832968913	5.077190083
H64	1.875881787	3.214106495	5.839133824
H65	0.121438478	2.667350904	4.18348419

$Tp_2LuTePh$

atom	x	y	z
Lu1	0.34504121	0.442405883	-0.751196551
N2	2.107617969	-0.9561983	-1.730382742
N3	3.401022511	-0.524709162	-1.768123907
C4	2.121956636	-2.236057973	-2.126991766
C5	3.423915924	-2.644636197	-2.44070905
C6	4.202455755	-1.523319672	-2.196949133
N7	1.649833775	1.805584336	-2.551750839
N8	3.01548408	1.818954287	-2.510751587
C9	1.31498611	2.605733064	-3.577627975
C10	2.450308939	3.148710535	-4.1924758
C11	3.511111169	2.618860033	-3.479250058
N12	2.210248201	1.451789596	0.427703851
N13	3.478038824	1.407603419	-0.07328936
C14	2.302419975	1.987874174	1.653655035
C15	3.630567085	2.308927681	1.954889417
C16	4.341120384	1.92295512	0.827982048
B17	3.798234811	0.954167696	-1.520599336
N18	0.944900217	-1.264114062	0.978447896
N19	-0.000190014	-1.96924342	1.651033319
C20	2.13126301	-1.72281446	1.396349267

C21	1.962117191	-2.734746875	2.350283754
C22	0.586559254	-2.858058396	2.481021641
N23	-1.22462107	-1.326834716	-1.086862298
N24	-1.867034146	-1.916910548	-0.039867234
C25	-1.780391024	-1.812786836	-2.208003239
C26	-2.784389996	-2.734113095	-1.897789079
C27	-2.804426241	-2.764554654	-0.509279131
N28	-1.053701157	0.852308133	1.174346649
N29	-1.71026501	-0.157048393	1.813713262
C30	-1.397253098	1.989146039	1.799225599
C31	-2.266685934	1.724401198	2.861743736
C32	-2.442881655	0.349512163	2.827867559
B33	-1.491025826	-1.643589031	1.446953861
Te34	-1.635001083	2.530147836	-1.982916305
C35	-3.464003604	2.543687853	-0.875198872
C36	-3.932505181	3.772971725	-0.384869904
C37	-5.143851913	3.856712985	0.302249004
C38	-5.908677128	2.710201442	0.520705383
C39	-5.452147981	1.482939312	0.037096028
C40	-4.244100476	1.399362341	-0.659279461
H41	1.200640792	-2.800612059	-2.15675596
H42	3.752324371	-3.610304524	-2.793100004
H43	5.264852971	-1.360251312	-2.306151796

H44	0.278623016	2.765837365	-3.837081052
H45	2.488243891	3.828223478	-5.0304826
H46	4.578241926	2.748496272	-3.588870074
H47	1.414231892	2.108896218	2.257354738
H48	4.017715103	2.758194313	2.856567448
H49	5.395183677	1.986366513	0.600013404
H50	4.979134701	1.07403748	-1.701867369
H51	3.044816605	-1.307618647	0.995433967
H52	2.727399286	-3.29186866	2.868948414
H53	-0.012470641	-3.506105696	3.103784005
H54	-1.449948565	-1.457447519	-3.175082672
H55	-3.410195088	-3.287658918	-2.580458745
H56	-3.420287234	-3.328658214	0.175259188
H57	-1.034247495	2.937723575	1.428253777
H58	-2.72347254	2.4332005	3.534818252
H59	-3.040115522	-0.301912476	3.448645671
H60	-2.171621615	-2.335957535	2.151182601
H61	-3.34374165	4.672314593	-0.545523791
H62	-5.487462396	4.8214851	0.668993196
H63	-6.852079949	2.774509207	1.056952889
H64	-6.042037721	0.583178608	0.196516586
H65	-3.908907848	0.439852537	-1.040386257

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