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SUPPORTING INFORMATION

The Synthesis and Structures of *Tris*(2-pyridylseleno)methyl Zinc Compounds with κ^2-, κ^3- and κ^4-Coordination Modes

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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.[1] Solvents were purified and degassed by standard procedures. NMR spectra were measured on Bruker 300 DRX, Bruker Avance III 400, Bruker Avance III 400SL and Bruker Avance III 500 DMX spectrometers. ^{1}H NMR spectra 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, δ 5.32 for $CDHCl_2$ and δ 1.72 for THF-d_8).[2] ^{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_6, δ 53.84 for CD_2Cl_2 and δ 25.31 for THF-d_8).[2] Coupling constants are given in hertz. Pyridine-2(1*H*)-selone[3] and $Zn[N(SiMe_3)_2]_2$[4] were prepared by the literature methods. Mass spectra were obtained on a JEOL JMS-HX110HF tandem mass spectrometer using fast atom bombardment (FAB). Infrared spectra were recorded on PerkinElmer Spectrum Two spectrometer and are reported in cm^{-1}.

X-ray structure determinations

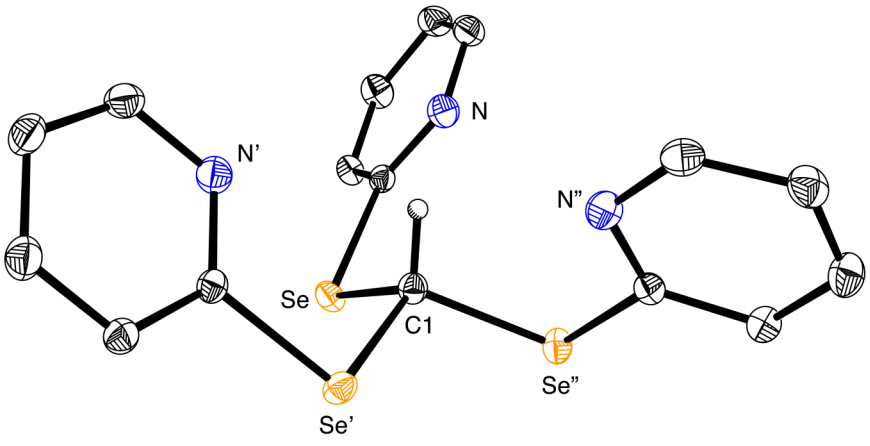
Single crystal X-ray diffraction data were collected on a Bruker Apex II diffractometer and crystal data, data collection and refinement parameters are summarized in Table 1. The structures were solved using direct methods and standard difference map techniques, and were refined by full-matrix least-squares procedures on F^2 with SHELXTL (Version 2008/4).[5]

Computational Details

Calculations were carried out using DFT as implemented in the Jaguar 7.6 (release 110) suite of *ab initio* quantum chemistry programs.[6] Geometry optimizations were performed with the B3LYP density functional[7] using the 6-31G** (H, C, N, S) and LAV3P (Se, Zn) basis sets,[8] and atomic coordinates are listed in Table 2.

Synthesis of [Tpsem]H

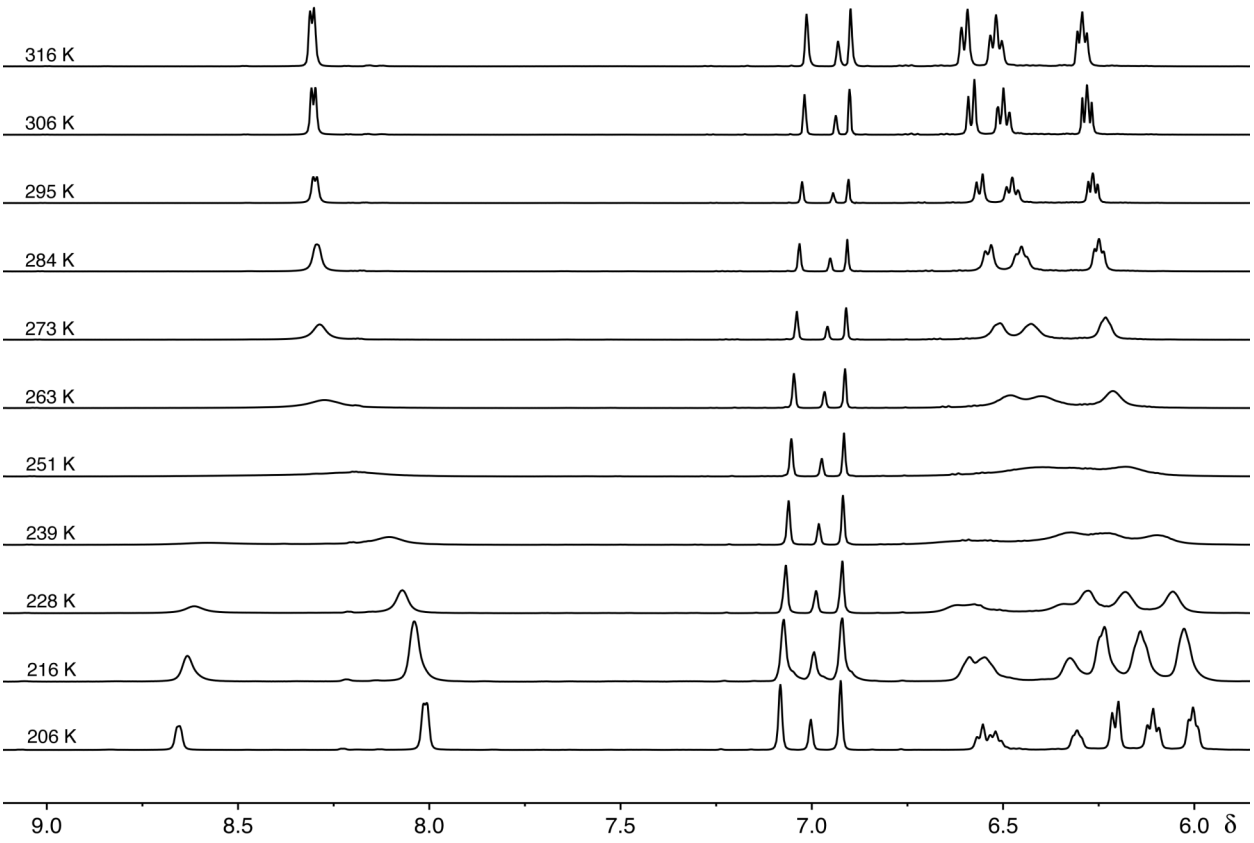
Tris(2-pyridylseleno)methane has been previously reported[9] but was synthesized by an alternative method based on that for *tris*(2-pyridylthio)methane.[10] A mixture of $CHBr_3$ (184 μL, 2.1 mmol), KOH (529 mg, 9.5 mmol) and pyridine-2(1*H*)-selone (1.0 g, 6.3 mmol) was treated with benzene (6 mL) and heated at 60 ˚C for 3 hours, resulting in the formation of a red-brown solution with an oily layer that contained a brown solid, both of which were removed by filtration. The volatile components were removed from the filtrate by lyophilization to give a brown solid that was washed with benzene and dried *in vacuo* to give [Tpsem]H as a brown solid (642 mg, 63%) that is pure according to ^{1}H NMR spectroscopy. The compound may be obtained as pale yellow crystals from toluene and has been authenticated by X-ray diffraction.[9a] ^{1}H NMR ($CDCl_3$): 7.06 [m, 3H, $HC(SeC_5\underline{H}_4N)_3$], 7.37 [d, $^3J_{H-H}$ = 4 Hz, 3H, $HC(SeC_5\underline{H}_4N)_3$], 7.39 [s, 1H, $\underline{H}C(SeC_5H_4N)_3$], 7.49 [dt, $^4J_{H-H}$ = 2 Hz, $^3J_{H-H}$ = 8 Hz, 3H, $HC(SeC_5\underline{H}_4N)_3$], 8.53 [d, $^3J_{H-H}$ = 4 Hz, 3H, $HC(SeC_5\underline{H}_4N)_3$]. ^{1}H NMR ($C_6D_6$): 6.36 [m, 3H, $HC(SeC_5\underline{H}_4N)_3$], 6.69 [dt, $^4J_{H-H}$ = 2 Hz, $^3J_{H-H}$ = 8 Hz, 3H, $HC(SeC_5\underline{H}_4N)_3$], 6.98 [d, $^3J_{H-H}$ = 8 Hz, 3H, $HC(SeC_5\underline{H}_4N)_3$], 7.99 [s, 1H, $\underline{H}C(SeC_5H_4N)_3$], 8.36 [d, $^3J_{H-H}$ = 4 Hz, 3H, $HC(SeC_5\underline{H}_4N)_3$]. $^{13}C\{^1H\}$ NMR (C_6D_6): 22.5 [s, 1C, $H\underline{C}(SeC_5H_4N)_3$], 120.6 [s, 3C, $HC(Se\underline{C}_5H_4N)_3$], 125.2 [s, 3C, $HC(Se\underline{C}_5H_4N)_3$], 136.3 [s, 3C, $HC(Se\underline{C}_5H_4N)_3$], 150.3 [s, 3C, $HC(Se\underline{C}_5H_4N)_3$], 158.1 [s, 3C, $HC(Se\underline{C}_5H_4N)_3$]. MS: m/z = 486.0 $[M]^+$, M = [Tpsem]H.



Molecular structure of [Tpsem]H

Synthesis of [κ^3-Tpsem]ZnN(SiMe$_3$)$_2$

A mixture of [Tpsem]H (10 mg, 0.02 mmol) and Zn[N(SiMe$_3$)$_2$]$_2$ (8 mg, 0.02 mmol) in an NMR tube equipped with a J. Young valve was dissolved in benzene-d_6 (1 mL) and heated at 60 ˚C. The reaction was monitored by ^{1}H NMR spectroscopy, thereby demonstrating the formation of [κ^3-Tpsem]ZnN(SiMe$_3$)$_2$ over a period of 6 hours. ^{1}H NMR (C_6D_6): 0.47 [s, 18H, [(C$\underline{H}_3$)$_3$Si]$_2$NZnC(SeC$_5$H$_4$N)$_3$], 6.28 [t, $^3J_{H–H}$ = 6 Hz, 3H, (Me$_3$Si)$_2$NZnC(SeC$_5\underline{H}_4$N)$_3$], 6.48 [t, $^3J_{H–H}$ = 7 Hz, 3H, (Me$_3$Si)$_2$NZnC(SeC$_5\underline{H}_4$N)$_3$], 6.66 [d, $^3J_{H–H}$ = 8 Hz, 3H, (Me$_3$Si)$_2$NZnC(SeC$_5\underline{H}_4$N)$_3$], 8.39 [d, $^3J_{H–H}$ = 4 Hz, 3H, (Me$_3$Si)$_2$NZnC(SeC$_5\underline{H}_4$N)$_3$]. ^{1}H NMR (THF-d_8): -0.04 [s, 18H, [(C$\underline{H}_3$)$_3$Si]$_2$NZnC(SeC$_5$H$_4$N)$_3$], 7.11 [m, 3H, (Me$_3$Si)$_2$NZnC(SeC$_5\underline{H}_4$N)$_3$], 7.34 [d, $^3J_{H–H}$ = 8 Hz, 3H, (Me$_3$Si)$_2$NZnC(SeC$_5\underline{H}_4$N)$_3$], 7.54 [m, 3H, (Me$_3$Si)$_2$NZnC(SeC$_5\underline{H}_4$N)$_3$], 8.62 [dt, $^3J_{H–H}$ = 5 Hz, $^4J_{H–H}$ = 1 Hz, 3H, (Me$_3$Si)$_2$NZnC(SeC$_5\underline{H}_4$N)$_3$]. ^{13}C{^{1}H} NMR (C_6D_6): 6.7 [s, 6C, [(C$\underline{H}_3$)$_3$Si]$_2$NZnC(SeC$_5$H$_4$N)$_3$], not observed [1C, (Me$_3$Si)$_2$NZn$\underline{C}$(SeC$_5$H$_4$N)$_3$], 119.7 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$], 124.5 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$], 136.6 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$], 148.3 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$], 163.4 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$]. ^{13}C{^{1}H} NMR (THF- d_8): 6.4 [s, 6C, [(C$\underline{H}_3$)$_3$Si]$_2$NZnC(SeC$_5$H$_4$N)$_3$], not observed [1C, (Me$_3$Si)$_2$NZn$\underline{C}$(SeC$_5$H$_4$N)$_3$], 120.8 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$], 124.7 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$], 137.9 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$], 149.3 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$], 163.9 [s, 3C, (Me$_3$Si)$_2$NZnC(Se$\underline{C}_5$H$_4$N)$_3$].

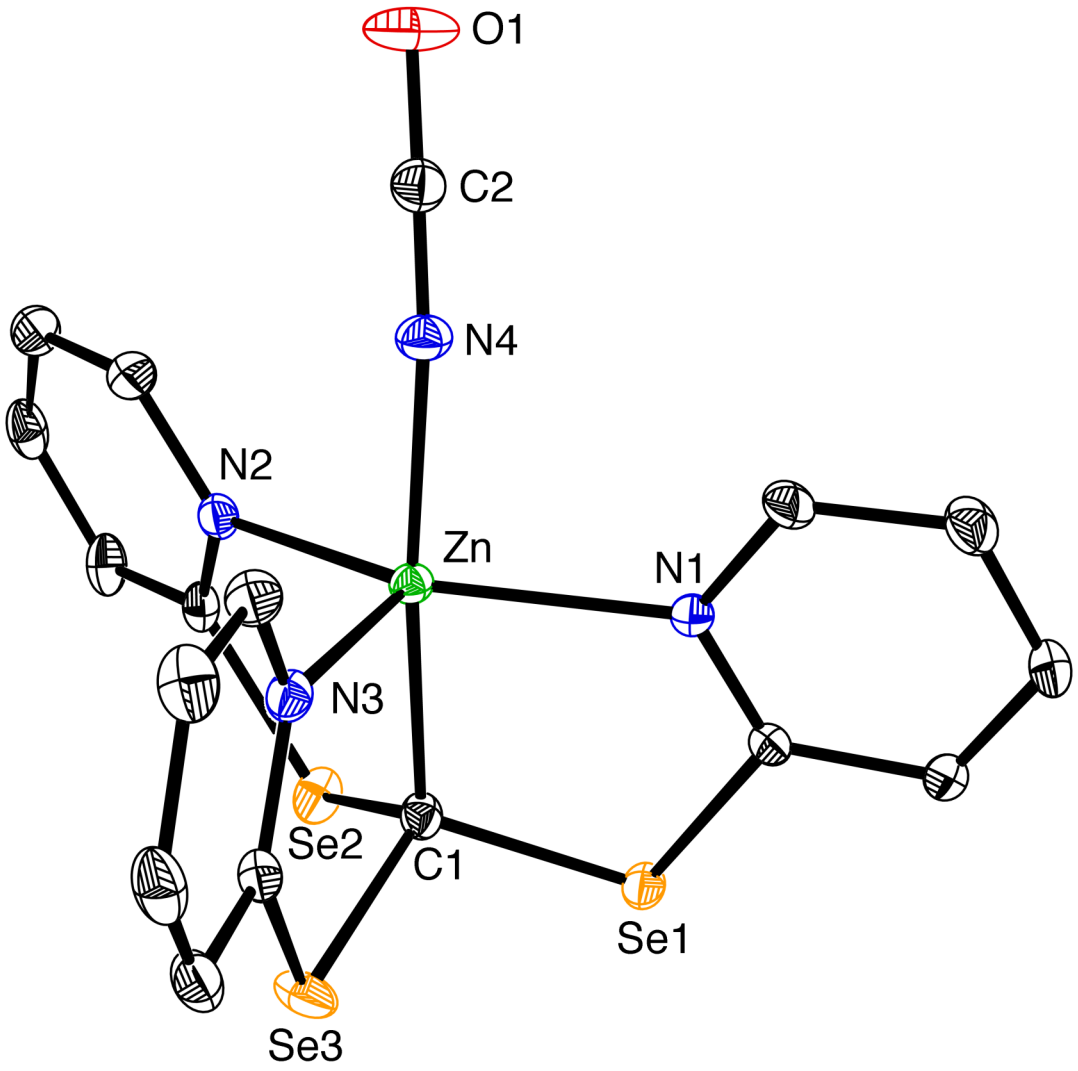


Variable temperature ^{1}H NMR spectra of [κ^3-Tpsem]ZnN(SiMe$_3$)$_2$ in d_8-toluene.

Synthesis of [κ^4-Tpsem]ZnNCO

A mixture of [Tpsem]H (10 mg, 0.02 mmol) and Zn[N(SiMe$_3$)$_2$]$_2$ (8 mg, 0.02 mmol) in an NMR tube equipped with a J. Young valve was dissolved in benzene-d_6 (1 mL) and heated at 60 ˚C for 2 hours to generate [κ^3-Tpsem]ZnN(SiMe$_3$)$_2$. The solution was frozen and the atmosphere removed *in vacuo*. The sample was treated with CO_2 (1 atm) and allowed to stand at room temperature for 2 days. The reaction was monitored by ^{1}H NMR spectroscopy, thereby demonstrating the quantitative conversion to [κ^4-Tpsem]ZnNCO, together with the formation of (Me$_3$SiO)$_2$CO (δ 0.21).[11] The sample was lyophilized and the solid obtained was dissolved in benzene (*ca.* 1 mL) and allowed to evaporate, thereby depositing colorless crystals of [κ^4-Tpsem]ZnNCO suitable for X-ray diffraction (5 mg, 40%). ^{1}H NMR (C_6D_6): 6.24 [m, 3H, OCNZnC(SeC$_5$H$_4$N)$_3$], 6.42 [dt, $^3J_{H–H}$ = 7 Hz, $^4J_{H–H}$ = 2 Hz, 3H, OCNZnC(SeC$_5$H$_4$N)$_3$], 6.47 [d, $^3J_{H–H}$ = 8 Hz, 3H,

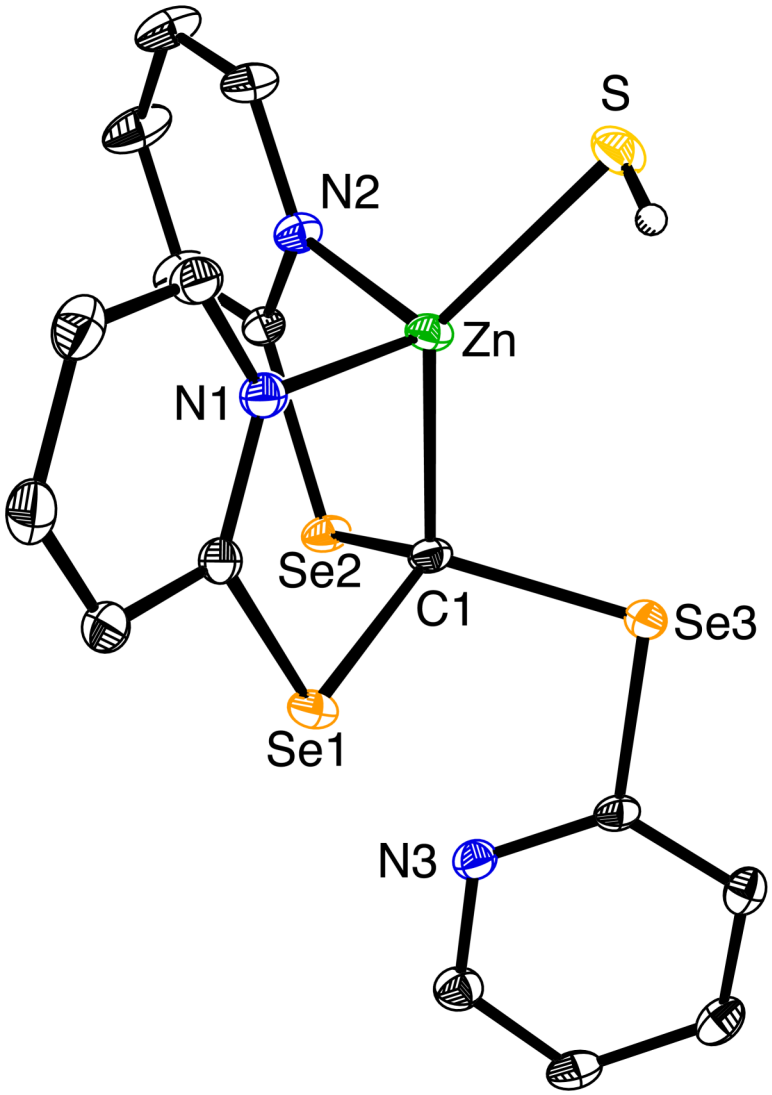
OCNZnC(SeC$_5$H$_4$N)$_3$], 9.13 [d, $^3J_{H-H}$ = 6 Hz, 3H, OCNZnC(SeC$_5$H$_4$N)$_3$]. ^{13}C{^{1}H} NMR (C_6D_6): not observed [1C, OCNZnC(SeC$_5$H$_4$N)$_3$], 120.5 [s, 3C, OCNZnC(SeC$_5$H$_4$N)$_3$], 124.0 [s, 3C, OCNZnC(SeC$_5$H$_4$N)$_3$], not observed [1C, OCNZnC(SeC$_5$H$_4$N)$_3$], 137.7 [s, 3C, OCNZnC(SeC$_5$H$_4$N)$_3$], 149.6 [s, 3C, OCNZnC(SeC$_5$H$_4$N)$_3$], 158.6 [s, 3C, OCNZnC(SeC$_5$H$_4$N)$_3$]. MS: *m*/*z* = 591.9 [M]$^+$. IR Data (cm^{-1}): 3056 (w), 2951 (w), 2205 (s), 1655 (w), 1584 (s), 1553 (s), 1452 (s), 1413 (s), 1340 (m), 1277 (m), 1244 (w), 1152 (m), 1116 (s), 1085 (m), 1044 (m), 1002 (m), 891 (m), 836 (m), 752 (s), 729 (m), 700 (m), 679 (m), 651 (w), 620 (m), 569 (m), 469 (s), 406 (s).



Molecular structure of [κ^4-Tpsem]ZnNCO

Synthesis of [κ^3-Tpsem]ZnSH

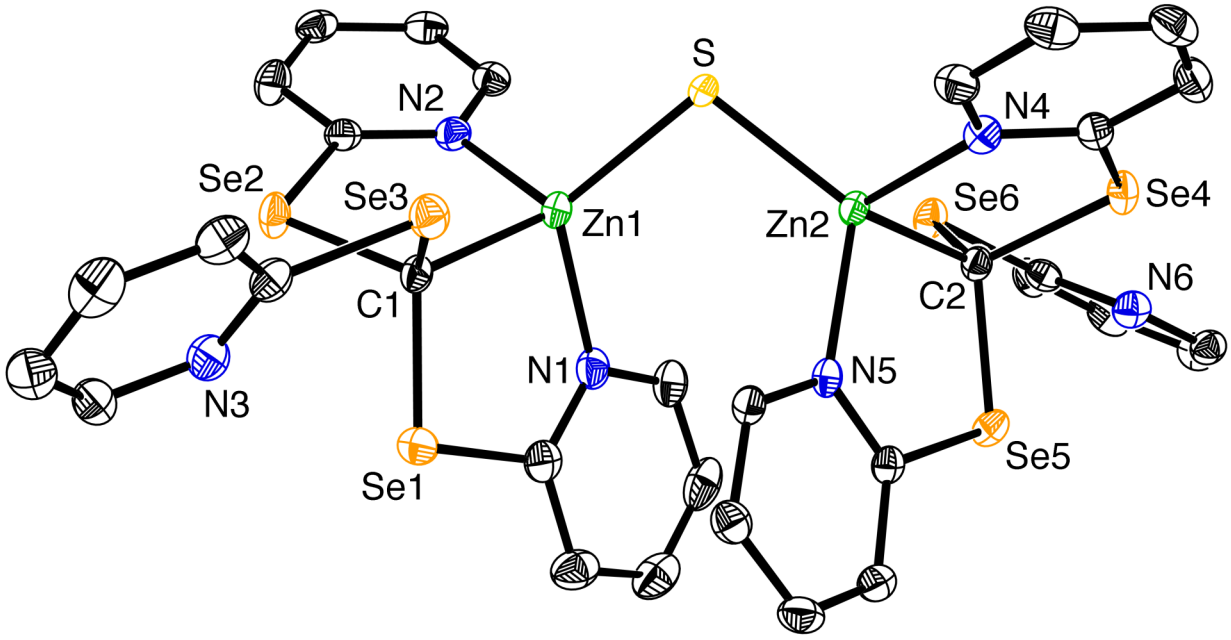
A mixture of [Tpsem]H (25 mg, 0.05 mmol) and Zn[N(SiMe$_3$)$_2$]$_2$ (20 mg, 0.05 mmol) in an NMR tube equipped with a J. Young valve was dissolved in benzene-d_6 (3 mL) and heated at 60 ˚C for 5 hours to generate [κ^3-Tpsem]ZnN(SiMe$_3$)$_2$. The solution was transferred to a small Schlenk tube and treated with H_2S, slowly allowing the pressure to reach 1 atm, thereby depositing [κ^3-Tpsem]ZnSH as a microcrystalline solid. The H_2S was removed *in vacuo* and the mixture was filtered to give [κ^3-Tpsem]ZnSH as a light yellow solid that was washed with hexane (2 × 3 mL) and dried *in vacuo* (16 mg, 53%). Crystals suitable for X-ray diffraction were obtained by treating a frozen solution of [κ^3-Tpsem]ZnN(SiMe$_3$)$_2$ in benzene with H_2S (*ca*. 24cm Hg) H_2S for 15 minutes, during which period the solution was allowed to warm to room temperature slowly. Anal. calcd. for [κ^3-Tpsem]ZnSH: C, 33.0%; H, 2.3%; N, 7.2%. Found: C, 33.1%; H, 1.9%; N, 6.8%. ^{1}H NMR (CD_2Cl_2): -1.65 [s, 1H, HSZnC(SeC$_5$H$_4$N)$_3$], 7.15 [t, $^3J_{H–H}$ = 6 Hz, 3H, HSZnC(SeC$_5$H$_4$N)$_3$], 7.32 [d, $^3J_{H–H}$ = 8 Hz, 3H, HSZnC(SeC$_5$H$_4$N)$_3$], 7.55 [t, $^3J_{H–H}$ = 7 Hz, 3H, HSZnC(SeC$_5$H$_4$N)$_3$], 8.66 [d, $^3J_{H–H}$ = 5 Hz, 3H, HSZnC(SeC$_5$H$_4$N)$_3$]. ^{13}C{^{1}H} NMR (CD_2Cl_2): not observed [1C, HSZnC(SeC$_5$H$_4$N)$_3$], 120.9 [s, 3C, HSZnC(SeC$_5$H$_4$N)$_3$], 124.5 [s, 3C, HSZnC(SeC$_5$H$_4$N)$_3$], 137.9 [s, 3C, HSZnC(SeC$_5$H$_4$N)$_3$], 149.0 [s, 3C, HSZnC(SeC$_5$H$_4$N)$_3$], 161.5 [s, 3C, HSZnC(SeC$_5$H$_4$N)$_3$]. MS: m/z = 549.9 [M – SH]$^+$.



Molecular structure of [κ³-Tpsem]ZnSH

Synthesis of {[κ³-Tpsem]Zn}$_2$(μ–S)

A solution of [κ³-Tpsem]ZnSH (6 mg, 0.01 mmol) in CH_2Cl_2 (*ca.* 0.5 mL) was allowed to evaporate slowly at room temperature, thereby depositing orange crystals of {[κ³-Tpsem]Zn}$_2$(μ–S) suitable for X-ray diffraction (2 mg, 31%). ^{1}H NMR (CD_2Cl_2): 7.05 [t, $^3J_{H–H}$ = 6 Hz, 6H, [ZnC(SeC$_5$H$_4$N)$_3$]$_2$(μ-S)], 7.18 [d, $^3J_{H–H}$ = 8 Hz, 6H, [ZnC(SeC$_5$H$_4$N)$_3$]$_2$(μ-S)], 7.43 [t, $^3J_{H–H}$ = 7 Hz, 6H, [ZnC(SeC$_5$H$_4$N)$_3$]$_2$(μ-S)], 8.78 [d, $^3J_{H–H}$ = 5 Hz, 6H, [ZnC(SeC$_5$H$_4$N)$_3$]$_2$(μ-S)].



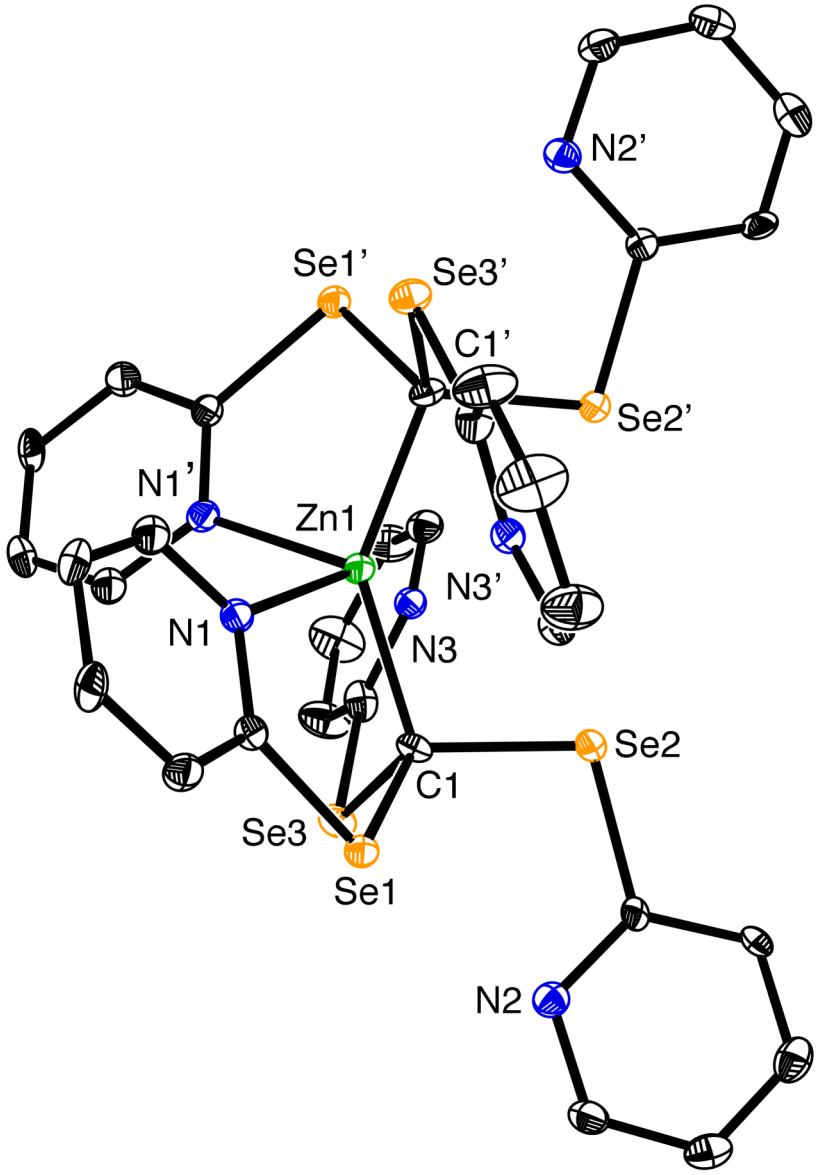
Molecular structure of {[κ³-Tpsem]Zn}₂S.

Interconversion of [κ³-Tpsem]ZnSH and {[κ³-Tpsem]Zn}₂(μ–S)

A mixture composed of {[κ³-Tpsem]Zn}₂(μ–S) and [κ³-Tpsem]ZnSH (2.5:1, *ca.* 5 mg) was dissolved in CD_2Cl_2 in an NMR tube equipped with J. Young valve and treated with H_2S (*ca.* 20 cm Hg) at room temperature. The reaction was monitored by ^1H NMR spectroscopy, thereby demonstrating the complete conversion of {[κ³-Tpsem]Zn}₂(μ–S) into [κ³-Tpsem]ZnSH within a period of 5 minutes. The volatile components were removed *in vacuo* and the resulting yellow solid was redissolved in CD_2Cl_2 and analyzed by ^1H NMR spectroscopy, thereby demonstrating that the formation of a mixture of {[κ³-Tpsem]Zn}₂(μ–S) and [κ³-Tpsem]ZnSH (0.4:1).

Synthesis of [κ^2-Tpsem]$_2$Zn

A solution of [κ^3-Tpsem]ZnN(SiMe$_3$)$_2$ (*ca.* 10 mg, 0.02 mmol) in benzene (*ca.* 1 mL) was allowed to evaporate slowly, thereby depositing colorless crystals of [κ^2-Tpsem]$_2$Zn suitable for X-ray diffraction.

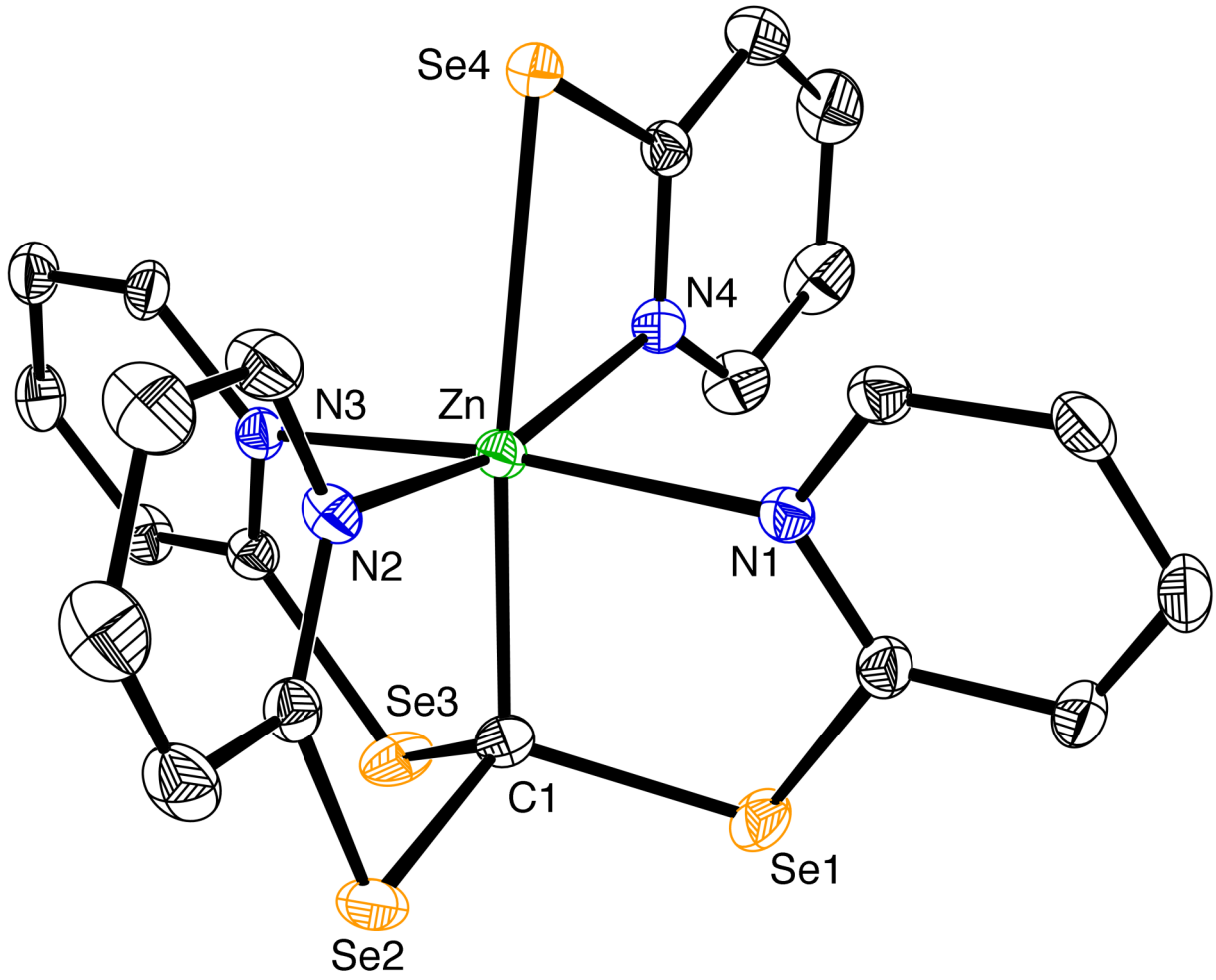


Molecular structure of [κ^2-Tpsem]$_2$Zn

Synthesis of [κ^4-Tpsem]Zn(κ^2–SeC$_6$H$_4$N)

A mixture of [Tpsem]H (10 mg, 0.02 mmol) and Zn[N(SiMe$_3$)$_2$]$_2$ (8 mg, 0.02 mmol) in an NMR tube equipped with a J. Young valve was dissolved in benzene-d_6 (1 mL) and heated at 60 ˚C for a period of 6 hours. The solvent was allowed to evaporate slowly at

room temperature, thereby depositing pale yellow crystals of [κ^4-Tpsem]Zn(κ^2–SeC_6H_4N) suitable for X-ray diffraction.



Molecular structure of [κ^4-Tpsem]Zn(κ^2–SeC_6H_4N)

Table 1. Crystal, intensity collection and refinement data.

	[κ⁴-Tpsem]ZnNCO•0.5C₆H₆	**[κ³-Tpsem]ZnSH**
lattice	Monoclinic	Orthorhombic
formula	$C_{20}H_{15}N_4OSe_3Zn$	$C_{16}H_{13}N_3SSe_3Zn$
formula weight	629.61	581.60
space group	*C2/c*	*Pbca*
a / Å	33.545(5)	8.4549(7)
b / Å	9.1886(14)	17.4460(15)
c / Å	14.125(2)	25.563(2)
α / °	90	90
β / °	102.036(2)	90
γ / °	90	90
V / Å³	4258.1(11)	3770.6(5)
Z	8	8
temperature (K)	150(2)	130(2)
radiation (λ, Å)	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.964	2.049
μ (Mo Kα), mm^{-1}	6.301	7.208
θ max, deg.	32.77	30.65
no. of data collected	36250	57778
no. of data used	7522	5819
no. of parameters	271	221
R_1 [$I > 2\sigma(I)$]	0.0430	0.0374
wR_2 [$I > 2\sigma(I)$]	0.0891	0.0772
R_1 [all data]	0.0889	0.0671
wR_2 [all data]	0.1042	0.0878
GOF	1.011	1.029
R_{int}	0.0708	0.0859

Table 1 (cont). Crystal, intensity collection and refinement data.

	{[κ³-Tpsem]Zn}₂(μ–S)•THF	**[κ²-Tpsem]₂Zn•2C₆H₆**
lattice	Monoclinic	Monoclinic
formula	$C_{36}H_{32}N_6OSSe_6Zn_2$	$C_{44}H_{36}N_6Se_6Zn$
formula weight	1201.24	1187.92
space group	*Cc*	*P*2/*c*
a / Å	22.1822(19)	20.788(8)
b / Å	16.4386(14)	8.263(3)
c / Å	13.2756(12)	25.940(10)
α / °	90	90
β / °	122.6530(10)	101.114(6)
γ / °	90	90
V / Å³	4075.8(6)	4372(3)
Z	4	4
temperature (K)	130(2)	149(2)
radiation (λ, Å)	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.958	1.805
μ (Mo Kα), mm^{-1}	6.624	5.596
θ max, deg.	30.75	29.57
no. of data collected	32923	63502
no. of data used	12653	12248
no. of parameters	424	515
R_1 [$I > 2\sigma(I)$]	0.0430	0.0579
wR_2 [$I > 2\sigma(I)$]	0.0803	0.0655
R_1 [all data]	0.0621	0.1860
wR_2 [all data]	0.0847	0.0857
GOF	1.000	1.000
R_{int}	0.0437	0.2340

Table 1 (cont). Crystal, intensity collection and refinement data.

	[κ⁴-Tpsem]Zn(κ²–SeC₆H₄N)•0.5C₆H₆	**[Tpsem]H**
lattice	Monoclinic	Rhombohedral (hexagonal setting)
formula	$C_{24}H_{19}N_4Se_4Zn$	$C_{16}H_{13}N_3Se_3$
formula weight	744.64	484.17
space group	*C2/c*	*R-3c*
a / Å	32.015(9)	12.0529(17)
b / Å	9.029(3)	12.0529(17)
c / Å	17.758(5)	39.847(6)
α / °	90	90
β / °	95.383(4)	90
γ / °	90	120
V / Å^3	5110(3)	5013.2(12)
Z	8	12
temperature (K)	150(2)	150(2)
radiation (λ, Å)	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.936	1.924
μ (Mo Kα), mm^{-1}	6.679	6.602
θ max, deg.	31.52	32.64
no. of data collected	42494	26789
no. of data used	8503	2007
no. of parameters	299	67
R_1 [$I > 2\sigma(I)$]	0.0392	0.0266
wR_2 [$I > 2\sigma(I)$]	0.0780	0.0594
R_1 [all data]	0.0769	0.0467
wR_2 [all data]	0.0891	0.0677
GOF	1.013	1.063
R_{int}	0.0598	0.0535

Table 2. **Cartesian coordinates for geometry optimized structures.**

[κ^4-Tpsem]ZnNCO

-1042.58578004512 Hartrees

atom	x	y	z
Zn	9.659852419	9.65856473	13.15607933
Se	6.588905011	8.126380906	13.42232943
Se	6.663877534	11.32707099	12.86530211
Se	7.497339313	9.248860575	10.51378871
N	8.98937985	8.4693997	14.93973043
N	9.451662891	11.88772038	13.18066101
N	10.16752713	8.559788849	11.2689682
C	7.56321371	9.589716214	12.47892957
C	7.783790737	7.893850209	14.94953031
C	7.345930371	7.099123328	16.01823332
H	6.355963931	6.655206668	15.99465319
C	8.197610347	6.906136021	17.09673707
H	7.882140365	6.295229814	17.93791751
C	9.458809473	7.511883429	17.08976942
H	10.15205341	7.389047685	17.91436517
C	9.812443318	8.28236411	15.99182515
H	10.77831755	8.769499675	15.90853144
C	8.244568752	12.45203632	13.08726701
C	8.06322985	13.83999863	13.1642448
H	7.067774696	14.26295444	13.07586592
C	9.176922271	14.64774031	13.34545956
H	9.063441019	15.72636097	13.40805738
C	10.4423503	14.0580553	13.43929695

H	11.33768811	14.65379186	13.57746082
C	10.53207488	12.67674582	13.35338899
H	11.47601893	12.14768809	13.43238918
C	9.26837719	8.456647658	10.28629609
C	9.558502937	7.812292618	9.075914015
H	8.798969044	7.738623743	8.304396892
C	10.82277048	7.267697715	8.898308797
H	11.07241731	6.761111565	7.970199724
C	11.76376179	7.371402145	9.928415799
H	12.76041299	6.955555149	9.830926
C	11.39369877	8.026281104	11.09396648
H	12.0730547	8.159824399	11.92942125
N	11.59935422	9.712159349	13.77814823
O	13.86596181	9.819045784	14.55694226
C	12.73370222	9.766595657	14.16819493

[κ^4-Tptm]ZnNCO

-2209.50406484924 Hartrees

atom	x	y	z
Zn	4.058521167	4.961734928	0.733194009
S	6.307492586	3.979253671	3.033510559
S	7.199175375	3.868043952	0.201787851
S	6.940966996	6.485249041	1.57934715
N	2.120758455	5.099707965	0.122708217
N	3.626091202	3.877948249	2.576983242
N	4.751176786	3.795984673	-0.986754995
N	4.431767658	7.124310843	0.736981722
O	-0.122506728	5.352991562	-0.68859579

C	0.998021656	5.228182133	-0.28432173
C	6.251305096	4.815958895	1.425275495
C	4.62618862	3.540350626	3.399785558
C	4.392048532	2.827213002	4.589682109
H	5.225525561	2.565941392	5.233652664
C	3.092341069	2.471036949	4.908993317
H	2.889662889	1.918821533	5.822419315
C	2.047322799	2.826396691	4.045511233
H	1.017712773	2.564292478	4.261130158
C	2.36114963	3.527770718	2.893492684
H	1.610911071	3.8397045	2.173747362
C	6.03461852	3.423411645	-1.062037687
C	6.520385233	2.66527056	-2.143238832
H	7.566699672	2.378872844	-2.172664208
C	5.642552359	2.300676875	-3.150261513
H	5.997025403	1.71514807	-3.994011735
C	4.299436134	2.69242782	-3.069397804
H	3.58250126	2.426220871	-3.837819729
C	3.900470267	3.436725644	-1.971725069
H	2.878768331	3.776751777	-1.835935604
C	5.636269221	7.586870267	1.092610784
C	5.925897895	8.963569127	1.098661293
H	6.913869088	9.304060081	1.39146227
C	4.93469191	9.855967011	0.725709266
H	5.138763271	10.92308556	0.722628838
C	3.673775393	9.370336451	0.353237655
H	2.872854557	10.03681791	0.054409217
C	3.469906473	8.000169234	0.374334277

H	2.523054242	7.54669839	0.100013724

$\{[\kappa^3\text{-Tpsem}]Zn\}_2(\mu\text{–S})$

-2147.16211527580 Hartrees

atom	x	y	z
Zn	-3.310487369	11.2401442	17.13192359
Zn	-6.145254621	13.63452561	17.84881329
Se	-3.652639096	9.2866434	14.37612345
Se	-0.787076442	9.302087223	15.92533222
Se	-1.752397915	11.96223944	14.25368384
Se	-9.010691198	15.26677604	18.69054511
Se	-9.175906384	12.81362309	16.55671653
Se	-8.516506684	12.18451466	19.71241473
N	-4.966803052	9.826870033	16.87482872
N	-1.776759649	10.3376468	18.41146882
N	-0.989465571	9.729989028	12.67546194
N	-6.201220382	15.76068764	18.38552113
N	-6.490661839	13.38314626	15.70092106
N	-11.1839683	12.83344668	19.00606113
S	-3.986659294	13.04911881	18.37816323
C	-2.342999576	10.43769675	15.36023253
C	-8.275708168	13.45821	18.22369205
C	-5.047403722	9.12945582	15.73670158
C	-6.12641653	8.268783447	15.48013188
H	-6.163744834	7.709930924	14.55028924
C	-7.130865934	8.151433819	16.42961595
H	-7.977664229	7.494990809	16.24848937
C	-7.044642289	8.886936941	17.61785908

H	-7.815682908	8.840264574	18.37791587
C	-5.945464564	9.71125831	17.79533759
H	-5.826239927	10.32522549	18.68382542
C	-0.818973943	9.588754914	17.85706096
C	0.189020088	8.995123233	18.63341753
H	0.957102817	8.392994764	18.1584973
C	0.183625844	9.20191275	20.00515668
H	0.954037362	8.752087628	20.62573333
C	-0.812961619	10.00125449	20.5786351
H	-0.841544969	10.19541507	21.64520235
C	-1.771188564	10.55320642	19.74277455
H	-2.563035743	11.20405703	20.10627725
C	-0.918990369	11.05562705	12.7196093
C	-0.279784211	11.82390244	11.73525873
H	-0.239630779	12.90584278	11.81681398
C	0.303234424	11.15944131	10.66313992
H	0.808549365	11.72112727	9.882023816
C	0.23564908	9.762965098	10.60549594
H	0.680344236	9.207377445	9.786465897
C	-0.42026312	9.098334087	11.63658708
H	-0.499791575	8.013129418	11.64078347
C	-7.368079644	16.32253262	18.71501076
C	-7.451866796	17.67232102	19.09178175
H	-8.411654871	18.10336226	19.35839647
C	-6.289866667	18.42933334	19.12405125
H	-6.331013973	19.47606782	19.41321934
C	-5.067540223	17.83138653	18.79333676
H	-4.137430242	18.38829683	18.8204185

C	-5.069314895	16.49231148	18.43483906
H	-4.159571128	15.94892493	18.19045212
C	-7.706944058	13.01645544	15.2831068
C	-7.970030789	12.76481059	13.92719464
H	-8.967963236	12.47373674	13.61449696
C	-6.938385964	12.89374213	13.00900491
H	-7.119183132	12.69811338	11.95554938
C	-5.665349146	13.27322354	13.45191722
H	-4.826584761	13.36725323	12.77223849
C	-5.489561655	13.5064853	14.80599449
H	-4.52411016	13.7837552	15.22043095
C	-10.47403842	12.13836877	19.88765576
C	-11.05385266	11.38923111	20.92204998
H	-10.43319585	10.84210528	21.6250879
C	-12.43962593	11.37549492	21.02098102
H	-12.92605539	10.80756018	21.80954921
C	-13.19771609	12.10371369	20.09767864
H	-14.28180437	12.11973494	20.14289484
C	-12.52177761	12.81513378	19.11249386
H	-13.06474784	13.39826332	18.37147424

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