From elusive thio- and selenosilanoic acids to copper(I) complexes with unprecedented Si=E→Cu—O—Si coordination mode (E = S, Se)

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Electronic Supplementary Information

Contents:

1. Synthesis of compounds 3-5.

All experiments were carried out under dry oxygen-free nitrogen using standard Schlenk techniques. Solvents were dried by standard methods and freshly distilled and degassed prior to use. The NMR spectra were recorded on Bruker spectrometers (AV400 or AV200) referenced to residual solvent signals as internal standards (^{1}H NMR: $CDCl_3$, 7.27 ppm and $^{13}C\{H\}$ NMR: $CDCl_3$, 77.0 ppm) or with an external standard ($SiMe_4$ for ^{29}Si NMR; $SeMe_2$ for ^{77}Se NMR). Concentrated solutions of samples in $CDCl_3$ were sealed off in a Young-type NMR tube for measurements. Melting points were recorded on a "Melting point tester" device from BSGT company and are uncorrected. All the samples are sealed off in capillary under vacuum and each sample was measured in duplicate. High resolution ESI mass spectra were recorded on an Orbitrap LTQ XL of Thermo Scientific mass spectrometer and the raw data evaluated using the Xcalibur computer program. For the single crystal X-ray structure analyses the crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data of compounds **3-5** were collected on an Oxford Diffraction Xcalibur S Sapphire at 150 K (MoKa radiation, λ= 0.71073 Å). The structures were solved by direct methods and refined on F^2 with the SHELX-97[1] software package. The positions of the H atoms were calculated and considered isotropically according to a riding model.

Commercially available reagents were purchased from Aldrich (triethylhydridoborate, trimethylammonium chloride), Acros (4-dimethylaminopyridine (dmap), selenium element) and used as received. L'Si(=S)(OH)(dmap), **1** (L = CH[C(Me)NR]$_2$, R = 2,6-*i*Pr$_2$C$_6$H$_3$),[2] L'Si(=O)(dmap), **2** (L' = CH[C(Me)(C=CH$_2$)(NR)$_2$]),[2] $(MesCu)_4$ (Mes = 2,4,6-$Me_3C_6H_2$)[3] were synthesized according to published procedures.

Compound LSi(=Se)OH(dmap), 3

$Li(HBEt_3)$ (1 mL, 1 mmol, 1 M THF solution) was added dropwise to a suspension of Se (40mg, 0.5 mmol) in THF (20 mL) at –20 ^{o}C. This mixture was allowed to warm to room temperature and stirred for another 12 hours. All volatiles were removed in vacuo, then THF (30 mL) and **3** (0.285 g, 0.5 mmol) was added at –20 ^{o}C. The mixture was stirred at room temperature for 12 hours and a yellow suspension

was formed. The suspension was cooled to –78 ^{o}C and two molar equivalents of $Me_3N{\cdot}HCl$ (95.6 mg, 1 mmol) were added, affording to a clear yellow solution after warming to room temperature. After 12 hours at ambient temperature, all volatiles were removed in vacuo and toluene (20 mL) was added to the solid residue. Filtration by cannula resulted in a yellow filtrate which was concentrated to ca. 5 mL, and *n*-hexane (3 mL) was added to the clear solution. After standing at 0 ^{o}C for 24 hours, a yellow crystalline product was separated from the yellow mother liquor by filtration, and dried in vacuo for three hours. Yield: 0.25 g (75%). Mp: 192-194 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C, ppm): δ = 1.08 (d, 6 H, ^{3}J = 7.2 Hz, (CH_3)$_2$CH), 1.21 (d, 6 H, ^{3}J = 6.4 Hz, (CH_3)$_2$CH), 1.24 (d, 6 H, ^{3}J = 6.8 Hz, (CH_3)$_2$CH), 1.41 (d, 6 H, ^{3}J = 6.8 Hz, (CH_3)$_2$CH), 2.00 (s, 6 H, α-CH_3), 2.96 (s, 6 H, N(CH_3)$_2$), 3.27 (sept, 2 H, ^{3}J = 6.8 Hz, C*H*(CH$_3$)$_2$), 3.44 (sept, 2 H, ^{3}J = 6.8 Hz, C*H*(CH$_3$)$_2$), 5.73 (s, 1 H, *γ*-*H*), 6.42-6.44 (m, 3 H, Py-*H* and O*H*), 7.22-7.25 (m, 4 H, Ar-*H*), 7.32-7.36 (m, 2 H, Ar-*H*), 8.29-8.31 (m, 2 H, Py-*H*); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 25 ^{o}C, ppm): δ = 23.7, 24.0, 24.1, 24.4 (CH*Me*$_2$,), 26.2 (NC*Me*), 27.9 (*C*HMe$_2$), 29.3 (*C*HMe$_2$), 38.9 (N*Me*$_2$), 100.8 (*γ*-*C*), 106.2, 124.5, 124.6, 128.6, 137.1, 144.3, 145.4, 149.2, 154.1, 170.0; ^{29}Si{^{1}H} NMR (79 Hz, $CDCl_3$, 25 ^{o}C, ppm): δ = –25.5. ESI-MS, *m/z*: 665.3138, ([M + H]$^{+}$), calcd: 665.3154; 543.2294 ([M – dmap + H]$^{+}$), calcd: 543.2310. Elemental analysis (%): calcd for $C_{36}H_{52}N_4OSeSi$: C, 65.13; H, 7.90; N, 8.44. Found: C, 65.28; H, 8.19; N, 7.95. IR (KBr, cm^{-1}): 536 (w), 585 (s), 654 (w), 761 (m), 799 (s), 897 (s), 1002 (s), 1028 (m), 1060 (w), 1103 (w), 1173 (w), 1228 (s), 1251 (m), 1320 (s), 1378 (vs), 1439 (s), 1462 (m), 1543 (vs), 1607 (vs) (C=N), 2866 (s), 2926 (s), 2958 (vs), 3059 (w), 3424 (m) (OH).

Compound [LSi(=S)OCu]$_2$, 4

To a mixture of (MesCu)$_4$ (0.106 g, 0.125 mmol) (Mes = 2,4,6-Me$_3$C$_6$H$_2$) and **1** (0.309 g, 0.5 mmol) was added THF (30 mL) at –20 ^{o}C, and a clear yellow solution formed instantly. It was left to warm to room temperature and stirred for another 12 hours. All volatiles were removed in vacuo, and the obtained residue was washed with *n*-hexane (5 mL) to remove dmap and then extracted with toluene (15 mL). The obtained yellow filtrate was concentrated to ca. 4 mL and left at –20 ^{o}C for 24 hours to afford yellow crystalline product, which was separated from the mother liquor by filtration and dried in vacuo for four hours. Yield: 0.21 g (76%). Mp: 320-323 ^{o}C (decomp.). There are two isomers that have equilibrium present in the solution, so two

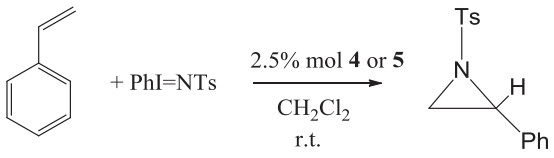
sets of signal for each moiety observed, and the ratio of isomers **4a** and **4b** is 1:0.62 according to the integral of γ-H of β-diketiminato ligand. ^{1}H NMR ($CDCl_3$, 25 ^{o}C, 400 MHz, ppm): isomer **4b**: δ = 1.06 (d, 12 H, ^{3}J = 6.8 Hz, CH(CH_3)$_2$), 1.13 (d, 24 H, ^{3}J = 6.8 Hz, CH(CH_3)$_2$), 1.36 (d, 12 H, ^{3}J = 6.8 Hz, CH(CH_3)$_2$), 1.89 (s, 12 H, α-CH_3), 3.10 (sept, 4 H, ^{3}J = 6.8 Hz, CH(CH$_3$)$_2$), 3.42 (sept, 4 H, ^{3}J = 6.8 Hz, CH(CH$_3$)$_2$), 5.55 (s, 2 H, γ-H), 7.19-7.42 (m, 12 H, Ar-*H*); isomer **4a**: δ = 1.08 (d, 12 H, ^{3}J = 6.8 Hz, CH(CH_3)$_2$), 1.12 (d, 24 H, ^{3}J = 6.8 Hz, CH(CH_3)$_2$), 1.34 (d, 12 H, ^{3}J = 6.8 Hz, CH(CH_3)$_2$), 1.86 (s, 12 H, α-CH_3), 3.26 (sept, 4 H, ^{3}J = 6.8 Hz, CH(CH$_3$)$_2$) , 3.48 (sept, 4 H, ^{3}J = 6.8 Hz, CH(CH$_3$)$_2$), 5.49 (s, 2 H, γ-H), 7.19-7.42 (m, 12 H, Ar-*H*); ^{13}C{^{1}H} NMR ($CDCl_3$, 25 ^{o}C, 50 MHz, ppm): δ = 23.6, 23.81, 24.2, 24.7, 24.8, 25.7, 26.2, 27.6, 28.0, 28.6, 29.2 (^{13}C resonance signals for *i*Pr and α-CH_3 groups in **4b** and **4b**), 100.0 (γ-C in **4a**), 100.1 (γ-C in **4b**), 124.0, 124.5, 124.6, 124.9, 127.9, 128.1, 136.7, 137.9, 144.8, 145.3, 146.3, 168.7, 168.8 (Ar-^{13}C signals for **4a** and **4b**). ^{29}Si{^{1}H} NMR ($CDCl_3$, 25 ^{o}C, 79 MHz, ppm): δ = –39.1 (isomer **4b**); –38.4 (isomer **4a**). ESI-MS: *m/z* 1113.4071(2, [M + H]$^{+}$), calcd: 1113.4088; 1051.4857 ([M – Cu + 2 H]$^{+}$), calcd: 1051.4870. Elemental analysis (%): calcd for $C_{58}H_{82}Cu_2N_4O_2S_2Si_2$: C, 62.49; H, 7.41; N, 5.03; S, 5.75. Found: C, 62.98; H, 7.79; N, 5.72; S, 5.11. IR (KBr, cm^{-1}): 504 (w), 542 (w), 614 (vs), 660 (s), 721 (w), 756 (s), 802 (s), 901 (m), 932 (w), 950 (w), 1028 (s), 1057 (vs), 1106 (w), 1173 (w), 1248 (m), 1323 (vs), 1387 (vs), 1436 (s), 1468 (m), 1552 (vs), 1587 (w), 1627 (w) (C=N), 2866 (m), 2926 (s), 2962 (vs), 3022 (w), 3062 (w).

Compound [LSi(=Se)OCu]$_2$, 5

To a mixture of (MesCu)$_4$ (0.144 g, 0.17 mmol) and **3** (0.451 g, 0.68 mmol) was added THF (30 mL) at –20 ^{o}C. The mixture was allowed to warm to room temperature and stirred for another 12 hours. All volatiles were removed in vacuo, and the residue was washed with *n*-hexane (5 mL) and extracted into toluene (20 mL). The obtained yellow filtrate was concentrated to ca. 5 mL and left at –20 ^{o}C for 24 hours to afford a yellow crystalline product. Yield: 0.67 g, 82%. Mp: 295-296 ^{o}C (dec.). There are *cis* and *trans* isomers that have equilibrium present in the solution, so two sets of signal for each moiety observed, and the ratio of isomers **5a** and **5b** is 1:0.49 according to the integral of γ-H of β-diketiminato ligand. ^{1}H NMR ($CDCl_3$, 25 ^{o}C, 400 MHz, ppm): isomer **5b**: δ = 1.01 (d, 12 H, ^{3}J = 6.8 Hz, CH(CH_3)$_2$), 1.09 (d,

24 H, ^3J = 6.8Hz, CH(CH_3)$_2$), 1.33 (d, 12 H, ^3J = 6.8 Hz, CH(CH_3)$_2$), 1.86 (s, 12 H, α-CH_3), 3.03 (sept, 4 H, ^3J = 6.8 Hz, CH(CH$_3$)$_2$) , 3.40 (sept, 4 H, ^3J = 6.8 Hz, CH(CH$_3$)$_2$), 5.56 (s, 2 H, γ-H), 7.17-7.39 (m, 12 H, Ar-*H*); isomer **5a**: δ = 1.02 (d, 12 H, ^3J = 6.8 Hz, CH(CH_3)$_2$), 1.14 (d, 24 H, ^3J = 6.8 Hz, CH(CH_3)$_2$), 1.33 (d, 12 H, ^3J = 6.8 Hz, CH(CH_3)$_2$), 1.86 (s, 12 H, α-CH_3), 3.22 (sept, 4 H, ^3J = 6.8 Hz, CH(CH$_3$)$_2$) , 3.48 (sept, 4 H, ^3J = 6.8 Hz, CH(CH$_3$)$_2$), 5.47 (s, 2 H, γ-H), 7.17-7.39 (m, 12 H, Ar-*H*); ^{13}C{^{1}H} NMR (CDCl$_3$, 25 ^{o}C, 100 MHz, ppm): 23.2, 23.7, 24.0, 24.1, 24.4, 24.5, 24.5, 24.6, 24.7, 25.7, 26.5, 27.6, 28.1, 28.2, 28.6, 28.7, 29.3 (^{13}C resonance signals for *i*Pr and α-CH$_3$ groups in **5a** and **5b**), 100.3 (γ-C in **5a**), 100.7 (γ-C in **5b**), 123.0, 124.0, 124.4, 124.5, 124.7, 124.9, 128.1, 136.7, 137.8, 144.4, 145.2, 146.2, 146.3, 146.4, 168.3, 168.6 (Ar-^{13}C signals for **5a** and **5b**). ^{29}Si{^{1}H} NMR (CDCl$_3$, 25 ^{o}C, 79 MHz, ppm): δ = –42.2 (isomer **5b**), –40.1 (isomer **5a**). ESI-MS: *m/z* 1209.2968 ([M + H]$^+$), calcd: 1209.2977. 1147.3765 ([M – Cu + 2 H]$^+$), calcd: 1147.3759. Elemental analysis (%): calcd for $C_{65}H_{90}Cu_2N_4O_2Se_2Si_2$: C, 60.02; H, 6.97; N, 4.31. Found: C, 59.82; H, 6.95; N, 4.46. IR (KBr, cm^{-1}): 501 (w), 527 (m), 568 (m), 660 (w), 724 (w), 759 (m), 799 (s), 898 (m), 932 (w), 947 (w), 1022 (s), 1066 (s), 1176 (w), 1231 (w), 1251 (m), 1323 (s), 1387 (vs), 1445 (s), 1462 (s), 1546 (vs), 1587 (w), 1621 (w), 2866 (m), 2926 (s), 2964 (vs), 3022 (w), 3062 (w).

Procedure for aziridination reactions with 4 and 5[4]



Under N_2 atmosphere, the pre-catalyst **4** or **5** (11 mg for **4** and 12 mg for **5**, 0.005 mmol) was placed in a Schlenk flask with molecular sieves, and dry CH_2Cl_2 (10 mL) was added to the flask followed with styrene (0.5 mL, 4 mmol). After the mixture was stirred for 15 min., PhI=NTs (0.15 g, 0.4 mmol) was added portion-wise in 1 hour. The mixture was stirred for another 3 hours, and then it was purified with silica-column chromatography using CH_2Cl_2 as eluent. The product is characterized with NMR spectroscopy and they are identical to that reported in the literatures.[5] The yields were determined by ^{1}H NMR spectra using mesitylene as internal standard.

2. Selected spectra of compounds 3-5.

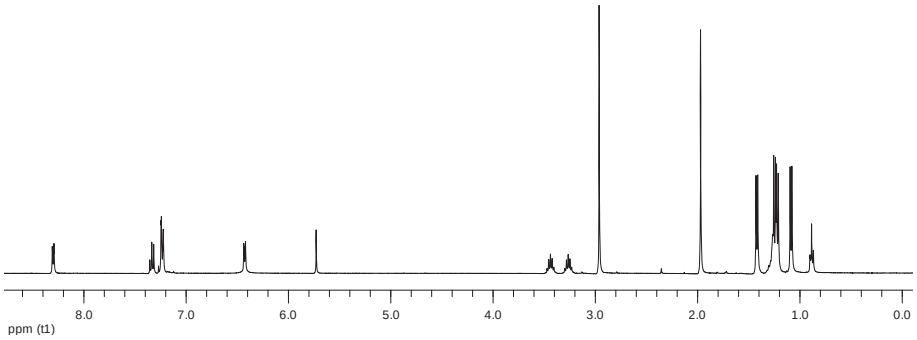


Figure 1s. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

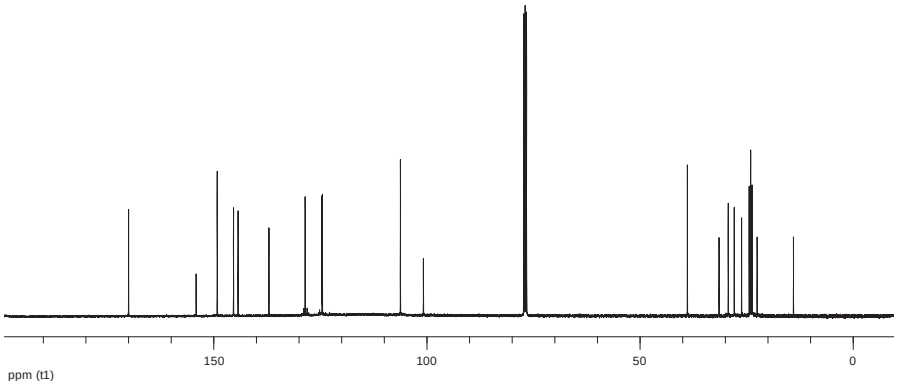


Figure 2s. ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

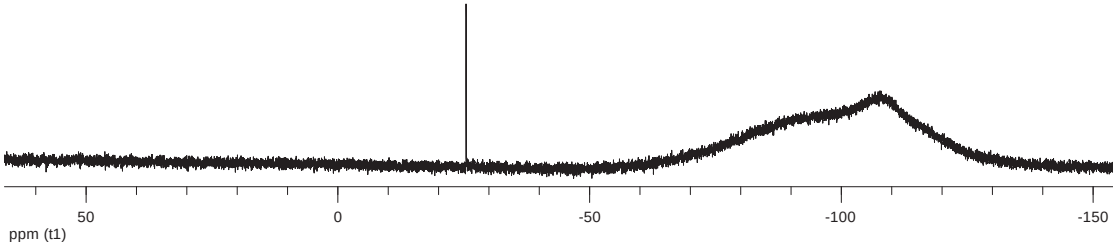


Figure 3s. ^{29}Si NMR spectrum of compound **3** in $CDCl_3$.

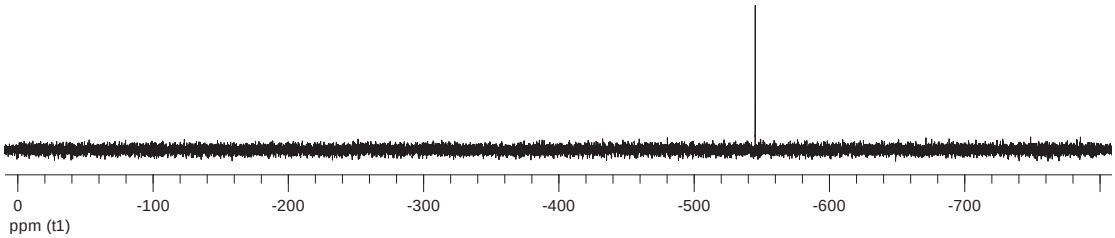


Figure 4s. ^{77}Se NMR spectrum of compound **3** in $CDCl_3$.

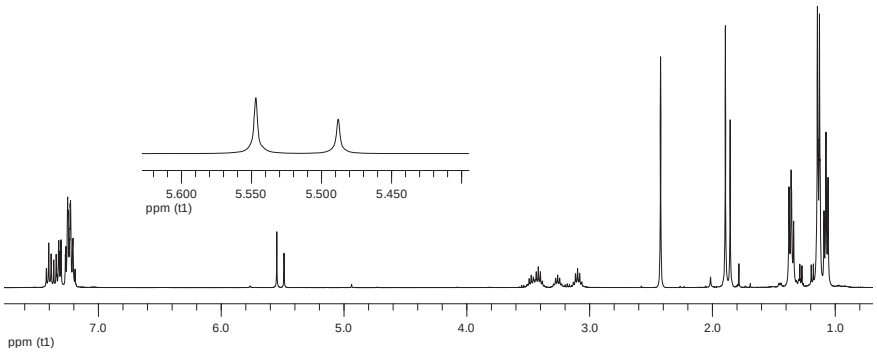


Figure 5s. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

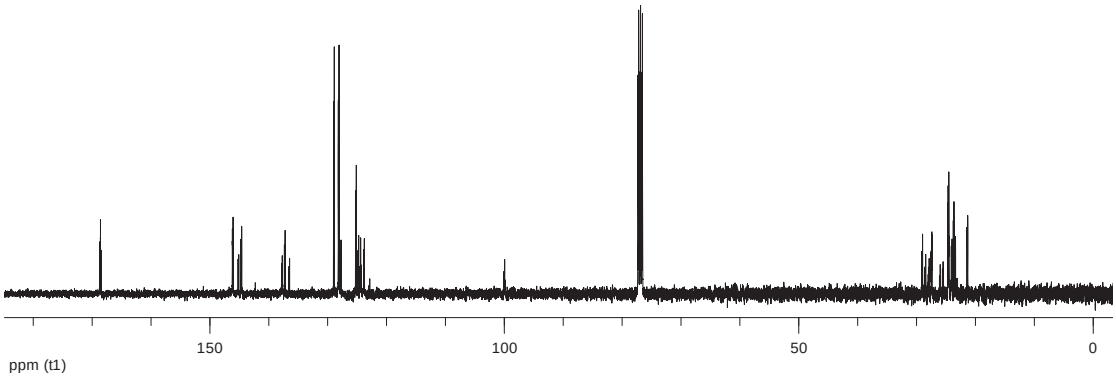


Figure 6s. ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

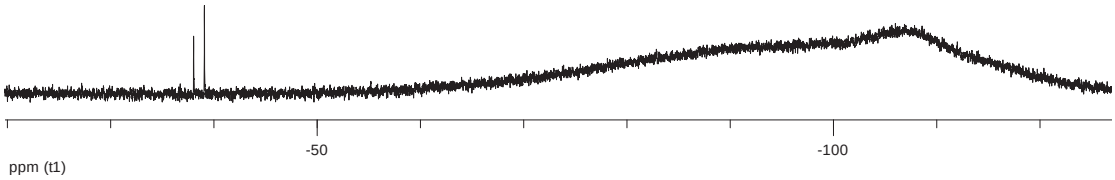


Figure 7s. ^{29}Si NMR spectrum of compound **4** in $CDCl_3$.

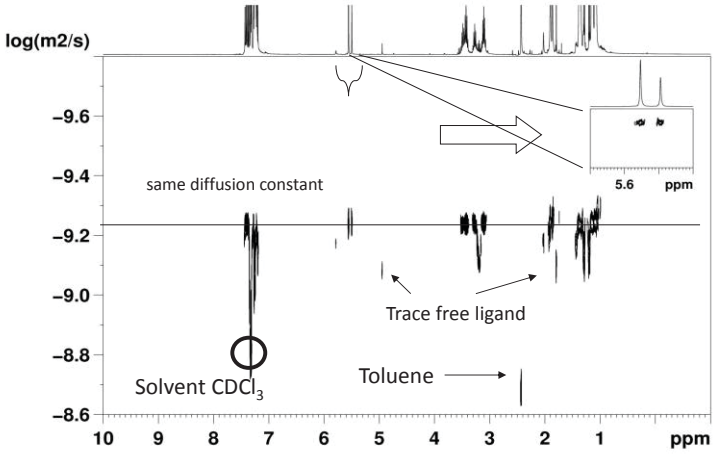


Figure 8s. ^{1}H- DOSY spectrum of compound **4** in $CDCl_3$.

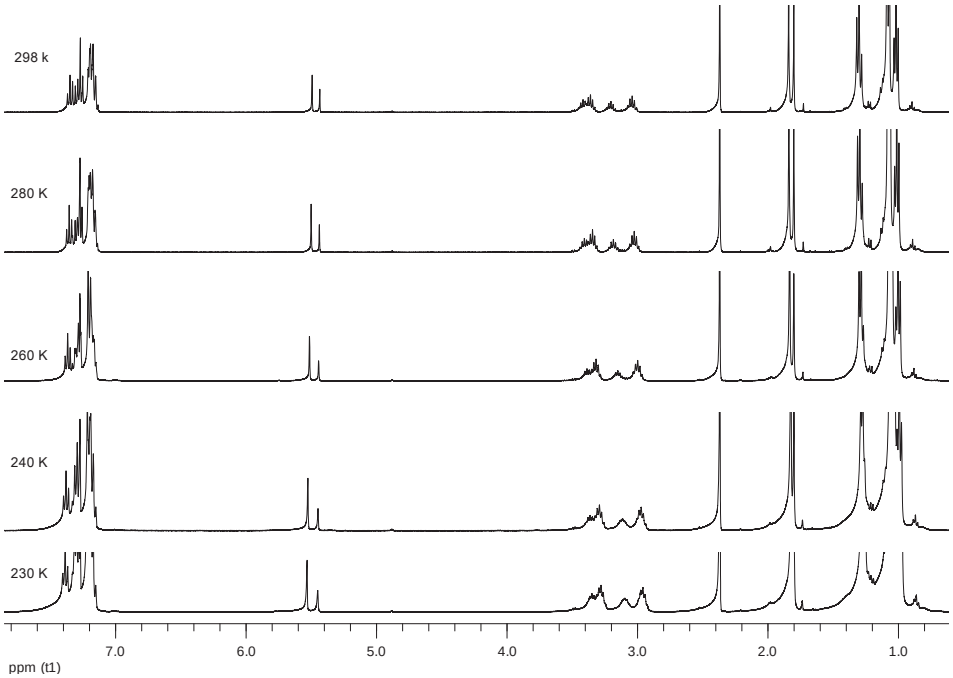


Figure 9s. Varied temperature ^{1}H NMR spectra of **4** in $CDCl_3$. From 298 K to 230 K, the the ratios of the the ring proton in γ-position of L at δ = 5.55 and 5.49 ppm decreased from 1:0.62 to 1:0.42.

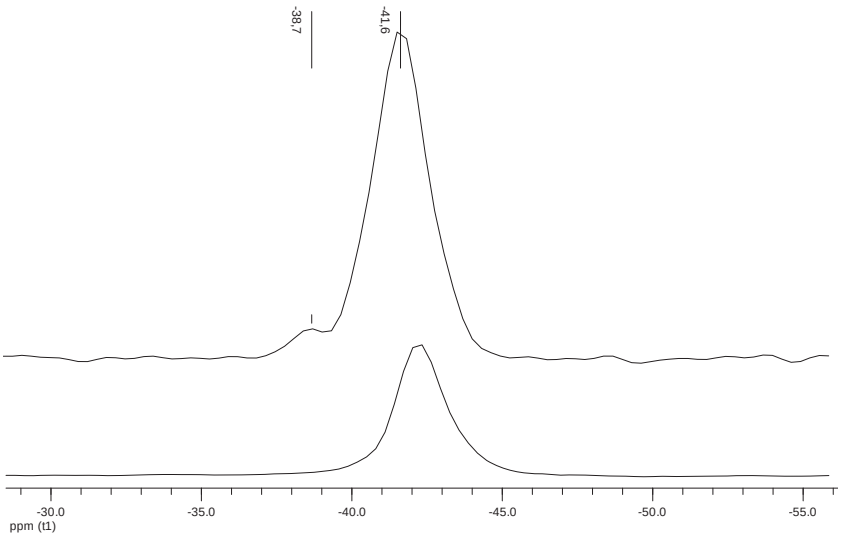


Figure 10s. Solid state ^{29}Si NMR spectra of **4** in crystalline (bottom) and fine powder (top) form.

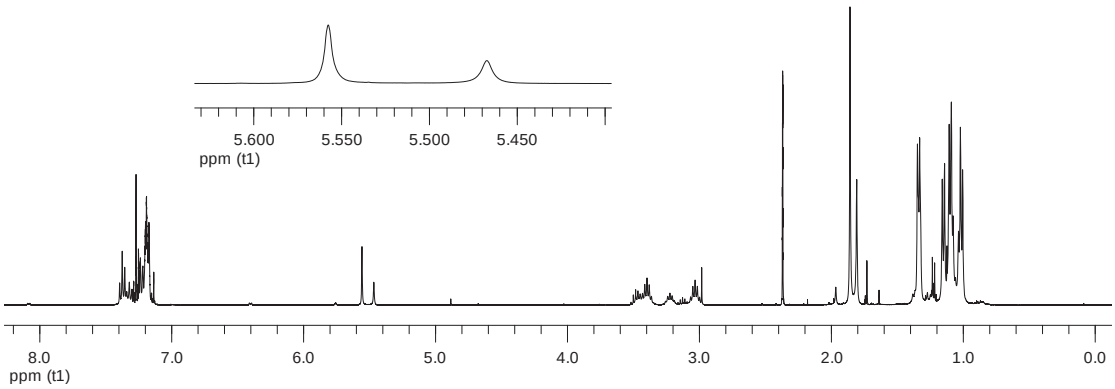


Figure 11s. ^{1}H NMR spectrum of compound **5** in $CDCl_3$.

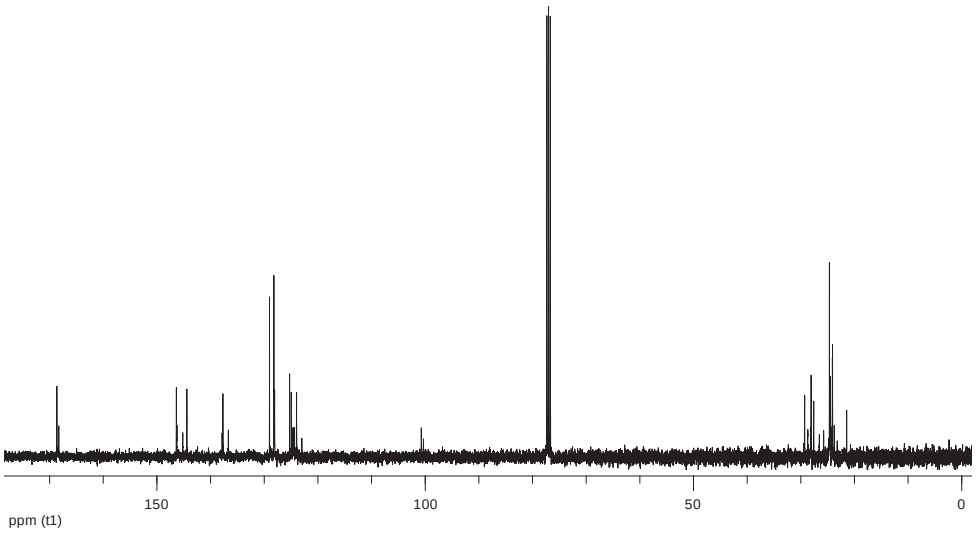


Figure 12s. ^{13}C NMR spectrum of compound **5** in $CDCl_3$.

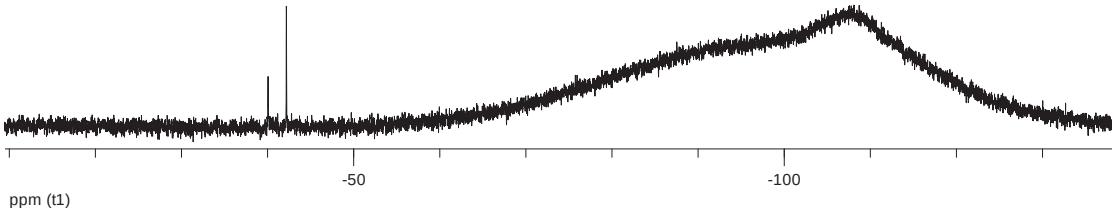


Figure 13s. ^{29}Si NMR spectrum of compound **5** in $CDCl_3$.

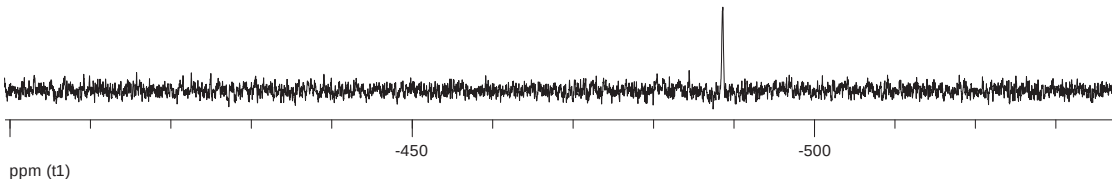


Figure 14s. ^{77}Se NMR spectrum of compound **5** in $CDCl_3$.

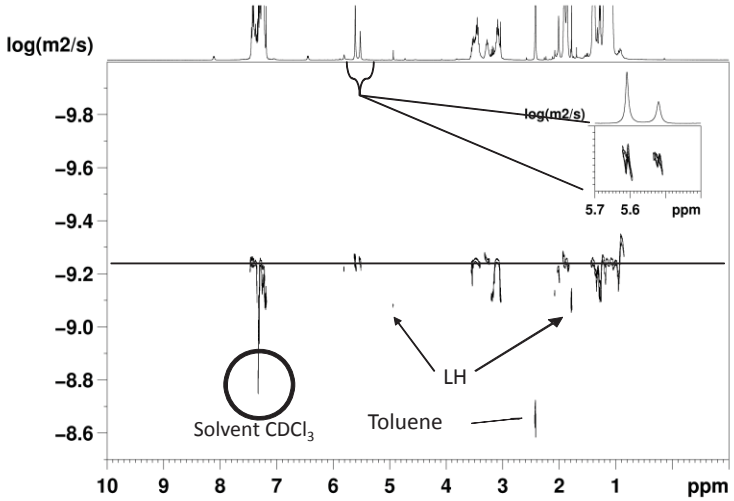


Figure 15s. ^{1}H- DOSY spectrum of compound **5** in $CDCl_3$.

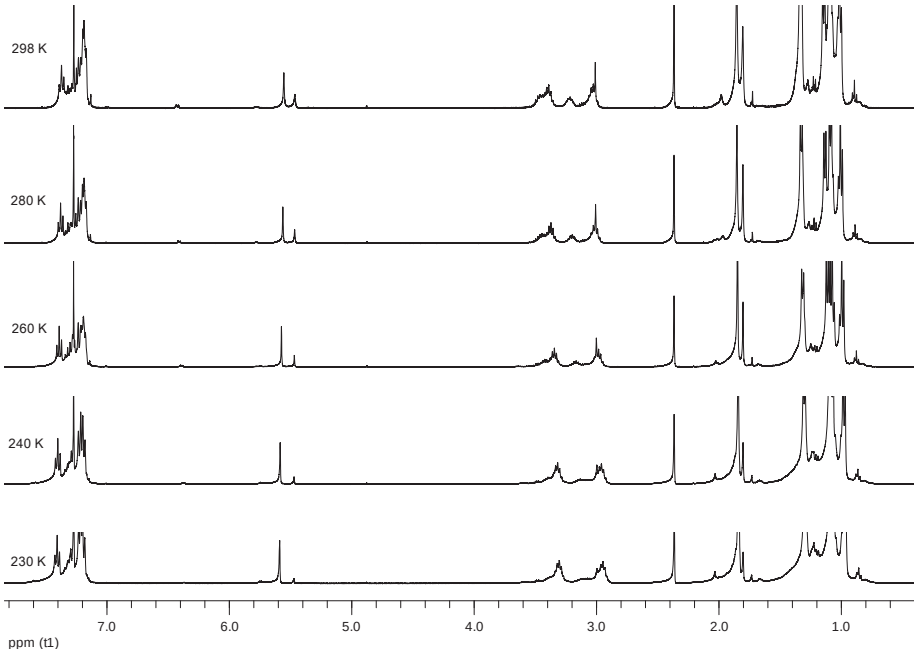


Figure 16s. Varied temperature ^{1}H NMR spectra of **5** in $CDCl_3$. From 298 K to 230 K, the the ratios of the the ring proton in γ-position of L at δ = 5.55 and 5.46 ppm decreased from 1:0.49 to 1:0.11.

3. Crystal data and refinement of compounds 3-5.

Table 1s. Crystal Data and Structure Refinement for **3-5** [a]

	3·0.5 *n*-hexane	**4**·2 Toluene	0.5 **5**·2 Toluene
formula	$C_{39}H_{59}N_4OSeSi$	$C_{72}H_{98}Cu_2N_4O_2S_2Si_2$	$C_{43}H_{57}Cu\ N_2OSeSi$
formula weight	706.95	1298.92	788.50
crystal system	Triclinic	Monoclinic	Triclinic
space group	*P-1*	*C2/c*	*P-1*
a/Å	10.6226(7)	25.8234(12)	11.9792(5)
b/Å	13.2004(7)	16.4939(5)	12.6053(6)
c/Å	14.9165(8)	18.2042(8)	14.1703(5)
α/deg	76.004(4)		79.437(3)
β/deg	75.594(5)	116.278(6)	85.487(3)
γ/deg	73.587(5)		73.996(4)
V/Å^3	1909.89(19)	6952.4(5)	2021.05(15)
Z	2	4	2
ρ_{calcd}/g·cm^{-3}	1.229	1.241	1.296
μ/mm^{-1}	1.049	0.752	1.504
F(000)	754	2768	828
crystal size/mm^3	0.28 x 0.13 x 0.11	0.15 x 0.11 x 0.07	0.16 x 0.14 x 0.08
θ range/deg	3.28–26.00	3.24–26.00	3.32–25.00
index ranges	-13 ≤ h ≤ 8	–27 ≤ *h* ≤ 31	–9 ≤ *h* ≤ 14
	–16 ≤ *k* ≤15	–20 ≤ *k* ≤ 20	–14 ≤ *k* ≤ 14
	–18 ≤ *l* ≤ 17	–22 ≤ *l* ≤ 21	–16 ≤ *l* ≤ 16
collected data	14582	26083	14701
unique data	7489 (R_{int} = 0.0344)	6820 (R_{int} = 0.0523)	7105 (R_{int} = 0.0404)
completeness to *θ*	99.8%	99.8%	99.8 %
data/restraints/parameters	7489 / 0 / 419	6820 / 0 / 379	7105 / 0 / 433
GOF on F^2	1.049	1.077	1.037
final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0463	R_1 = 0.0494	R_1 = 0.0463
	wR_2 = 0.1032	wR_2 = 0.1026	wR_2 = 0.1005

R indices (all data)	R_1 = 0.0578	R_1 = 0.0641	R_1 = 0.0631
	wR_2 = 0.1076	wR_2 = 0.1079	wR_2 = 0.1075
Largest diff peak/hole ($e \cdot Å^{-3}$)	0.642/–0.547	0.479/–0.517	0.948/–0.779

[a] All data were collected at 173(2) K using Mo K_α (λ = 0.71073 Å) radiation. $R_1 = \sum(||F_o| - |F_c||)/\sum|F_o|$, $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2/\sum[w(F_o^2)^2]\}^2\}^{1/2}$, GOF = $\{\sum[w(F_o^2 - F_c^2)^2]/(N_o - N_p)\}^{1/2}$.

Table 2s. Bond lengths (Å) and angles (°) in compound **3**

O(1)-Si(1)	1.619(2)
Se(1)-Si(1)	2.1348(7)
Si(1)-N(1)	1.816(2)
Si(1)-N(2)	1.823(2)
N(1)-C(2)	1.346(3)
N(1)-C(6)	1.465(3)
N(2)-C(4)	1.338(3)
N(2)-C(18)	1.460(3)
N(3)-C(34)	1.340(4)
N(3)-C(30)	1.343(4)
N(4)-C(32)	1.362(4)
N(4)-C(35)	1.444(4)
N(4)-C(36)	1.448(4)
C(1)-C(2)	1.506(4)
C(2)-C(3)	1.395(3)
C(3)-C(4)	1.392(4)
C(4)-C(5)	1.507(3)
C(6)-C(7)	1.406(4)
C(6)-C(11)	1.415(4)
C(7)-C(8)	1.400(4)
C(7)-C(15)	1.522(4)
C(8)-C(9)	1.373(4)
C(9)-C(10)	1.388(4)
C(10)-C(11)	1.390(4)
C(11)-C(12)	1.518(4)
C(12)-C(14)	1.528(4)
C(12)-C(13)	1.535(4)
C(15)-C(17)	1.530(4)
C(15)-C(16)	1.538(4)
C(18)-C(19)	1.403(4)

C(18)-C(23)	1.410(4)
C(19)-C(20)	1.403(4)
C(19)-C(27)	1.525(4)
C(20)-C(21)	1.385(4)
C(21)-C(22)	1.375(4)
C(22)-C(23)	1.393(4)
C(23)-C(24)	1.525(4)
C(24)-C(25)	1.525(4)
C(24)-C(26)	1.531(4)
C(27)-C(28)	1.525(4)
C(27)-C(29)	1.537(4)
C(30)-C(31)	1.372(4)
C(31)-C(32)	1.413(4)
C(32)-C(33)	1.409(4)
C(33)-C(34)	1.374(4)
C(41)-C(42)	1.520(5)
C(42)-C(43)	1.514(5)
C(43)-C(43)#1	1.519(7)

O(1)-Si(1)-N(1)	102.40(10)
O(1)-Si(1)-N(2)	102.63(10)
N(1)-Si(1)-N(2)	96.87(10)
O(1)-Si(1)-Se(1)	120.13(9)
N(1)-Si(1)-Se(1)	116.11(7)
N(2)-Si(1)-Se(1)	115.28(7)
C(2)-N(1)-C(6)	118.4(2)
C(2)-N(1)-Si(1)	121.39(17)
C(6)-N(1)-Si(1)	119.75(17)
C(4)-N(2)-C(18)	118.7(2)
C(4)-N(2)-Si(1)	121.98(17)
C(18)-N(2)-Si(1)	118.87(17)
C(34)-N(3)-C(30)	115.1(3)
C(32)-N(4)-C(35)	120.8(3)
C(32)-N(4)-C(36)	120.1(2)
C(35)-N(4)-C(36)	118.4(3)
N(1)-C(2)-C(3)	122.1(2)
N(1)-C(2)-C(1)	120.3(2)
C(3)-C(2)-C(1)	117.5(2)
C(4)-C(3)-C(2)	125.4(2)
N(2)-C(4)-C(3)	122.1(2)
N(2)-C(4)-C(5)	120.1(2)

C(3)-C(4)-C(5)	117.7(2)
C(7)-C(6)-C(11)	122.1(2)
C(7)-C(6)-N(1)	119.9(2)
C(11)-C(6)-N(1)	118.0(2)
C(8)-C(7)-C(6)	117.5(2)
C(8)-C(7)-C(15)	119.1(2)
C(6)-C(7)-C(15)	123.4(2)
C(9)-C(8)-C(7)	121.5(2)
C(8)-C(9)-C(10)	120.0(2)
C(9)-C(10)-C(11)	121.7(3)
C(10)-C(11)-C(6)	117.2(2)
C(10)-C(11)-C(12)	121.1(2)
C(6)-C(11)-C(12)	121.7(2)
C(11)-C(12)-C(14)	113.1(2)
C(11)-C(12)-C(13)	112.8(2)
C(14)-C(12)-C(13)	109.8(2)
C(7)-C(15)-C(17)	110.1(2)
C(7)-C(15)-C(16)	112.1(2)
C(17)-C(15)-C(16)	109.8(2)
C(19)-C(18)-C(23)	121.9(2)
C(19)-C(18)-N(2)	119.6(2)
C(23)-C(18)-N(2)	118.5(2)
C(18)-C(19)-C(20)	117.8(2)
C(18)-C(19)-C(27)	123.7(2)
C(20)-C(19)-C(27)	118.5(3)
C(21)-C(20)-C(19)	121.1(3)
C(22)-C(21)-C(20)	119.8(3)
C(21)-C(22)-C(23)	122.0(3)
C(22)-C(23)-C(18)	117.4(3)
C(22)-C(23)-C(24)	120.1(2)
C(18)-C(23)-C(24)	122.5(2)
C(23)-C(24)-C(25)	112.2(3)
C(23)-C(24)-C(26)	111.7(2)
C(25)-C(24)-C(26)	110.1(3)
C(19)-C(27)-C(28)	111.3(2)
C(19)-C(27)-C(29)	111.8(2)
C(28)-C(27)-C(29)	110.4(3)
N(3)-C(30)-C(31)	124.8(3)
C(30)-C(31)-C(32)	119.9(3)
N(4)-C(32)-C(33)	122.7(3)
N(4)-C(32)-C(31)	122.0(3)

C(33)-C(32)-C(31)	115.3(3)
C(34)-C(33)-C(32)	119.7(3)
N(3)-C(34)-C(33)	125.0(3)
C(43)-C(42)-C(41)	113.7(3)
C(42)-C(43)-C(43)#1	114.0(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1.

Table 3s. Bond lengths (Å) and angles (^{o}) in compound **4**

O(1)-Si(1)	1.568(2)
O(1)-Cu(1)#1	1.8404(19)
S(1)-Si(1)	2.0609(9)
S(1)-Cu(1)	2.1299(8)
Si(1)-N(2)	1.810(2)
Si(1)-N(1)	1.816(2)
Cu(1)-O(1)#1	1.8404(19)
Cu(1)-Cu(1)#1	2.8135(7)
C(1)-C(2)	1.501(4)
C(2)-N(2)	1.347(3)
C(2)-C(3)	1.401(4)
C(3)-C(4)	1.391(4)
C(4)-N(1)	1.343(3)
C(4)-C(5)	1.505(4)
C(11)-C(12)	1.402(4)
C(11)-C(16)	1.407(4)
C(11)-N(2)	1.466(3)
C(12)-C(13)	1.402(4)
C(12)-C(122)	1.527(4)
C(13)-C(14)	1.372(5)
C(14)-C(15)	1.384(5)
C(15)-C(16)	1.392(4)
C(16)-C(162)	1.521(4)
C(21)-C(22)	1.399(4)
C(21)-C(26)	1.406(4)
C(21)-N(1)	1.465(3)
C(22)-C(23)	1.397(4)
C(22)-C(222)	1.524(4)
C(23)-C(24)	1.380(5)
C(24)-C(25)	1.374(4)

C(25)-C(26)	1.398(4)
C(26)-C(262)	1.524(4)
C(121)-C(122)	1.539(4)
C(122)-C(123)	1.527(5)
C(161)-C(162)	1.535(4)
C(162)-C(163)	1.533(4)
C(221)-C(222)	1.536(5)
C(222)-C(223)	1.529(4)
C(261)-C(262)	1.526(4)
C(262)-C(263)	1.540(4)
C(51)-C(52)	1.382(5)
C(51)-C(56)	1.391(5)
C(51)-C(57)	1.500(5)
C(52)-C(53)	1.375(6)
C(53)-C(54)	1.376(6)
C(54)-C(55)	1.387(6)
C(55)-C(56)	1.363(6)

Si(1)-O(1)-Cu(1)#1	130.06(11)
Si(1)-S(1)-Cu(1)	99.28(4)
O(1)-Si(1)-N(2)	106.96(10)
O(1)-Si(1)-N(1)	108.89(11)
N(2)-Si(1)-N(1)	97.58(10)
O(1)-Si(1)-S(1)	120.98(8)
N(2)-Si(1)-S(1)	111.03(8)
N(1)-Si(1)-S(1)	108.85(8)
O(1)#1-Cu(1)-S(1)	170.62(6)
O(1)#1-Cu(1)-Cu(1)#1	88.08(6)
S(1)-Cu(1)-Cu(1)#1	100.94(2)
N(2)-C(2)-C(3)	121.7(2)
N(2)-C(2)-C(1)	120.2(2)
C(3)-C(2)-C(1)	118.1(2)
C(4)-C(3)-C(2)	126.0(2)
N(1)-C(4)-C(3)	121.9(2)
N(1)-C(4)-C(5)	120.6(2)
C(3)-C(4)-C(5)	117.5(2)
C(12)-C(11)-C(16)	122.3(2)
C(12)-C(11)-N(2)	119.7(2)
C(16)-C(11)-N(2)	118.0(2)
C(13)-C(12)-C(11)	117.4(3)
C(13)-C(12)-C(122)	118.7(3)

C(11)-C(12)-C(122)	123.9(2)
C(14)-C(13)-C(12)	121.4(3)
C(13)-C(14)-C(15)	120.2(3)
C(14)-C(15)-C(16)	121.4(3)
C(15)-C(16)-C(11)	117.4(3)
C(15)-C(16)-C(162)	120.2(3)
C(11)-C(16)-C(162)	122.5(2)
C(22)-C(21)-C(26)	122.3(2)
C(22)-C(21)-N(1)	118.0(2)
C(26)-C(21)-N(1)	119.6(2)
C(23)-C(22)-C(21)	117.9(3)
C(23)-C(22)-C(222)	118.6(3)
C(21)-C(22)-C(222)	123.4(2)
C(24)-C(23)-C(22)	120.8(3)
C(25)-C(24)-C(23)	120.2(3)
C(24)-C(25)-C(26)	121.8(3)
C(25)-C(26)-C(21)	116.9(3)
C(25)-C(26)-C(262)	119.2(3)
C(21)-C(26)-C(262)	123.9(2)
C(12)-C(122)-C(123)	111.5(2)
C(12)-C(122)-C(121)	111.4(3)
C(123)-C(122)-C(121)	108.7(3)
C(16)-C(162)-C(163)	112.4(2)
C(16)-C(162)-C(161)	112.1(2)
C(163)-C(162)-C(161)	109.7(3)
C(22)-C(222)-C(223)	112.1(2)
C(22)-C(222)-C(221)	110.4(3)
C(223)-C(222)-C(221)	109.7(3)
C(26)-C(262)-C(261)	112.9(2)
C(26)-C(262)-C(263)	110.1(2)
C(261)-C(262)-C(263)	110.0(3)
C(2)-N(2)-C(11)	118.9(2)
C(2)-N(2)-Si(1)	122.10(18)
C(11)-N(2)-Si(1)	118.41(16)
C(4)-N(1)-C(21)	120.3(2)
C(4)-N(1)-Si(1)	122.12(18)
C(21)-N(1)-Si(1)	117.59(17)
C(52)-C(51)-C(56)	117.5(4)
C(52)-C(51)-C(57)	121.9(3)
C(56)-C(51)-C(57)	120.6(4)
C(53)-C(52)-C(51)	121.6(3)

C(52)-C(53)-C(54)	120.4(4)
C(53)-C(54)-C(55)	118.3(4)
C(56)-C(55)-C(54)	121.2(4)
C(55)-C(56)-C(51)	121.0(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+3/2,-y+1/2,-z.

Table 4s. Bond lengths (Å) and angles (^{o}) in compound **5**

Cu(1)-O(1)#1	1.844(2)
Cu(1)-Se(1)	2.2531(5)
Cu(1)-Cu(1)#1	2.9271(8)
Si(1)-O(1)	1.567(2)
Si(1)-N(2)	1.817(3)
Si(1)-N(1)	1.824(3)
Si(1)-Se(1)	2.2011(9)
O(1)-Cu(1)#1	1.844(2)
N(1)-C(4)	1.347(4)
N(1)-C(18)	1.460(4)
N(2)-C(2)	1.352(4)
N(2)-C(6)	1.453(4)
C(1)-C(2)	1.502(5)
C(2)-C(3)	1.387(5)
C(3)-C(4)	1.395(5)
C(4)-C(5)	1.501(5)
C(6)-C(7)	1.396(5)
C(6)-C(11)	1.407(5)
C(7)-C(8)	1.403(5)
C(7)-C(15)	1.524(5)
C(8)-C(9)	1.380(5)
C(9)-C(10)	1.383(6)
C(10)-C(11)	1.393(5)
C(11)-C(12)	1.518(5)
C(12)-C(14)	1.531(5)
C(12)-C(13)	1.537(6)
C(15)-C(17)	1.535(6)
C(15)-C(16)	1.540(5)
C(18)-C(19)	1.410(5)
C(18)-C(23)	1.412(5)

C(19)-C(20)	1.393(5)
C(19)-C(27)	1.526(5)
C(20)-C(21)	1.385(5)
C(21)-C(22)	1.389(5)
C(22)-C(23)	1.384(5)
C(23)-C(24)	1.532(5)
C(24)-C(25)	1.525(5)
C(24)-C(26)	1.528(5)
C(27)-C(28)	1.519(6)
C(27)-C(29)	1.545(5)
C(30)-C(35)	1.374(6)
C(30)-C(31)	1.391(6)
C(30)-C(36)	1.511(5)
C(31)-C(32)	1.378(7)
C(32)-C(33)	1.368(7)
C(33)-C(34)	1.387(7)
C(34)-C(35)	1.369(7)
C(37)-C(42)	1.3802
C(37)-C(38)	1.4471
C(38)-C(39)	1.4288
C(39)-C(40)	1.3531
C(40)-C(41)	1.4049
C(41)-C(42)	1.3778
C(42)-C(43)	1.3706

O(1)#1-Cu(1)-Se(1)	172.07(7)
O(1)#1-Cu(1)-Cu(1)#1	83.61(7)
Se(1)-Cu(1)-Cu(1)#1	104.17(2)
O(1)-Si(1)-N(2)	108.67(13)
O(1)-Si(1)-N(1)	106.31(13)
N(2)-Si(1)-N(1)	97.19(13)
O(1)-Si(1)-Se(1)	120.89(10)
N(2)-Si(1)-Se(1)	109.54(9)
N(1)-Si(1)-Se(1)	111.61(9)
Si(1)-Se(1)-Cu(1)	93.49(3)
Si(1)-O(1)-Cu(1)#1	137.07(14)
C(4)-N(1)-C(18)	120.3(3)
C(4)-N(1)-Si(1)	120.5(2)
C(18)-N(1)-Si(1)	117.9(2)
C(2)-N(2)-C(6)	119.7(3)
C(2)-N(2)-Si(1)	120.2(2)

C(6)-N(2)-Si(1)	120.0(2)
N(2)-C(2)-C(3)	121.6(3)
N(2)-C(2)-C(1)	120.3(3)
C(3)-C(2)-C(1)	118.1(3)
C(2)-C(3)-C(4)	126.6(3)
N(1)-C(4)-C(3)	121.7(3)
N(1)-C(4)-C(5)	121.1(3)
C(3)-C(4)-C(5)	117.2(3)
C(7)-C(6)-C(11)	122.6(3)
C(7)-C(6)-N(2)	120.2(3)
C(11)-C(6)-N(2)	117.1(3)
C(6)-C(7)-C(8)	117.3(3)
C(6)-C(7)-C(15)	123.2(3)
C(8)-C(7)-C(15)	119.5(3)
C(9)-C(8)-C(7)	121.2(4)
C(8)-C(9)-C(10)	120.3(3)
C(9)-C(10)-C(11)	121.1(3)
C(10)-C(11)-C(6)	117.5(3)
C(10)-C(11)-C(12)	120.7(3)
C(6)-C(11)-C(12)	121.8(3)
C(11)-C(12)-C(14)	113.0(3)
C(11)-C(12)-C(13)	111.5(3)
C(14)-C(12)-C(13)	110.5(3)
C(7)-C(15)-C(17)	111.3(3)
C(7)-C(15)-C(16)	111.4(3)
C(17)-C(15)-C(16)	109.3(3)
C(19)-C(18)-C(23)	121.7(3)
C(19)-C(18)-N(1)	119.5(3)
C(23)-C(18)-N(1)	118.8(3)
C(20)-C(19)-C(18)	117.4(3)
C(20)-C(19)-C(27)	118.8(3)
C(18)-C(19)-C(27)	123.8(3)
C(21)-C(20)-C(19)	121.7(3)
C(20)-C(21)-C(22)	119.8(4)
C(23)-C(22)-C(21)	121.2(3)
C(22)-C(23)-C(18)	118.2(3)
C(22)-C(23)-C(24)	120.6(3)
C(18)-C(23)-C(24)	121.2(3)
C(25)-C(24)-C(26)	110.6(3)
C(25)-C(24)-C(23)	111.4(3)
C(26)-C(24)-C(23)	113.5(3)

C(28)-C(27)-C(19)	112.9(3)
C(28)-C(27)-C(29)	109.2(3)
C(19)-C(27)-C(29)	110.0(3)
C(35)-C(30)-C(31)	117.2(4)
C(35)-C(30)-C(36)	122.2(4)
C(31)-C(30)-C(36)	120.6(4)
C(32)-C(31)-C(30)	121.2(4)
C(33)-C(32)-C(31)	120.5(5)
C(32)-C(33)-C(34)	119.0(5)
C(35)-C(34)-C(33)	120.0(5)
C(34)-C(35)-C(30)	122.1(5)
C(42)-C(37)-C(38)	115.7
C(39)-C(38)-C(37)	122.5
C(40)-C(39)-C(38)	117.0
C(39)-C(40)-C(41)	122.4
C(42)-C(41)-C(40)	119.8
C(43)-C(42)-C(41)	119.8
C(43)-C(42)-C(37)	117.5
C(41)-C(42)-C(37)	122.5

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y,-z.

4. Computational (DFT) Details

DFT calculations of the compounds **4a** and isomer **4b** were performed at the B3LYP level using 6-31G(d) basis set for H, C, N, O, S and Si atoms and the LANL2DZ level for the Cu atom with the Gaussian 03 program.[6] Cartesian coordinates of optimized structures of compounds **4a** and **4b** are shown in Table 5s and 6s, respectively. The structure obtained by X-ray analysis was used as the input for the calculation of compound **4a**. Optimized structure of model compounds were obtained without symmetry constraints.

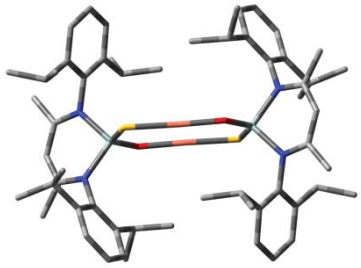


Figure 17s. Optimized structure of compound **4a**. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Si−O 1.5904, Si−S 2.0760, O−Cu 1.8877, S−Cu 2.2208, S−Si−O 121.40, Si−O−Cu 130.04, Si−S−Cu 102.13.

Table 5s. Cartesian coordinates (x, y, z) for the optimized structure of **4a**.

O	1.73800565	-0.00003518	1.61810461	C	5.77142632	-2.46356175	2.24939383
S	2.36308047	-0.00113466	-1.52663833	H	6.08780192	-3.11954926	1.43541129
Si	2.85848327	-0.00021610	0.48942167	H	5.12042923	-3.05708615	2.89832918
Cu	0.14322215	-0.00043317	-1.46176687	H	6.64926586	-2.16185626	2.82432063
C	5.77081305	2.46495460	2.24798259	C	3.76502240	2.71801806	0.30012049
H	6.08684649	3.12058811	1.43358366	C	2.89132302	3.60436454	0.97267121
H	6.64886231	2.16375826	2.82285657	C	2.70486269	4.88190682	0.42493190
H	5.11984255	3.05867234	2.89676373	H	2.03714217	5.57664443	0.92643876
C	5.03303486	1.25013208	1.73635450	C	3.35599132	5.27894954	-0.73654323
C	5.45563736	0.00064854	2.20499469	H	3.19985400	6.27710651	-1.13771465
H	6.25510628	0.00096316	2.93395156	C	4.20904663	4.39070757	-1.38395358
C	5.03344369	-1.24919648	1.73699021	H	4.71471919	4.70367045	-2.29276398

C	4.42863953	3.09894530	-0.89153903	H	3.58823253	-4.19046935	3.63819088
C	3.76635341	-2.71805461	0.30092313	H	2.21334278	-5.22010460	3.23056318
C	4.43058736	-3.09903562	-0.89038614	H	1.99721170	-3.86075148	4.34084490
C	4.21164973	-4.39098296	-1.38258301	N	4.02697526	1.39194865	0.85373861
H	4.71775720	-4.70397174	-2.29114306	N	4.02756127	-1.39174213	0.85427743
C	3.35865399	-5.27938515	-0.73530032	O	-1.73802789	-0.00021728	-1.61810610
H	3.20301252	-6.27767839	-1.13632470	S	-2.36307385	-0.00080967	1.52662364
C	2.70694155	-4.88231041	0.42582790	Si	-2.85850644	-0.00016548	-0.48942615
H	2.03927245	-5.57716260	0.92724353	Cu	-0.14322269	-0.00059410	1.46175471
C	2.89273841	-3.60456653	0.97333054	C	-5.77193083	-2.46326201	-2.24892838
C	2.51209086	4.18436282	3.42819112	H	-6.08974109	-3.11812164	-1.43458196
H	3.58768929	4.19120713	3.63716101	H	-6.64891242	-2.16149031	-2.82512406
H	1.99704483	3.86115013	4.34047730	H	-5.12067632	-3.05803077	-2.89644092
H	2.21230895	5.22026952	3.22974186	C	-5.03368005	-1.24892743	-1.73684806
C	2.13989323	3.25167686	2.25645618	C	-5.45577135	0.00093156	-2.20489060
H	2.39109777	2.22636093	2.53696390	H	-6.25528059	0.00130522	-2.93379983
C	0.61582648	3.29090045	2.03320197	C	-5.03300705	1.25039019	-1.73631444
H	0.31757582	2.63509752	1.21096652	C	-5.77070854	2.46527806	-2.24788829
H	0.26430978	4.30355482	1.80087626	H	-6.08733386	3.12049297	-1.43337052
H	0.09155942	2.95259344	2.93433021	H	-5.11949891	3.05942652	-2.89601599
C	5.03085034	2.06909580	-3.14042615	H	-6.64838679	2.16415970	-2.82336729
H	3.99612086	1.74059882	-3.26502262	C	-3.76662208	-2.71791702	-0.30095597
H	5.68466427	1.33510576	-3.62666220	C	-2.89314188	-3.60446281	-0.97351012
H	5.16337661	3.02261937	-3.66556555	C	-2.70750682	-4.88229666	-0.42617684
C	5.39074308	2.18222727	-1.64680939	H	-2.03993231	-5.57717371	-0.92768475
H	5.30514935	1.17984043	-1.21970514	C	-3.35925434	-5.27944105	0.73491400
C	6.85656025	2.63828848	-1.48743346	H	-3.20374615	-6.27781550	1.13578740
H	7.17512511	2.65239902	-0.43945658	C	-4.21208570	-4.39100134	1.38234794
H	7.00390542	3.64633394	-1.89363473	H	-4.71820820	-4.70403189	2.29088759
H	7.52645467	1.95982754	-2.02939027	C	-4.43084688	-3.09894442	0.89033690
C	6.85853064	-2.63761702	-1.48556407	C	-3.76481046	2.71818574	-0.30017649
H	7.17669968	-2.65157745	-0.43747130	C	-4.42834306	3.09923404	0.89150163
H	7.52837993	-1.95893256	-2.02729805	C	-4.20855696	4.39096927	1.38388438
H	7.00638176	-3.64562183	-1.89167461	H	-4.71414100	4.70400841	2.29271723
C	5.39259467	-2.18211720	-1.64552588	C	-3.35540053	5.27908833	0.73643153
H	5.30649166	-1.17967700	-1.21864814	H	-3.19910727	6.27722467	1.13759363
C	5.03318791	-2.06943649	-3.13929036	C	-2.70437124	4.88193964	-0.42505810
H	3.99839126	-1.74131691	-3.26434791	H	-2.03656790	5.57657288	-0.92659806
H	5.16619913	-3.02303981	-3.66416725	C	-2.89102648	3.60441103	-0.97276971
H	5.68694587	-1.33535737	-3.62547254	C	-2.51308393	-4.18364217	-3.42910627
C	0.61669927	-3.29161475	2.03274490	H	-3.58857598	-4.18976458	-3.63865690
H	0.31869159	-2.63619804	1.21011127	H	-1.99736821	-3.86038150	-4.34099543
H	0.09186649	-2.95315534	2.93348748	H	-2.21401293	-5.21980012	-3.23088755
H	0.26564031	-4.30446399	1.80059536	C	-2.14098462	-3.25161113	-2.25682404
C	2.14064865	-3.25181223	2.25670380	H	-2.39159653	-2.22606839	-2.53703725
H	2.39136710	-2.22632756	2.53704424	C	-0.61705619	-3.29158434	-2.03280771
C	2.51270323	-4.18403879	3.42883681	H	-0.31901818	-2.63627884	-1.21009296

H	-0.26609112	-4.30448760	-1.80075406	H	-5.30510485	1.18025461	1.21974989
H	-0.09215064	-2.95307112	-2.93349022	C	-5.03051985	2.06948890	3.14044494
C	-5.03262220	-2.06938377	3.13943093	H	-3.99583155	1.74083864	3.26497945
H	-3.99774083	-1.74140602	3.26412967	H	-5.16286489	3.02304329	3.66557979
H	-5.68611284	-1.33523604	3.62586832	H	-5.68441100	1.33560732	3.62674191
H	-5.16557705	-3.02299872	3.66429685	C	-0.61562376	3.29062544	-2.03344969
C	-5.39257329	-2.18196885	1.64577712	H	-0.31740380	2.63456667	-1.21140520
H	-5.30653283	-1.17952076	1.21890019	H	-0.09146079	2.95247400	-2.93470110
C	-6.85860282	-2.63731989	1.48634190	H	-0.26396761	4.30317070	-1.80089678
H	-7.17721965	-2.65106030	0.43837787	C	-2.13970876	3.25161142	-2.25659655
H	-7.00640568	-3.64537879	1.89233892	H	-2.39106219	2.22631804	-2.53707153
H	-7.52816323	-1.95866249	2.02846428	C	-2.51185704	4.18433382	-3.42831761
C	-6.85628492	2.63894130	1.48764561	H	-3.58747591	4.19140749	-3.63717403
H	-7.17496721	2.65315631	0.43971144	H	-2.21183605	5.22018653	-3.22992987
H	-7.52621898	1.96054884	2.02963898	H	-1.99697559	3.86099719	-4.34065153
H	-7.00342980	3.64698325	1.89392073	N	-4.02772140	-1.39153672	-0.85422572
C	-5.39051146	2.18265478	1.64685785	N	-4.02690376	1.39213265	-0.85374265

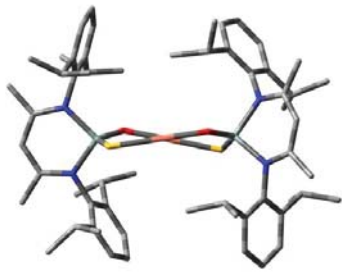


Figure 18s. Optimized structure of compound **4b**. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Si−O 1.5872, Si−S 2.0800, O−Cu 1.8858, S−Cu 2.2350, S−Si−O 119.69, Si−O−Cu 128.41, Si−S−Cu 100.32.

Table 6s. Cartesian coordinates (x, y, z) for the optimized structure of **4b**.

O	1.75488514	-0.27927341	-1.70176236	C	7.10410820	1.84526711	1.52784399
S	2.08711756	0.23399349	1.44285539	C	5.56605728	1.72512624	1.55210695
Si	2.75123999	-0.26856927	-0.45912891	C	5.03690920	1.96621162	2.97952655
Cu	-0.09520881	0.00651582	1.11769926	C	1.35372563	3.13840368	-2.65567826
C	5.19174833	-3.53593264	-1.44362188	C	2.82428182	2.68697522	-2.74873244
C	4.68945727	-2.12684017	-1.23350245	C	3.44710627	3.22986136	-4.05161258
C	5.38079857	-1.09492094	-1.87969504	N	3.63418889	-1.89787312	-0.43020863
C	5.21493393	0.27753288	-1.65885513	N	4.21321268	0.77739159	-0.91022503
C	6.24397181	1.20367357	-2.26325525	O	-1.97014390	-0.17684835	1.03234106
C	3.10315016	-3.01149965	0.35053655	S	-2.23093451	0.74059364	-2.00193250
C	2.10213859	-3.84463622	-0.19937388	Si	-2.96085760	0.33617438	-0.09664265
C	1.67188948	-4.94201290	0.56025102	Cu	-0.08536059	0.17318662	-1.73774352
C	2.20614549	-5.21407584	1.81367037	C	-6.77445951	-1.49744802	-0.10887484
C	3.17954467	-4.37263546	2.34319596	C	-5.67710375	-0.46491475	-0.00329318
C	3.64165109	-3.25614994	1.63679572	C	-6.05887397	0.83711085	0.32295221
C	4.22380771	2.20802495	-0.61350205	C	-5.20874573	1.90595410	0.64121294
C	4.90182198	2.66111047	0.54341359	C	-5.89280629	3.16199410	1.13584701
C	4.96941277	4.04110281	0.77017448	C	-4.09838621	-2.25271542	-0.37061571
C	4.38015354	4.94985518	-0.10226685	C	-4.10911813	-2.81187075	-1.67307819
C	3.69948487	4.48409961	-1.22055844	C	-3.87033444	-4.18787448	-1.79660429
C	3.60191678	3.11467631	-1.50432486	C	-3.62727682	-4.98994379	-0.68777684
C	1.66690268	-4.79080791	-2.52989488	C	-3.61751254	-4.42135076	0.58103537
C	1.45642166	-3.60731307	-1.56308536	C	-3.85157969	-3.05367183	0.77204254
C	-0.05039428	-3.32657485	-1.40948360	C	-3.03759437	2.94895583	0.96997049
C	4.29093704	-1.90781205	3.68933325	C	-2.52245030	2.94109237	2.28971220
C	4.70791192	-2.37139883	2.28057653	C	-1.69784000	4.00434886	2.67819210
C	6.08203934	-3.07140398	2.33299613	C	-1.39199715	5.04265147	1.80497278

C	-1.92992331	5.04462337	0.52351029	H	3.94817973	1.87466604	3.00941177
C	-2.76196510	4.01006971	0.07371401	H	5.31604453	2.95938521	3.35119112
C	-5.67877479	-2.48397852	-3.65897955	H	5.46342103	1.22703567	3.66790858
C	-4.38730148	-2.01839236	-2.95186241	H	0.88266314	2.77971818	-1.73599036
C	-3.20748051	-2.10755183	-3.94040085	H	0.78352627	2.74013102	-3.50292082
C	-2.50707393	-2.76136877	2.90678088	H	1.26388593	4.23153936	-2.67618720
C	-3.85636522	-2.51748435	2.20422860	H	2.81473403	1.59610142	-2.79723922
C	-5.00648096	-3.12379089	3.03575389	H	4.48270189	2.90124534	-4.19282495
C	-3.96255167	2.41494274	4.29865885	H	3.44376939	4.32629369	-4.07397802
C	-2.89105640	1.87845693	3.32508283	H	2.86920783	2.87941774	-4.91503810
C	-1.67589337	1.36176049	4.11619502	H	-6.74158337	-2.02265231	-1.06505003
C	-2.29792364	4.31921029	-2.41602824	H	-6.66671728	-2.25883263	0.66949923
C	-3.36839832	4.12890639	-1.32548597	H	-7.75247924	-1.02472694	0.00108466
C	-4.38382451	5.29117497	-1.39546906	H	-7.12061160	1.02252589	0.42720908
N	-4.39208330	-0.83257268	-0.17883475	H	-5.19524196	3.90952556	1.50850682
N	-3.87461941	1.82992664	0.53854559	H	-6.47452185	3.60414727	0.31910219
H	5.39479679	-4.03686223	-0.49381176	H	-6.59908890	2.90523317	1.93176312
H	6.10493694	-3.53009133	-2.04216415	H	-3.87930664	-4.63637603	-2.78581608
H	4.43911640	-4.13747094	-1.96149265	H	-3.44914302	-6.05517698	-0.81189144
H	6.19666162	-1.38756924	-2.52708603	H	-3.42876161	-5.05005130	1.44661376
H	6.78058813	1.75716485	-1.48737637	H	-1.29173406	4.01826753	3.68475963
H	5.77311100	1.94905105	-2.90843023	H	-0.74481194	5.85408936	2.12733153
H	6.96820326	0.63529209	-2.85013239	H	-1.70425742	5.86783765	-0.14782906
H	0.90260531	-5.59315788	0.15526015	H	-6.56657218	-2.39689760	-3.02349623
H	1.86171618	-6.07542203	2.38027620	H	-5.85315361	-1.87591325	-4.55445435
H	3.58813268	-4.58291509	3.32725379	H	-5.60553877	-3.53022814	-3.97868582
H	5.49160591	4.40743999	1.64934433	H	-4.50160186	-0.96478901	-2.68700526
H	4.44617210	6.01707860	0.09327109	H	-2.28368875	-1.75583230	-3.47682074
H	3.23052224	5.19568024	-1.89411187	H	-3.05949495	-3.13381108	-4.29854373
H	2.72626302	-5.02296626	-2.68729949	H	-3.40482975	-1.47464041	-4.81376061
H	1.22928332	-4.55592574	-3.50739683	H	-1.69594736	-2.29335780	2.34603890
H	1.18315424	-5.70374978	-2.16253457	H	-2.52499154	-2.32215408	3.91189434
H	1.90026686	-2.71422306	-2.00868692	H	-2.29432718	-3.83158897	3.01766238
H	-0.23428828	-2.48640202	-0.73336818	H	-4.00015860	-1.43646080	2.16432197
H	-0.58891644	-4.19590759	-1.01510383	H	-5.98982084	-2.92512060	2.59449637
H	-0.48848205	-3.07756916	-2.38213075	H	-4.90220773	-4.21101608	3.13219899
H	3.32413561	-1.39858350	3.65706857	H	-5.00449325	-2.70019240	4.04723852
H	5.03485107	-1.20801346	4.08827418	H	-4.87419721	2.72713232	3.77809866
H	4.22345882	-2.74742019	4.39118863	H	-4.23849617	1.64147937	5.02570163
H	4.81307899	-1.47371018	1.66623948	H	-3.58762229	3.28142567	4.85700490
H	6.44931915	-3.33734262	1.33569123	H	-3.30509348	1.02024573	2.79459744
H	6.03577443	-3.99211079	2.92708101	H	-0.88682486	1.01054442	3.44482501
H	6.82691754	-2.41319042	2.79653842	H	-1.25121979	2.13026470	4.77320981
H	7.52344593	1.60277151	0.54524806	H	-1.97892813	0.52095994	4.75140637
H	7.55011900	1.15862717	2.25745845	H	-1.57425662	3.50270193	-2.39655587
H	7.42779153	2.86071134	1.78556930	H	-2.77360168	4.32806733	-3.40411597
H	5.30850185	0.69791036	1.28049050	H	-1.76474675	5.27036218	-2.29823726

H	-3.89294099	3.19743869	-1.55358675	H	-3.88865119	6.25652209	-1.23548904
H	-5.17607792	5.20218787	-0.64608105	H	-4.85547643	5.32101853	-2.38508267

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