

**Use of Thio and Seleno Germanones as Ligands:
Silver(I) Halide Complexes with Ge=E→Ag-I (E = S,
Se) Moieties and Chalcogen Dependent
Argentophilic Interaction**

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Table S1. Crystal data and structure refinement parameters for compounds 3-6.

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empirical formula	C ₂₁ H ₂₈ GeN ₂ S	C ₂₁ H ₂₈ GeN ₂ Se	C ₄₂ H ₅₆ Ag ₂ Ge ₂ I ₂ N ₄ S ₂	C ₄₂ H ₅₆ Ag ₂ Ge ₂ I ₂ N ₄ Se ₂
fw	413.13	460.02	1295.81	1389.59
temperature, K	100(2)	100(2)	298(2)	100(2)
Wavelength, Å	0.71073	0.71073	0.71073	0.71073
cryst syst	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic
space group	<i>P2₁2₁2₁</i>	<i>P2₁2₁2₁</i>	<i>Pbca</i>	<i>P2₁/n</i>
a, Å	8.7901(18)	8.8178(11)	12.4060(19)	12.6196(17)
b, Å	11.461(2)	11.6655(14)	18.128(3)	13.5552(18)
c, Å	20.172(4)	20.231(3)	21.255(3)	13.8275(19)
β , deg	----	----	----	95.258(2)
volume, Å ³	2032.2(7)	2081.0(5)	4780.2(13)	2355.4(6)
Z	4	4	4	2
density (cald), Mg/m ³	1.350	1.468	1.801	1.959
absorption coefficient, mm ⁻¹	1.616	3.227	3.464	4.972
F(000)	864	936	2528	1336

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crystal size, mm ³	0.45 x 0.41 x 0.32	0.55 x 0.42 x 0.22	0.35 x 0.27 x 0.15	0.31 x 0.21 x 0.19
θ range for data collection, deg	2.04 to 25.00	2.01 to 24.99	2.21 to 25.00	2.09 to 24.99
limiting indices	-10 \leq h \leq 9, -13 \leq k \leq 10, -23 \leq l \leq 19	-10 \leq h \leq 8, -11 \leq k \leq 13, -23 \leq l \leq 24	-13 \leq h \leq 14, -21 \leq k \leq 21, -23 \leq l \leq 25	-14 \leq h \leq 14, -12 \leq k \leq 16, -16 \leq l \leq 16
no of reflns collected	5751	10896	23765	12128
no of indep reflns	3154 [$R_{\text{(int)}} = 0.0223$]	3662 [$R_{\text{(int)}} = 0.0264$]	4204 [$R_{\text{(int)}} = 0.0599$]	4134 [$R_{\text{(int)}} = 0.0327$]
max. and min. transmission	0.596 and 0.488	0.173 and 0.025	0.314 and 0.094	0.389 and 0.295
refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
no of data / restraints / parameters	3154 / 0 / 232	3662 / 0 / 232	4203 / 0 / 250	4129 / 0 / 250
goodness-of-fit on F^2	1.018	1.039	1.083	1.049
final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0221$, $wR_2 = 0.0557$	$R_1 = 0.0212$, $wR_2 = 0.0493$	$R_1 = 0.0523$, $wR_2 = 0.1292$	$R_1 = 0.0286$, $wR_2 = 0.0693$
R indices (all data)	$R_1 = 0.0253$, $wR_2 = 0.0563$	$R_1 = 0.0226$, $wR_2 = 0.0499$	$R_1 = 0.0773$, $wR_2 = 0.1516$	$R_1 = 0.0356$, $wR_2 = 0.0717$
Largest diff. peak and hole, e. \AA^{-3}	0.314 and -0.254	0.374 and -0.205	1.138 and -0.459	0.753 and -0.419
Flack parameter	0.010(9)	0.002(8)	---	---

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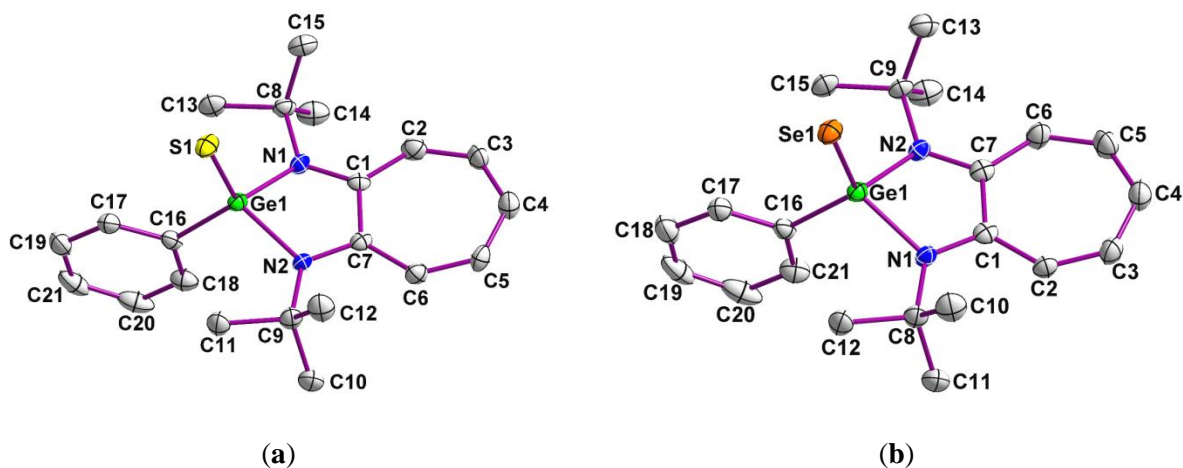


Figure S1. (a) Molecular structure of compound **3**. Thermal ellipsoids are drawn at the 30% probability level. All hydrogen atoms are omitted for clarity. Selected bond lengths (\AA) and angles (deg): Ge1-N1 1.918(2), Ge1-N2 1.902(2), Ge1-C16 1.941(3), Ge1-S1 2.102(7); N2-Ge1-N1 84.40(9), N2-Ge1-S1 116.36(7), N1-Ge1-S1 115.57(6), C16-Ge1-S1 116.53(8). (b) Molecular structure of compound **4**. Thermal ellipsoids are drawn at the 30% probability level. All hydrogen atoms are omitted for clarity. Selected bond lengths (\AA) and angles (deg): Ge1-N1 1.912(2), Ge1-N2 1.916(2), Ge1-C16 1.946(2), Ge1-Se1 2.235(4); N1-Ge1-N2 84.61(8), N1-Ge1-Se1 116.02(6), N2-Ge1-Se1 115.09(6), C16-Ge1-Se1 117.02(8).

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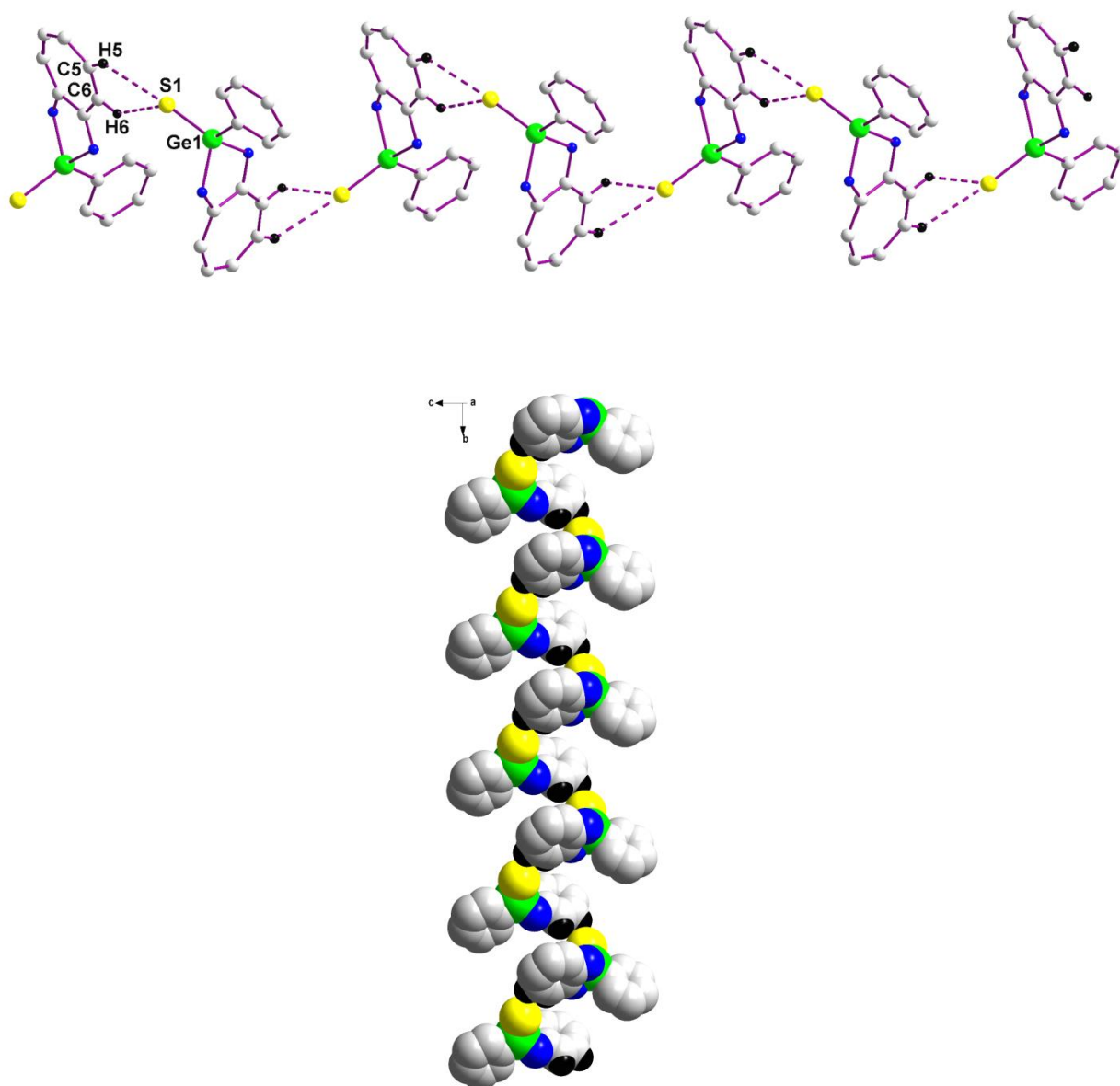


Figure S2. Helix formation in compound **3** via C-H...S interactions.

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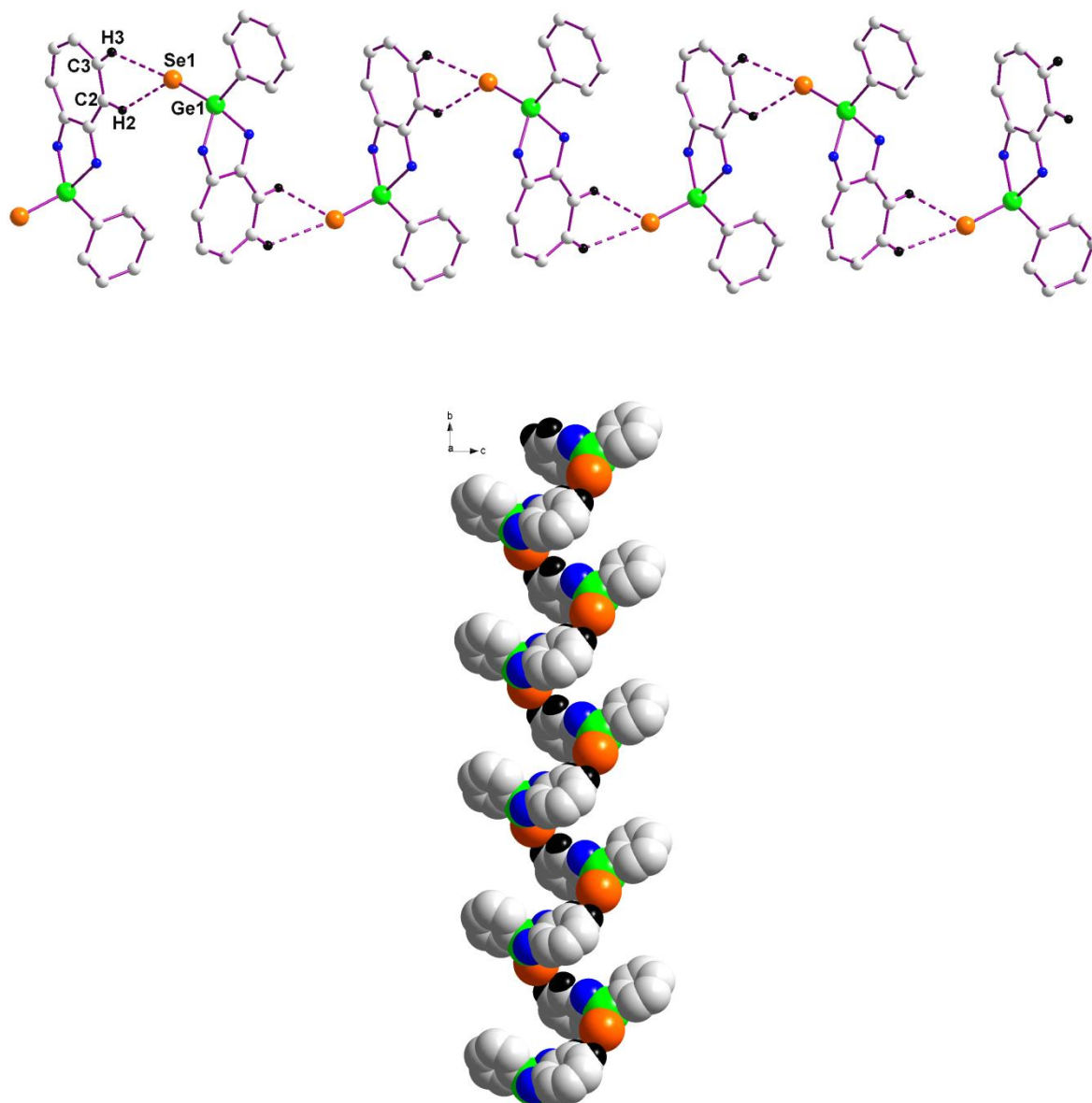


Figure S3. Helix formation in compound **4** via C-H...Se interactions.

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Table S2. Metric parameters for the weak C-H...E interactions in compounds **3** (E = S) and **4** (E = Se).

	Interactions	Distances (Å)			Angle (°)	
Compound	D-H...A ^a	D-H	H...A	D...A	D-H...A	Symmetry
3	C5-H5...S1	0.930	2.941	3.634	132.49	x, -2+y, z
	C6-H6...S1	0.930	2.915	3.631	134.86	x, -2+y, z
4	C2-H2...Se1	0.931	2.997	3.692	132.69	1-x, -0.5+y, 0.5-z
	C3-H3...Se1	0.929	2.944	3.652	134.13	1-x, -0.5+y, 0.5-z

^aD = donor; A = acceptor.

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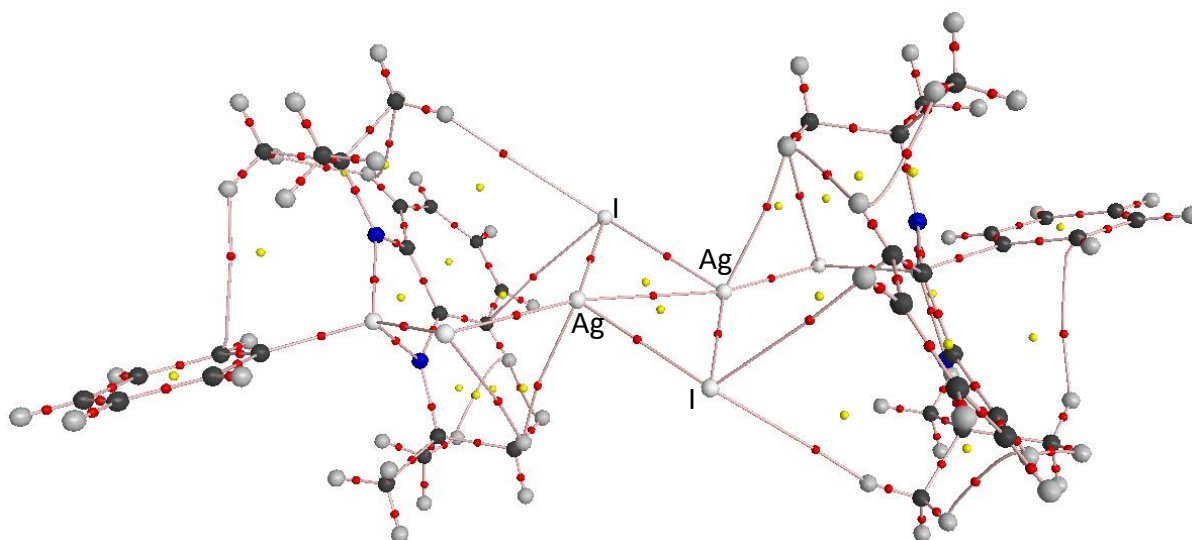


Figure S4. Representation of bond critical point between two silver atoms in compound 6.

Complete list of authors for reference 10

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