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Electronic Supplementary Information for New Journal of Chemistry

2,6-Dihalo-9-selenabicyclo[3.3.1]nonanes and Their Complexes with Selenium Dihalides: Synthesis and Structural Characterisation

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Table S1. Crystal data and structure refinement parameters for compounds **1-3**.

Compound	**1**	**2**	**3**
Empirical formula	$C_8H_{12}Cl_2Se$	$C_8H_{12}Br_2Se$	$C_{16}H_{24}Cl_6Se_3$
Formula weight	258.04	346.96	665.93
Crystal colour, habit	colorless prism	colorless prism	pink prism
Crystal size (mm)	$0.43 \times 0.28 \times 0.19$	$0.40 \times 0.30 \times 0.05$	$0.42 \times 0.10 \times 0.10$
Temperature (K)	100(2)	100(2)	100(2)
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	*Pnma*	C2/c	$P2_1/n$
a (Å)	15.5132(15)	12.724(1)	7.5401(5)
b (Å)	7.6193(8)	10.1559(8)	11.0902(7)
c (Å)	7.9082(8)	7.6780(6)	12.9721(8)
b (°)	90.0	95.932(2)	90.3850(15)
V (Å^3)	934.75(16)	986.89(13)	1084.72(12)
$Z(Z')$	4(0.5)	4(0.5)	2(0.5)
$F(000)$	512	656	648
D_{calc} (g cm^{-1})	1.834	2.335	2.039
Linear absorption, m (cm^{-1})	45.21	118.39	58.26
Absorption correction	multi-scan	multi-scan	multi-scan
T_{min}/T_{max}	0.239/0.428	0.088/ 0.589	0.193/0.594
Scan type	ω	ω	ω
q Range (°)	2.63−29.50	2.57−29.00	2.42-29.00
Completeness of dataset (%)	99.9	99.5	99.9
Reflections measured	5930	3672	7145
Independent reflections [R_{int}]	1402 [0.0336]	1309 [0.0234]	2890 [0.0397]
Observed reflections [$I > 2\sigma(I)$]	1191	1135	2473
Parameters	91	51	115
Final $R(F_{hkl})$: R_1	0.0273	0.0260	0.0317
wR_2	0.0664	0.0690	0.0858
GOF	1.020	1.009	0.962
Δr_{max}, Δr_{min} (e Å^{-3})	0.629; -0.485	0.821, -0.677	1.139; -0.973

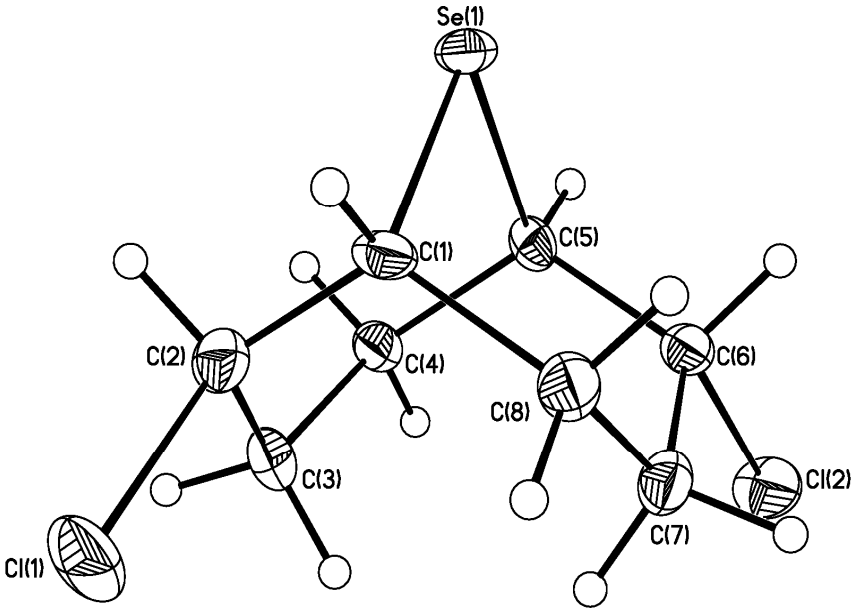


Fig. S1. X-ray crystal structure of compound **1**

Fig. S2. Crystals of compound **1**

Table S2. Crystal data and structure refinement for compound **1**.

Empirical formula	$C_8H_{12}Cl_2Se$	
Formula weight	258.04	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorombic	
Space group	P n m a	
Unit cell dimensions	a = 15.5132(15) Å	α= 90°.
	b = 7.6193(8) Å	β= 90°.
	c = 7.9082(8) Å	γ = 90°.
Volume	934.75(16) $Å^3$	
Z	4	
Density (calculated)	1.834 Mg/m^3	
Absorption coefficient	4.521 mm^{-1}	
F(000)	512	
Crystal size	0.43 x 0.28 x 0.19 mm^3	
Theta range for data collection	2.63 to 29.58°.	
Index ranges	-13<=h<=21, -10<=k<=10, -10<=l<=10	
Reflections collected	5930	
Independent reflections	1402 [R(int) = 0.0336]	
Completeness to theta = 29.58°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.428 and 0.239	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1402 / 0 / 91	
Goodness-of-fit on F^2	1.020	
Final R indices for 1191 refl. with [I>2sigma(I)]	R1 = 0.0273, wR2 = 0.0632	
R indices (all data)	R1 = 0.0374, wR2 = 0.0664	
Largest diff. peak and hole	0.629 and -0.485 $e.Å^{-3}$	

Table S3. Atomic coordinates ($x\ 10^4$) and equivalent isotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	7780(1)	2500	3566(1)	18(1)
Cl(2)	8213(1)	2500	-2048(1)	30(1)
Cl(1)	10665(1)	2500	4013(1)	38(1)
C(1)	8947(2)	1552(6)	3671(5)	17(1)
C(6)	8142(3)	1890(6)	153(5)	18(1)
C(7)	8934(3)	739(6)	473(6)	21(1)
C(8)	9052(3)	141(6)	2305(6)	20(1)
C(5)	8000(3)	3459(6)	1291(5)	16(1)
C(2)	9559(3)	3109(6)	3655(5)	21(1)
C(3)	9594(3)	4246(6)	2058(6)	22(1)
C(4)	8715(3)	4825(6)	1394(6)	18(1)

Table S4. Bond lengths [Å] and angles [°] for compound **1**.

Se(1)-C(1)	1.952(4)
Se(1)-C(5)	1.971(4)
Cl(2)-C(6)	1.805(4)
Cl(1)-C(2)	1.801(4)
C(1)-C(2)	1.519(6)
C(1)-C(8)	1.533(6)
C(1)-H(1A)	0.9600
C(6)-C(5)	1.512(6)
C(6)-C(7)	1.531(6)
C(6)-H(6A)	0.9600
C(7)-C(8)	1.530(6)
C(7)-H(7A)	0.9599
C(7)-H(7B)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9599
C(5)-C(4)	1.523(6)
C(5)-H(5A)	0.9600
C(2)-C(3)	1.533(6)
C(2)-H(2A)	0.9600
C(3)-C(4)	1.526(6)
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(4)-H(4A)	0.9601
C(4)-H(4B)	0.9599
C(1)-Se(1)-C(5)	90.85(17)
C(2)-C(1)-C(8)	118.4(3)
C(2)-C(1)-Se(1)	106.8(3)
C(8)-C(1)-Se(1)	109.2(3)
C(2)-C(1)-H(1A)	107.3
C(8)-C(1)-H(1A)	107.3
Se(1)-C(1)-H(1A)	107.3
C(5)-C(6)-C(7)	118.1(3)
C(5)-C(6)-Cl(2)	112.3(3)
C(7)-C(6)-Cl(2)	104.9(3)
C(5)-C(6)-H(6A)	107.0
C(7)-C(6)-H(6A)	107.0
Cl(2)-C(6)-H(6A)	107.0

C(8)-C(7)-C(6)	115.0(4)
C(8)-C(7)-H(7A)	108.7
C(6)-C(7)-H(7A)	108.5
C(8)-C(7)-H(7B)	108.6
C(6)-C(7)-H(7B)	108.1
H(7A)-C(7)-H(7B)	107.7
C(7)-C(8)-C(1)	116.5(4)
C(7)-C(8)-H(8A)	108.2
C(1)-C(8)-H(8A)	108.2
C(7)-C(8)-H(8B)	108.3
C(1)-C(8)-H(8B)	108.0
H(8A)-C(8)-H(8B)	107.3
C(6)-C(5)-C(4)	117.8(4)
C(6)-C(5)-Se(1)	106.0(3)
C(4)-C(5)-Se(1)	109.3(3)
C(6)-C(5)-H(5A)	107.9
C(4)-C(5)-H(5A)	107.6
Se(1)-C(5)-H(5A)	107.9
C(1)-C(2)-C(3)	118.1(3)
C(1)-C(2)-Cl(1)	113.1(3)
C(3)-C(2)-Cl(1)	104.0(3)
C(1)-C(2)-H(2A)	107.1
C(3)-C(2)-H(2A)	106.9
Cl(1)-C(2)-H(2A)	107.1
C(4)-C(3)-C(2)	114.6(4)
C(4)-C(3)-H(3A)	109.1
C(2)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3B)	108.5
C(2)-C(3)-H(3B)	108.3
H(3A)-C(3)-H(3B)	107.7
C(5)-C(4)-C(3)	118.1(4)
C(5)-C(4)-H(4A)	108.3
C(3)-C(4)-H(4A)	108.1
C(5)-C(4)-H(4B)	107.1
C(3)-C(4)-H(4B)	107.7
H(4A)-C(4)-H(4B)	107.1

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	15(1)	23(1)	15(1)	0	5(1)	0
Cl(2)	25(1)	52(1)	13(1)	0	-2(1)	0
Cl(1)	16(1)	64(1)	33(1)	0	-9(1)	0
C(1)	10(2)	25(2)	15(2)	2(2)	2(2)	1(2)
C(6)	15(2)	26(2)	13(2)	0(2)	0(2)	-3(2)
C(7)	20(2)	24(2)	19(2)	-7(2)	-3(2)	2(2)
C(8)	18(2)	18(2)	24(2)	-4(2)	-1(2)	2(2)
C(5)	12(2)	18(2)	16(2)	2(2)	-4(2)	0(2)
C(2)	19(2)	28(2)	16(2)	-3(2)	-2(2)	2(2)
C(3)	17(2)	24(2)	24(2)	-3(2)	-3(2)	-7(2)
C(4)	16(2)	23(2)	17(2)	0(2)	1(2)	-4(2)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **1**.

	x	y	z	U(eq)
H(1A)	9009	982	4747	20
H(6A)	7645	1149	269	21
H(7A)	9438	1378	130	25
H(7B)	8891	-281	-234	25
H(8A)	8644	-778	2528	24
H(8B)	9618	-357	2417	24
H(5A)	7486	4045	921	19
H(2A)	9391	3865	4569	25
H(3A)	9888	3603	1189	26
H(3B)	9929	5274	2303	26
H(4A)	8516	5780	2084	22
H(4B)	8797	5279	273	22

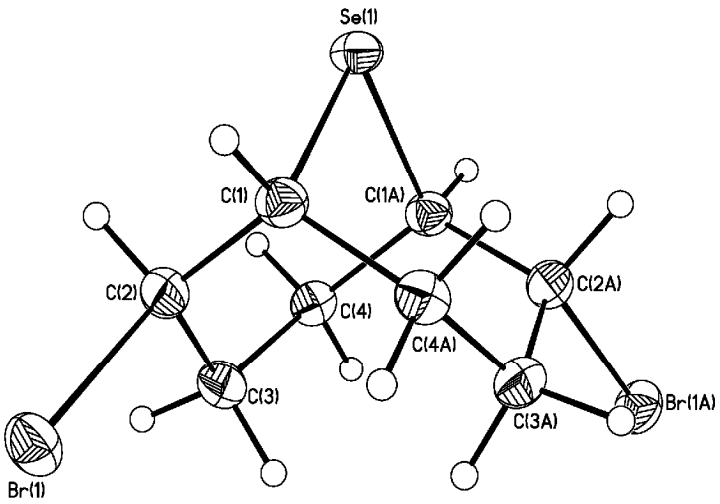


Fig. S3. X-ray crystal structure of compound **2**

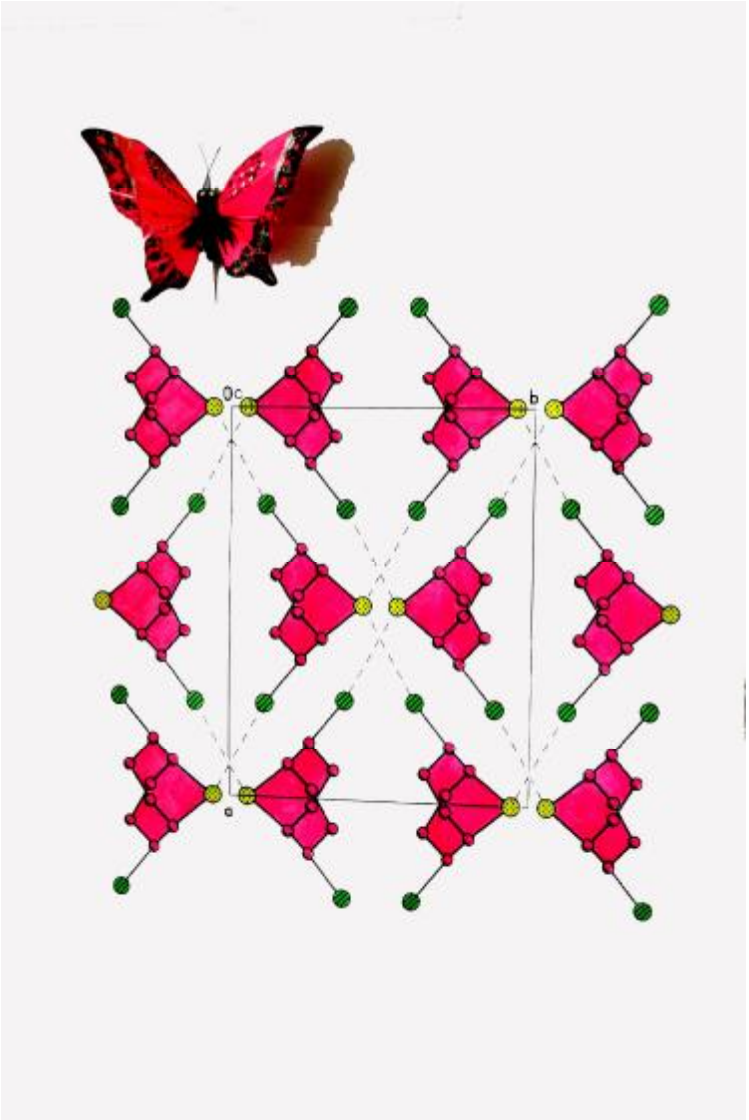


Fig. S4. Molecular packing in the crystal of compound **2**.

Table S7. Crystal data and structure refinement for compound **2**.

Empirical formula	$C_8H_{12}Br_2Se$	
Formula weight	346.96	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 12.7243(10) Å	α= 90°.
	b = 10.1559(8) Å	β= 95.9320(17)°.
	c = 7.6780(6) Å	γ = 90°.
Volume	986.89(13) $Å^3$	
Z	4	
Density (calculated)	2.335 Mg/m^3	
Absorption coefficient	11.839 mm^{-1}	
F(000)	656	
Crystal size	0.40 x 0.30 x 0.05 mm^3	
Theta range for data collection	2.57 to 28.99°.	
Index ranges	-17<=h<=17, -11<=k<=13, -10<=l<=10	
Reflections collected	3672	
Independent reflections	1309 [R(int) = 0.0234]	
Completeness to theta = 28.99°	99.5 %	
Absorption correction	Num	
Max. and min. transmission	0.589 and 0.088	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1309 / 0 / 51	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0260, wR2 = 0.0661	
R indices (all data)	R1 = 0.0317, wR2 = 0.0690	
Largest diff. peak and hole	0.821 and -0.677 $e.Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (E^2x 10^3) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	5000	4420(1)	2500	21(1)
Br(1)	7547(1)	1173(1)	2343(1)	26(1)
C(1)	5882(2)	3053(3)	1546(3)	20(1)
C(2)	6428(2)	2355(3)	3139(4)	21(1)
C(3)	5747(2)	1522(3)	4243(4)	23(1)
C(4)	4786(2)	2249(3)	4838(3)	21(1)

Table S9. Bond lengths [Å] and angles [°] for compound **2**.

Se(1)-C(1)	1.974(3)
Se(1)-C(1)#1	1.974(3)
Br(1)-C(2)	2.006(3)
C(1)-C(2)	1.518(4)
C(1)-C(4)#1	1.527(4)
C(1)-H(1A)	1.0000
C(2)-C(3)	1.528(4)
C(2)-H(2A)	1.0000
C(3)-C(4)	1.537(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(1)#1	1.527(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(1)-Se(1)-C(1)#1	90.56(15)
C(2)-C(1)-C(4)#1	119.1(2)
C(2)-C(1)-Se(1)	105.05(17)
C(4)#1-C(1)-Se(1)	109.70(17)
C(2)-C(1)-H(1A)	107.5
C(4)#1-C(1)-H(1A)	107.5
Se(1)-C(1)-H(1A)	107.5
C(1)-C(2)-C(3)	117.9(2)
C(1)-C(2)-Br(1)	108.28(18)
C(3)-C(2)-Br(1)	107.38(18)
C(1)-C(2)-H(2A)	107.6
C(3)-C(2)-H(2A)	107.6
Br(1)-C(2)-H(2A)	107.6
C(2)-C(3)-C(4)	114.4(2)
C(2)-C(3)-H(3A)	108.7
C(4)-C(3)-H(3A)	108.7
C(2)-C(3)-H(3B)	108.7
C(4)-C(3)-H(3B)	108.7
H(3A)-C(3)-H(3B)	107.6
C(1)#1-C(4)-C(3)	116.9(2)
C(1)#1-C(4)-H(4A)	108.1
C(3)-C(4)-H(4A)	108.1
C(1)#1-C(4)-H(4B)	108.1
C(3)-C(4)-H(4B)	108.1
H(4A)-C(4)-H(4B)	107.3

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

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	22(1)	15(1)	25(1)	0	5(1)	0
Br(1)	23(1)	27(1)	28(1)	-2(1)	3(1)	6(1)
C(1)	20(1)	18(1)	23(1)	1(1)	4(1)	0(1)
C(2)	19(1)	20(1)	24(1)	-2(1)	2(1)	2(1)
C(3)	24(1)	20(1)	24(1)	4(1)	1(1)	2(1)
C(4)	23(1)	20(1)	22(1)	0(1)	3(1)	-2(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2**.

	x	y	z	U(eq)
H(1A)	6440	3512	948	24
H(2A)	6789	3040	3922	26
H(3A)	6193	1207	5293	28
H(3B)	5494	739	3555	28
H(4A)	4322	1589	5319	26
H(4B)	5041	2848	5808	26

Table S12. Torsion angles [°] for compound **2**.

C(1)#1-Se(1)-C(1)-C(2)	-65.53(16)
C(1)#1-Se(1)-C(1)-C(4)#1	63.59(16)
C(4)#1-C(1)-C(2)-C(3)	-54.9(3)
Se(1)-C(1)-C(2)-C(3)	68.4(3)
C(4)#1-C(1)-C(2)-Br(1)	67.1(2)
Se(1)-C(1)-C(2)-Br(1)	-169.56(12)
C(1)-C(2)-C(3)-C(4)	-52.6(3)
Br(1)-C(2)-C(3)-C(4)	-175.12(19)
C(2)-C(3)-C(4)-C(1)#1	46.2(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

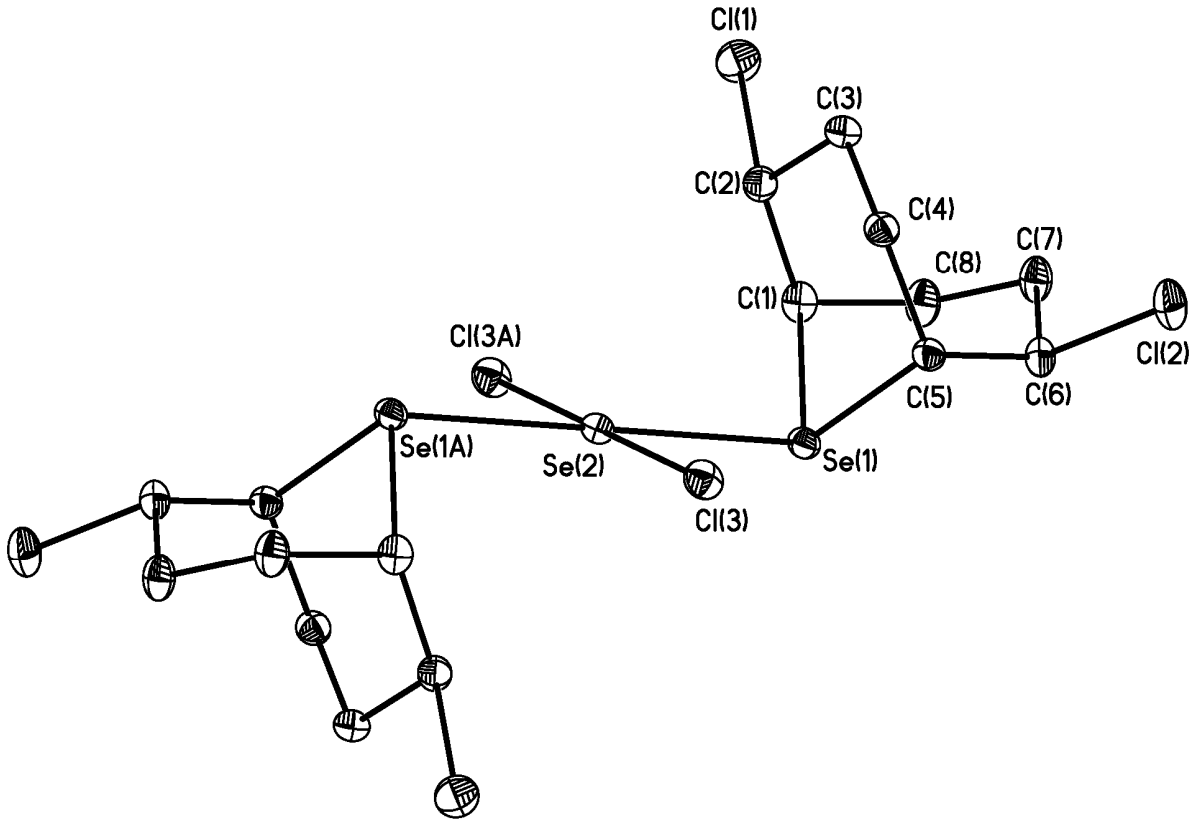


Fig. 5S. X-ray crystal structure of complex **3**.

Table S13. Crystal data and structure refinement for complex **3**.

Empirical formula	$C_{16}H_{24}Cl_6Se_3$	
Formula weight	665.93	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 7.5401(5) Å	α= 90°.
	b = 11.0902(7) Å	β= 90.3850(15)°.
	c = 12.9721(8) Å	γ = 90°.
Volume	1084.72(12) $Å^3$	
Z	2	
Density (calculated)	2.039 Mg/m^3	
Absorption coefficient	5.826 mm^{-1}	
F(000)	648	
Crystal size	0.42 x 0.10 x 0.10 mm^3	
Theta range for data collection	2.42 to 29.00°.	
Index ranges	-10<=h<=9, -14<=k<=15, -17<=l<=12	
Reflections collected	7145	
Independent reflections	2890 [R(int) = 0.0324]	
Completeness to theta = 29.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.594 and 0.193	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2890 / 0 / 115	
Goodness-of-fit on F^2	0.962	
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0812	
R indices (all data)	R1 = 0.0400, wR2 = 0.0858	
Largest diff. peak and hole	1.139 and -0.973 $e.Å^{-3}$	

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for complex **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	8051(1)	9192(1)	733(1)	13(1)
Se(2)	5000	10000	0	13(1)
Cl(1)	5372(1)	5853(1)	1925(1)	23(1)
Cl(2)	12018(1)	6768(1)	-703(1)	21(1)
Cl(3)	6367(1)	10317(1)	-1663(1)	18(1)
C(1)	7431(3)	7811(3)	1618(2)	15(1)
C(2)	6137(4)	7007(2)	1032(2)	15(1)
C(3)	6786(4)	6384(2)	54(2)	16(1)
C(4)	7665(3)	7230(2)	-729(2)	14(1)
C(5)	9067(3)	8093(2)	-311(2)	13(1)
C(6)	10718(3)	7585(3)	239(2)	15(1)
C(7)	10439(4)	6752(3)	1165(2)	18(1)
C(8)	9199(3)	7269(3)	1995(2)	18(1)

Table S15. Bond lengths [Å] and angles [°] for complex **3**.

Se(1)-C(1)	1.973(3)
Se(1)-C(5)	1.979(3)
Se(1)-Se(2)	2.6403(3)
Se(2)-Cl(3)#1	2.4228(7)
Se(2)-Cl(3)	2.4228(7)
Se(2)-Se(1)#1	2.6403(3)
Cl(1)-C(2)	1.823(3)
Cl(2)-C(6)	1.813(3)
C(1)-C(2)	1.522(4)
C(1)-C(8)	1.538(4)
C(1)-H(1A)	1.0000
C(2)-C(3)	1.528(4)
C(2)-H(2A)	1.0000
C(3)-C(4)	1.537(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.523(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.538(4)
C(5)-H(5A)	1.0000
C(6)-C(7)	1.531(4)
C(6)-H(6A)	1.0000
C(7)-C(8)	1.541(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(1)-Se(1)-C(5)	90.88(11)
C(1)-Se(1)-Se(2)	105.29(8)
C(5)-Se(1)-Se(2)	107.64(8)
Cl(3)#1-Se(2)-Cl(3)	180.00(3)
Cl(3)#1-Se(2)-Se(1)	90.298(18)
Cl(3)-Se(2)-Se(1)	89.702(18)
Cl(3)#1-Se(2)-Se(1)#1	89.702(18)
Cl(3)-Se(2)-Se(1)#1	90.298(18)
Se(1)-Se(2)-Se(1)#1	180.0
C(2)-C(1)-C(8)	118.8(2)
C(2)-C(1)-Se(1)	108.49(18)
C(8)-C(1)-Se(1)	106.23(18)
C(2)-C(1)-H(1A)	107.6
C(8)-C(1)-H(1A)	107.6
Se(1)-C(1)-H(1A)	107.6

C(1)-C(2)-C(3)	118.2(2)
C(1)-C(2)-Cl(1)	107.34(19)
C(3)-C(2)-Cl(1)	108.33(19)
C(1)-C(2)-H(2A)	107.5
C(3)-C(2)-H(2A)	107.5
Cl(1)-C(2)-H(2A)	107.5
C(2)-C(3)-C(4)	114.5(2)
C(2)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3A)	108.6
C(2)-C(3)-H(3B)	108.6
C(4)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.6
C(5)-C(4)-C(3)	116.8(2)
C(5)-C(4)-H(4A)	108.1
C(3)-C(4)-H(4A)	108.1
C(5)-C(4)-H(4B)	108.1
C(3)-C(4)-H(4B)	108.1
H(4A)-C(4)-H(4B)	107.3
C(4)-C(5)-C(6)	119.5(2)
C(4)-C(5)-Se(1)	111.05(17)
C(6)-C(5)-Se(1)	102.94(18)
C(4)-C(5)-H(5A)	107.6
C(6)-C(5)-H(5A)	107.6
Se(1)-C(5)-H(5A)	107.6
C(7)-C(6)-C(5)	118.1(2)
C(7)-C(6)-Cl(2)	107.78(19)
C(5)-C(6)-Cl(2)	108.03(19)
C(7)-C(6)-H(6A)	107.5
C(5)-C(6)-H(6A)	107.5
Cl(2)-C(6)-H(6A)	107.5
C(6)-C(7)-C(8)	114.2(2)
C(6)-C(7)-H(7A)	108.7
C(8)-C(7)-H(7A)	108.7
C(6)-C(7)-H(7B)	108.7
C(8)-C(7)-H(7B)	108.7
H(7A)-C(7)-H(7B)	107.6
C(1)-C(8)-C(7)	116.9(2)
C(1)-C(8)-H(8A)	108.1
C(7)-C(8)-H(8A)	108.1
C(1)-C(8)-H(8B)	108.1
C(7)-C(8)-H(8B)	108.1
H(8A)-C(8)-H(8B)	107.3

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

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	14(1)	11(1)	15(1)	-1(1)	-2(1)	0(1)
Se(2)	14(1)	10(1)	14(1)	-1(1)	0(1)	0(1)
Cl(1)	25(1)	20(1)	23(1)	7(1)	6(1)	-2(1)
Cl(2)	19(1)	25(1)	19(1)	3(1)	5(1)	7(1)
Cl(3)	21(1)	17(1)	16(1)	-1(1)	2(1)	0(1)
C(1)	16(1)	19(1)	11(1)	2(1)	0(1)	1(1)
C(2)	15(1)	14(1)	16(1)	3(1)	1(1)	0(1)
C(3)	17(1)	12(1)	18(1)	-2(1)	0(1)	-1(1)
C(4)	15(1)	14(1)	14(1)	-2(1)	-2(1)	0(1)
C(5)	14(1)	11(1)	15(1)	1(1)	1(1)	0(1)
C(6)	13(1)	17(1)	16(1)	-1(1)	1(1)	3(1)
C(7)	15(1)	23(2)	15(1)	4(1)	0(1)	5(1)
C(8)	15(1)	24(2)	15(1)	4(1)	-2(1)	4(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for complex **3**.

	x	y	z	U(eq)
H(1A)	6799	8135	2235	18
H(2A)	5088	7512	837	18
H(3A)	5765	5981	-285	19
H(3B)	7648	5750	252	19
H(4A)	8218	6729	-1270	17
H(4B)	6722	7715	-1065	17
H(5A)	9485	8599	-900	16
H(6A)	11446	8285	480	18
H(7A)	11606	6579	1486	21
H(7B)	9942	5978	916	21
H(8A)	8929	6618	2491	22
H(8B)	9854	7903	2377	22

Table S18. Torsion angles [°] for complex **3**.

C(1)-Se(1)-Se(2)-Cl(3)#1	40.21(9)
C(5)-Se(1)-Se(2)-Cl(3)#1	136.16(8)
C(1)-Se(1)-Se(2)-Cl(3)	-139.79(9)
C(5)-Se(1)-Se(2)-Cl(3)	-43.84(8)
C(5)-Se(1)-C(1)-C(2)	-61.14(19)
Se(2)-Se(1)-C(1)-C(2)	47.42(18)
C(5)-Se(1)-C(1)-C(8)	67.59(19)
Se(2)-Se(1)-C(1)-C(8)	176.16(16)
C(8)-C(1)-C(2)-C(3)	-56.9(3)
Se(1)-C(1)-C(2)-C(3)	64.4(3)
C(8)-C(1)-C(2)-Cl(1)	65.9(3)
Se(1)-C(1)-C(2)-Cl(1)	-172.82(12)
C(1)-C(2)-C(3)-C(4)	-51.4(3)
Cl(1)-C(2)-C(3)-C(4)	-173.62(19)
C(2)-C(3)-C(4)-C(5)	48.3(3)
C(3)-C(4)-C(5)-C(6)	58.9(3)
C(3)-C(4)-C(5)-Se(1)	-60.7(3)
C(1)-Se(1)-C(5)-C(4)	61.0(2)
Se(2)-Se(1)-C(5)-C(4)	-45.4(2)
C(1)-Se(1)-C(5)-C(6)	-68.04(18)
Se(2)-Se(1)-C(5)-C(6)	-174.40(14)
C(4)-C(5)-C(6)-C(7)	-55.9(3)
Se(1)-C(5)-C(6)-C(7)	67.6(3)
C(4)-C(5)-C(6)-Cl(2)	66.6(3)
Se(1)-C(5)-C(6)-Cl(2)	-169.83(13)
C(5)-C(6)-C(7)-C(8)	-51.7(3)
Cl(2)-C(6)-C(7)-C(8)	-174.3(2)
C(2)-C(1)-C(8)-C(7)	59.7(3)
Se(1)-C(1)-C(8)-C(7)	-62.8(3)
C(6)-C(7)-C(8)-C(1)	47.7(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z

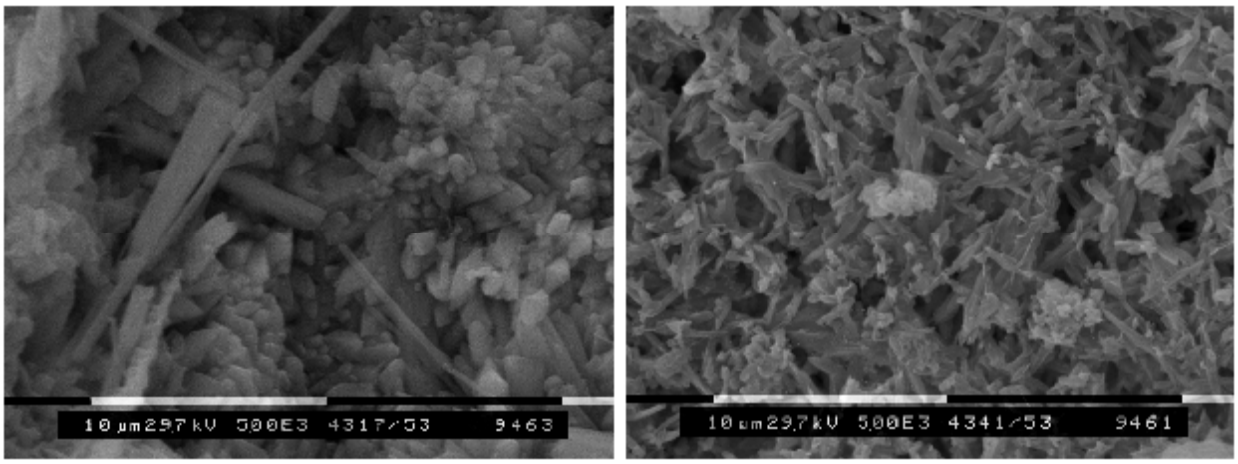
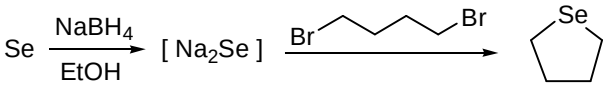


Fig. S6. SEM images of complexes **3** (left) and **4** (right).

Synthesis of tetrahydroselenophene (5).



5

Sodium borohydride (2.88 g, 76 mmol) was added portionwise to a mixture of selenium (3 g, 38 mmol) and degassed ethanol (100 mL) at room temperature under argon. Disappearance of selenium and discoloration was observed. A solution of 1,4-dibromobutane (8.21 g, 38 mmol) in ethanol (35 mL) was added dropwise for 20 min. The mixture was refluxed for 2 h and allowed to cool to room temperature. The mixture was diluted with degassed water (200 mL) and extracted with ether (4 x 30 mL). The organic phase was washed with water and dried over Na_2SO_4. Slow evaporation of ether on rotary evaporator gives the crude product, with was distilled under reduced pressure to afford pure compound **5** (4.36 g, 85% yield), bp 58-60 ºC (55 mm Hg). The spectral characteristics of compound **5** correspond to the literature data (A. L. Esteban and E. Diez, *J. Magn. Res.*, 1979, **36**, 113).