Electronic Supplementary Material (ESI) for New Journal of Chemistry.
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Table 1 Crystal data and structure refinement for 2.

Identification code	1
Empirical formula	$C_8H_{12}Br_4Se$
Formula weight	506.76
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	7.5472(14)
b/Å	7.8647(15)
c/Å	11.259(2)
α/°	77.095(3)
β/°	84.024(3)
γ/°	79.049(3)
Volume/Å^3	638.2(2)
Z	2
ρ_{calc}g/cm^3	2.6369
μ/mm^{-1}	15.420
F(000)	466.2
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.4 to 50
Index ranges	$-10 \leq h \leq 10$, $-10 \leq k \leq 10$, $-15 \leq l \leq 15$
Reflections collected	9185
Independent reflections	2206 [R_{int} = 0.0468, R_{sigma} = 0.0670]
Data/restraints/parameters	2206/0/117
Goodness-of-fit on F^2	1.231
Final R indexes [I>=2σ (I)]	R_1 = 0.0843, wR_2 = 0.2644
Final R indexes [all data]	R_1 = 0.1059, wR_2 = 0.2999
Largest diff. peak/hole / e Å^{-3}	2.53/-2.07

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br(1)	967.8(13)	7286.8(13)	4555.4(11)	40.2(6)
Br(2)	1464.3(13)	7828.8(14)	2166.1(11)	41.3(6)
Br(3)	5232.6(16)	9815.9(14)	6839.9(13)	63.3(7)
Br(4)	3243.6(15)	2265.5(14)	9666.5(12)	55.6(6)

Se(1)	450.8(13)	6837.3(15)	6834.4(11)	45.6(6)
C(1)	2021.1(19)	8347.7(19)	7265.5(19)	37(3)
C(2)	1984.5(19)	7937.2(19)	8628.8(19)	52(4)
C(3)	2712.5(19)	6008.3(19)	9275.4(19)	33(3)
C(4)	2035.7(19)	4596.7(19)	8800.9(19)	36(3)
C(5)	2194.7(19)	4677.9(19)	7467.9(19)	37(3)
C(6)	4058.5(19)	4721.3(19)	6771.6(19)	30(3)
C(7)	5003.9(19)	6291.2(19)	6829.9(19)	42(3)
C(8)	3814.6(19)	8122.1(19)	6527.4(19)	38(3)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	28.2(9)	45.4(9)	48.0(11)	-2.2(6)	-11.7(7)	-11.2(7)
Br(2)	29.6(8)	54.2(10)	43.2(10)	-3.4(6)	-4.4(6)	-18.8(7)
Br(3)	94.2(15)	46.2(10)	61.3(12)	-37.5(9)	-1.2(10)	-16.0(8)
Br(4)	70.7(12)	43.2(10)	52.8(11)	-16.2(8)	-13.6(9)	0.2(7)
Se(1)	21.1(8)	68.9(12)	42.8(10)	1.7(7)	-3.2(6)	-10.8(8)
C(1)	42(6)	36(6)	32(7)	5(5)	5(6)	-16(5)
C(2)	48(7)	41(7)	72(10)	-2(6)	8(7)	-33(7)
C(3)	28(6)	54(7)	20(6)	-14(5)	5(5)	-13(5)
C(4)	32(6)	49(7)	28(7)	-7(5)	-1(5)	-13(6)
C(5)	28(6)	29(6)	59(9)	-10(5)	-16(6)	-6(6)
C(6)	42(6)	32(6)	19(6)	-7(5)	0(5)	-12(5)
C(7)	21(6)	40(6)	67(10)	-2(5)	-1(6)	-19(6)
C(8)	53(7)	24(6)	40(8)	-11(5)	-2(6)	-11(5)

Table 4 Bond Lengths for 2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br(1)	Br(2)	2.6263(17)	C(1)	C(8)	1.515(2)
Br(1)	Se(1)	2.5099(17)	C(2)	C(3)	1.551(2)
Br(3)	C(8)	1.968(2)	C(3)	C(4)	1.522(3)
Br(4)	C(4)	1.9733(18)	C(4)	C(5)	1.481(3)
Se(1)	C(1)	1.991(2)	C(5)	C(6)	1.540(2)
Se(1)	C(5)	1.9825(17)	C(6)	C(7)	1.555(2)
C(1)	C(2)	1.495(3)	C(7)	C(8)	1.5325(19)

Table 5 Bond Angles for 2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Se(1)	Br(1)	Br(2)	178.71(5)	C(5)	C(4)	Br(4)	110.07(12)
C(1)	Se(1)	Br(1)	103.12(8)	C(5)	C(4)	C(3)	118.51(14)
C(5)	Se(1)	Br(1)	104.52(8)	C(4)	C(5)	Se(1)	103.01(11)
C(5)	Se(1)	C(1)	90.54(8)	C(6)	C(5)	Se(1)	110.89(11)
C(2)	C(1)	Se(1)	105.79(11)	C(6)	C(5)	C(4)	119.21(15)
C(8)	C(1)	Se(1)	108.99(14)	C(7)	C(6)	C(5)	116.40(15)
C(8)	C(1)	C(2)	119.65(14)	C(8)	C(7)	C(6)	114.68(13)
C(3)	C(2)	C(1)	117.75(16)	C(1)	C(8)	Br(3)	108.01(14)
C(4)	C(3)	C(2)	114.45(15)	C(7)	C(8)	Br(3)	106.26(12)
C(3)	C(4)	Br(4)	107.63(12)	C(7)	C(8)	C(1)	115.82(13)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2.

Atom	*x*	*y*	*z*	U(eq)
H(1)	1433.6(19)	9582.6(19)	7011.2(19)	45(4)
H(2a)	2676.2(19)	8709.9(19)	8871.5(19)	62(5)
H(2b)	742.9(19)	8243.5(19)	8937.7(19)	62(5)
H(3a)	4023.1(19)	5809.4(19)	9180.4(19)	39(3)
H(3b)	2369.3(19)	5872.9(19)	10141.5(19)	39(3)
H(4)	745.7(19)	4682.1(19)	9055.9(19)	43(3)
H(5)	1738.6(19)	3657.9(19)	7326.7(19)	45(4)
H(6a)	4854.4(19)	3626.1(19)	7088.6(19)	36(3)
H(6b)	3919.5(19)	4746.5(19)	5920.7(19)	36(3)
H(7a)	5412.2(19)	6112.6(19)	7644.5(19)	50(4)
H(7b)	6065.7(19)	6273.0(19)	6264.6(19)	50(4)
H(8)	3587.4(19)	8401.4(19)	5657.9(19)	46(4)

1.

Table 1 Crystal data and structure refinement for 3.

Identification code	1
Empirical formula	$C_8H_{12}Br_2I_2Se$
Formula weight	600.76
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.503(3)
b/Å	10.107(4)
c/Å	18.967(7)
α/°	90
β/°	99.587(5)
γ/°	90
Volume/Å^3	1418.2(9)
Z	4
ρ_{calc}g/cm^3	2.8134
μ/mm^{-1}	12.598
F(000)	1075.0
Crystal size/mm^3	0.5 × 0.3 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.58 to 58
Index ranges	$-10 \leq h \leq 10$, $-13 \leq k \leq 13$, $-25 \leq l \leq 25$
Reflections collected	15260
Independent reflections	3749 [R_{int} = 0.0368, R_{sigma} = 0.0329]
Data/restraints/parameters	3749/0/117
Goodness-of-fit on F^2	1.010
Final R indexes [I>=2σ (I)]	R_1 = 0.0310, wR_2 = 0.0675
Final R indexes [all data]	R_1 = 0.0470, wR_2 = 0.0745
Largest diff. peak/hole / e Å^{-3}	1.54/-1.69

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
I(1)	1466.2(4)	6689.1(3)	4779.50(14)	45.44(9)
I(2)	-2034.2(5)	6935.1(4)	3953.12(17)	58.66(11)
Br(1)	9289.1(7)	9685.4(6)	6025.3(4)	71.45(18)
Br(2)	3278.9(7)	7300.9(7)	7770.2(3)	68.08(17)

Se(1)	5035.2(6)	6390.5(5)	5578.0(2)	47.80(12)
C(1)	6056(6)	8202(4)	5647(2)	42.4(9)
C(2)	4775(6)	9166(4)	5921(2)	44.2(10)
C(3)	4264(6)	8890(4)	6655(2)	46.1(10)
C(4)	3695(6)	7475(5)	6765(2)	42.7(9)
C(5)	4975(6)	6390(4)	6615(2)	43.5(10)
C(6)	6931(6)	6419(5)	6995(3)	47.4(10)
C(7)	8076(6)	7631(5)	6859(2)	46.5(10)
C(8)	7946(6)	8014(5)	6075(2)	45.2(10)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I(1)	55.30(18)	42.67(16)	36.08(15)	1.62(12)	0.99(12)	-3.92(11)
I(2)	59.1(2)	67.2(2)	44.19(18)	-5.05(16)	-7.37(14)	3.94(15)
Br(1)	58.5(3)	65.1(4)	94.5(4)	-11.2(3)	23.7(3)	17.2(3)
Br(2)	54.5(3)	105.3(5)	45.9(3)	4.0(3)	12.5(2)	9.8(3)
Se(1)	52.8(3)	42.8(2)	44.4(2)	9.34(19)	-1.8(2)	-14.24(19)
C(1)	51(2)	42(2)	34(2)	5.8(19)	6.1(18)	1.1(17)
C(2)	48(2)	37(2)	45(2)	6.4(18)	0.3(19)	-0.9(18)
C(3)	49(2)	43(2)	46(2)	9.0(19)	7.9(19)	-10(2)
C(4)	35(2)	54(3)	37(2)	-1.4(18)	0.3(17)	-1.9(19)
C(5)	46(2)	37(2)	46(2)	-6.3(18)	0.7(19)	2.9(18)
C(6)	45(2)	46(3)	49(3)	3.3(19)	0.2(19)	11(2)
C(7)	36(2)	56(3)	46(2)	-3.1(19)	1.8(18)	5(2)
C(8)	42(2)	46(3)	49(3)	1.2(18)	13(2)	2(2)

Table 4 Bond Lengths for 3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I(1)	I(2)	2.8364(9)	C(1)	C(8)	1.524(6)
I(1)	Se(1)	2.8644(10)	C(2)	C(3)	1.529(6)
Br(1)	C(8)	1.977(5)	C(3)	C(4)	1.518(6)
Br(2)	C(4)	1.991(4)	C(4)	C(5)	1.515(6)
Se(1)	C(1)	1.980(4)	C(5)	C(6)	1.524(6)
Se(1)	C(5)	1.976(5)	C(6)	C(7)	1.542(6)
C(1)	C(2)	1.519(6)	C(7)	C(8)	1.525(6)

Table 5 Bond Angles for 3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Se(1)	I(1)	I(2)	178.156(16)	C(5)	C(4)	Br(2)	108.7(3)
C(1)	Se(1)	I(1)	104.76(13)	C(5)	C(4)	C(3)	117.0(4)
C(5)	Se(1)	I(1)	110.61(13)	C(4)	C(5)	Se(1)	107.8(3)
C(5)	Se(1)	C(1)	90.38(18)	C(6)	C(5)	Se(1)	106.9(3)
C(2)	C(1)	Se(1)	110.8(3)	C(6)	C(5)	C(4)	119.3(4)
C(8)	C(1)	Se(1)	103.6(3)	C(7)	C(6)	C(5)	117.1(4)
C(8)	C(1)	C(2)	118.9(4)	C(8)	C(7)	C(6)	114.7(4)
C(3)	C(2)	C(1)	117.6(4)	C(1)	C(8)	Br(1)	107.7(3)
C(4)	C(3)	C(2)	114.6(4)	C(7)	C(8)	Br(1)	108.2(3)
C(3)	C(4)	Br(2)	107.9(3)	C(7)	C(8)	C(1)	116.9(4)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3.

Atom	*x*	*y*	*z*	U(eq)
H(1)	6188(6)	8482(4)	5164(2)	50.9(11)
H(2a)	5316(6)	10039(4)	5935(2)	53.0(12)
H(2b)	3669(6)	9197(4)	5574(2)	53.0(12)
H(3a)	5291(6)	9103(4)	7020(2)	55.3(12)
H(3b)	3282(6)	9476(4)	6722(2)	55.3(12)
H(4)	2535(6)	7326(5)	6451(2)	51.3(11)
H(5)	4454(6)	5545(4)	6731(2)	52.2(11)
H(6a)	6930(6)	6359(5)	7505(3)	56.9(13)
H(6b)	7530(6)	5634(5)	6856(3)	56.9(13)
H(7a)	7699(6)	8381(5)	7118(2)	55.8(12)
H(7b)	9331(6)	7450(5)	7054(2)	55.8(12)
H(8)	8552(6)	7325(5)	5838(2)	54.2(12)

Table 1 Crystal data and structure refinement for 4.

Identification code	1
Empirical formula	$C_8H_{12}I_2Se$
Formula weight	440.95
Temperature/K	143.15
Crystal system	monoclinic
Space group	C2/c
a/Å	13.3579(7)
b/Å	10.2925(5)
c/Å	7.8592(4)
α/°	90
β/°	96.667(1)
γ/°	90
Volume/Å^3	1073.22(9)
Z	4
ρ_{calc}g/cm^3	2.7289
μ/mm^{-1}	9.194
F(000)	796.8
Crystal size/mm^3	0.4 × 0.4 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5 to 58
Index ranges	$-19 \leq h \leq 19$, $-14 \leq k \leq 14$, $-10 \leq l \leq 11$
Reflections collected	6364
Independent reflections	1409 [R_{int} = 0.0278, R_{sigma} = 0.0225]
Data/restraints/parameters	1409/0/50
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0186, wR_2 = 0.0464
Final R indexes [all data]	R_1 = 0.0197, wR_2 = 0.0469
Largest diff. peak/hole / e Å^{-3}	0.74/-1.09

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
I(1)	2446.86(12)	8867.56(17)	7714.9(2)	27.12(7)
Se(1)	5000	5587.6(3)	7500	19.80(9)
C(1)	4822.1(17)	7736(2)	9787(3)	19.2(4)
C(2)	4170.6(17)	6937(2)	8442(3)	17.2(4)

C(3)	3634.7(16)	7628(2)	6889(3)	18.1(4)
C(4)	4267.3(18)	8446(2)	5804(3)	20.7(4)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for 41. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I(1)	21.24(10)	31.15(11)	29.12(10)	9.28(6)	3.55(7)	-2.62(6)
Se(1)	19.43(16)	11.83(15)	29.51(17)	-0	8.68(12)	0
C(1)	19(1)	22.4(10)	16.8(9)	0.2(8)	4.2(8)	-1.2(8)
C(2)	15.5(9)	15.9(9)	20.9(10)	-0.2(8)	5.1(8)	-0.4(7)
C(3)	14.9(10)	18.7(10)	20.8(10)	3.0(8)	2.7(8)	-3.1(8)
C(4)	19.4(11)	21.8(11)	20.5(10)	3.1(8)	1.5(8)	3.1(8)

Table 4 Bond Lengths for 4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I(1)	C(3)	2.192(2)	C(1)	C(4)[1]	1.537(3)
Se(1)	C(2)[1]	1.974(2)	C(2)	C(3)	1.518(3)
Se(1)	C(2)	1.974(2)	C(3)	C(4)	1.522(3)
C(1)	C(2)	1.529(3)			

[1]1-X,+Y,3/2-Z

Table 5 Bond Angles for 41.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(2)	Se(1)	C(2)[1]	90.54(13)	C(2)	C(3)	I(1)	108.93(14)
C(4)[1]	C(1)	C(2)	116.98(18)	C(4)	C(3)	I(1)	108.14(14)
C(1)	C(2)	Se(1)[1]	109.79(15)	C(4)	C(3)	C(2)	117.95(19)
C(3)	C(2)	Se(1)[1]	105.11(14)	C(3)	C(4)	C(1)[1]	114.61(18)
C(3)	C(2)	C(1)	118.79(18)				

[1]1-X,+Y,3/2-Z

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4.

Atom	*x*	*y*	*z*	U(eq)
H(1a)	4385.1(17)	8391(2)	10254(3)	23.1(5)

H(1b)	5072.3(17)	7149(2)	10740(3)	23.1(5)
H(2)	3646.0(17)	6485(2)	9035(3)	20.7(5)
H(3)	3294.9(16)	6945(2)	6122(3)	21.7(5)
H(4a)	4512.7(18)	9221(2)	6474(3)	24.8(5)
H(4b)	3830.3(18)	8754(2)	4780(3)	24.8(5)

Table 1 Crystal data and structure refinement for 5.

Identification code	1
Empirical formula	$C_8H_{12}I_4Se$
Formula weight	694.76
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.7674(8)
b/Å	10.2154(10)
c/Å	18.8296(19)
α/°	90
β/°	101.236(2)
γ/°	90
Volume/Å^3	1465.4(3)
Z	4
ρ_{calc}g/cm^3	3.1488
μ/mm^{-1}	10.953
F(000)	1217.7
Crystal size/mm^3	0.5 × 0.3 × 0.3
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.42 to 61.2
Index ranges	$-11 \leq h \leq 11$, $-14 \leq k \leq 14$, $-26 \leq l \leq 26$
Reflections collected	17427
Independent reflections	4505 [R_{int} = 0.0384, R_{sigma} = 0.0360]
Data/restraints/parameters	4505/0/117
Goodness-of-fit on F^2	1.007
Final R indexes [I>=2σ (I)]	R_1 = 0.0271, wR_2 = 0.0475
Final R indexes [all data]	R_1 = 0.0410, wR_2 = 0.0512
Largest diff. peak/hole / e Å^{-3}	1.34/-1.53

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
I(1)	3522.9(3)	1637.4(2)	200.54(13)	21.88(6)
I(2)	6994.9(3)	1932.9(3)	1017.07(14)	26.66(7)
I(3)	1739.0(3)	2373.8(3)	-2866.11(14)	28.14(7)
I(4)	-4387.9(3)	4664.3(3)	-1025.19(15)	29.02(7)

Se(1)	28.2(5)	1322.3(4)	-587.7(2)	24.23(9)
C(1)	-1032(5)	3097(4)	-641(2)	21.5(8)
C(2)	176(5)	4101(4)	-888(2)	20.0(7)
C(3)	633(5)	3891(3)	-1636(2)	20.0(8)
C(4)	1252(5)	2514(4)	-1755.7(19)	19.4(7)
C(5)	75(5)	1385(3)	-1633(2)	20.7(8)
C(6)	-1854(5)	1375(4)	-2029(2)	22.5(8)
C(7)	-3002(5)	2519(4)	-1882(2)	22.0(8)
C(8)	-2869(5)	2885(4)	-1091(2)	20.8(8)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 5. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I(1)	25.27(13)	20.27(12)	18.54(12)	-0.89(10)	0.40(9)	2.47(9)
I(2)	24.92(13)	31.72(15)	20.54(13)	0.29(11)	-2.5(1)	-1.8(1)
I(3)	24.62(13)	36.48(15)	23.87(13)	-0.69(11)	6.08(10)	-5.53(11)
I(4)	25.21(14)	28.16(14)	36.19(15)	0.58(11)	12.16(11)	-6.39(11)
Se(1)	24.1(2)	22.2(2)	23.4(2)	-4.97(15)	-2.68(16)	9.62(15)
C(1)	27(2)	20.0(19)	17.4(18)	-3.3(15)	4.1(15)	-0.2(14)
C(2)	20.2(18)	19.3(18)	20.3(18)	-1.4(14)	3.1(14)	-2.1(14)
C(3)	22.2(19)	16.5(17)	21.3(19)	-1.0(14)	4.6(15)	3.7(14)
C(4)	21.7(19)	23.2(19)	13.1(16)	0.8(15)	2.5(14)	-0.1(14)
C(5)	21.6(19)	15.2(17)	24.3(19)	2.9(14)	2.0(15)	-1.7(14)
C(6)	20.9(19)	22(2)	23(2)	-2.9(15)	0.5(15)	-1.1(15)
C(7)	17.3(18)	25(2)	20.9(19)	-0.3(15)	-2.2(15)	-3.3(15)
C(8)	19.5(19)	20.8(19)	22.5(19)	-0.7(15)	4.7(15)	1.3(15)

Table 4 Bond Lengths for 5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I(1)	I(2)	2.8482(4)	C(1)	C(8)	1.526(5)
I(1)	Se(1)	2.8469(5)	C(2)	C(3)	1.534(5)
I(3)	C(4)	2.201(3)	C(3)	C(4)	1.517(5)
I(4)	C(8)	2.184(4)	C(4)	C(5)	1.517(5)
Se(1)	C(1)	1.985(4)	C(5)	C(6)	1.538(5)
Se(1)	C(5)	1.978(4)	C(6)	C(7)	1.527(5)
C(1)	C(2)	1.523(5)	C(7)	C(8)	1.521(5)

Table 5 Bond Angles for 5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Se(1)	I(1)	I(2)	178.740(13)	C(5)	C(4)	I(3)	108.4(2)
C(1)	Se(1)	I(1)	105.49(11)	C(5)	C(4)	C(3)	117.7(3)
C(5)	Se(1)	I(1)	108.34(11)	C(4)	C(5)	Se(1)	107.7(2)
C(5)	Se(1)	C(1)	90.46(15)	C(6)	C(5)	Se(1)	106.0(2)
C(2)	C(1)	Se(1)	110.9(3)	C(6)	C(5)	C(4)	119.4(3)
C(8)	C(1)	Se(1)	103.4(2)	C(7)	C(6)	C(5)	117.1(3)
C(8)	C(1)	C(2)	119.4(3)	C(8)	C(7)	C(6)	115.8(3)
C(3)	C(2)	C(1)	116.9(3)	C(1)	C(8)	I(4)	107.9(2)
C(4)	C(3)	C(2)	113.7(3)	C(7)	C(8)	I(4)	109.0(2)
C(3)	C(4)	I(3)	108.6(2)	C(7)	C(8)	C(1)	117.2(3)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5.

Atom	*x*	*y*	*z*	U(eq)
H(4)	2381(5)	2390(4)	-1425.3(19)	23.3(9)
H(2a)	-366(5)	4956(4)	-885(2)	24.0(9)
H(2b)	1264(5)	4122(4)	-533(2)	24.0(9)
H(5)	621(5)	574(3)	-1758(2)	24.8(9)
H(6a)	-1875(5)	1344(4)	-2545(2)	27(1)
H(6b)	-2389(5)	572(4)	-1901(2)	27(1)
H(3a)	-395(5)	4084(3)	-2004(2)	24.0(9)
H(3b)	1546(5)	4505(3)	-1697(2)	24.0(9)
H(8)	-3419(5)	2180(4)	-861(2)	25.0(9)
H(1)	-1163(5)	3339(4)	-151(2)	25.8(9)
H(7a)	-2694(5)	3280(4)	-2139(2)	26.4(9)
H(7b)	-4216(5)	2306(4)	-2084(2)	26.4(9)

Table 1 Crystal data and structure refinement for 6.

Identification code	1
Empirical formula	$C_8H_{12}Br_{6.5}Se$
Formula weight	706.52
Temperature/K	296.15
Crystal system	monoclinic
Space group	C2/m
a/Å	16.440(2)
b/Å	14.832(2)
c/Å	13.0060(19)
α/°	90
β/°	92.048(2)
γ/°	90
Volume/Å^3	3169.3(8)
Z	8
ρ_{calc}g/cm^3	2.9612
μ/mm^{-1}	18.730
F(000)	2560.8
Crystal size/mm^3	0.4 × 0.2 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.8 to 58
Index ranges	$-23 \leq h \leq 23$, $-21 \leq k \leq 21$, $-18 \leq l \leq 18$
Reflections collected	19170
Independent reflections	4359 [R_{int} = 0.0850, R_{sigma} = 0.0861]
Data/restraints/parameters	4359/0/150
Goodness-of-fit on F^2	0.991
Final R indexes [I>=2σ (I)]	R_1 = 0.0374, wR_2 = 0.0707
Final R indexes [all data]	R_1 = 0.0729, wR_2 = 0.0814
Largest diff. peak/hole / e Å^{-3}	1.91/-1.89

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Se(1)	7132.1(3)	2674.1(4)	3055.5(4)	16.45(13)
Br(2)	6346.9(4)	2366.8(4)	-340.4(4)	22.94(14)
Br(3)	7350.1(3)	1456.2(4)	4185.3(4)	17.74(13)
Br(6)	9295.0(5)	0	5109.7(6)	21.80(19)

Br(1)	4360.5(4)	2609.7(4)	3697.6(5)	26.49(15)
Br(7)	2214.1(6)	5000	8415.1(7)	28.4(2)
Br(8)	2851.6(5)	5000	10302.8(6)	23.2(2)
Br(9)	572.5(6)	5000	9481.2(6)	23.8(2)
Br(4)	7541.8(5)	0	5699.3(6)	21.00(19)
Br(5)	5697.0(6)	0	5235.4(8)	31.4(2)
Br(10)	3466.6(7)	5000	12075.6(8)	41.7(3)
C(7)	5376(4)	1573(4)	2417(4)	17.2(12)
C(2)	5804(3)	3723(4)	2464(4)	18.4(13)
C(5)	6785(3)	2051(4)	1746(4)	17.6(12)
C(1)	5981(3)	3014(4)	3291(4)	16.6(12)
C(6)	6183(4)	1294(4)	1950(4)	18.4(13)
C(4)	6524(3)	2858(4)	1050(4)	16.8(12)
C(8)	5457(3)	2179(4)	3360(4)	20.5(13)
C(3)	5776(4)	3383(4)	1339(4)	18.4(13)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 6. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Se(1)	18.4(3)	16.9(3)	13.9(3)	-1.4(2)	-1.5(2)	-1.5(2)
Br(2)	26.9(3)	29.4(4)	12.5(3)	-2.3(3)	-0.0(2)	-1.5(2)
Br(3)	19.3(3)	20.3(3)	13.5(3)	0.4(2)	-2.0(2)	-1.3(2)
Br(6)	30.5(5)	16.4(4)	18.6(4)	-0	3.0(4)	0
Br(1)	19.2(3)	36.4(4)	24.1(3)	3.9(3)	4.2(3)	-0.6(3)
Br(7)	37.7(6)	32.5(5)	15.2(4)	-0	5.1(4)	0
Br(8)	30.7(5)	20.3(5)	19.1(4)	-0	7.5(4)	0
Br(9)	36.3(5)	19.2(5)	15.3(4)	-0	-6.1(4)	0
Br(4)	26.1(5)	24.8(5)	11.9(4)	-0	-2.8(3)	0
Br(5)	27.1(5)	24.8(5)	42.9(6)	-0	9.4(4)	0
Br(10)	49.6(7)	52.4(7)	22.5(5)	-0	-4.8(5)	0
C(7)	27(3)	11(3)	14(3)	-3(2)	0(2)	1(2)
C(2)	16(3)	17(3)	22(3)	3(2)	2(2)	-1(2)
C(5)	22(3)	16(3)	15(3)	-3(2)	3(2)	-7(2)
C(1)	17(3)	14(3)	19(3)	3(2)	2(2)	-3(2)
C(6)	33(4)	17(3)	5(3)	0(3)	-1(2)	-6(2)
C(4)	22(3)	16(3)	13(3)	-6(2)	-1(2)	2(2)
C(8)	17(3)	28(4)	16(3)	2(3)	3(2)	1(2)
C(3)	25(3)	18(3)	12(3)	4(2)	1(2)	2(2)

Table 4 Bond Lengths for 6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Se(1)	Br(3)	2.3479(8)	Br(5)	Br(5)[3]	2.3510(19)
Se(1)	C(5)	2.003(5)	C(7)	C(6)	1.535(8)
Se(1)	C(1)	1.993(5)	C(7)	C(8)	1.523(8)
Br(2)	C(4)	1.962(5)	C(2)	C(1)	1.524(8)
Br(6)	Br(6)[1]	2.3456(18)	C(2)	C(3)	1.547(8)
Br(1)	C(8)	1.976(6)	C(5)	C(6)	1.526(8)
Br(7)	Br(8)	2.6347(13)	C(5)	C(4)	1.551(8)
Br(8)	Br(10)	2.4844(14)	C(1)	C(8)	1.512(8)
Br(9)	Br(9)[2]	2.3549(18)	C(4)	C(3)	1.514(8)

[1]2-X,+Y,1-Z; [2]-X,+Y,2-Z; [3]1-X,+Y,1-Z

Table 5 Bond Angles for 6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(5)	Se(1)	Br(3)	102.10(17)	C(8)	C(1)	Se(1)	110.4(4)
C(1)	Se(1)	Br(3)	102.90(16)	C(8)	C(1)	C(2)	120.8(5)
C(1)	Se(1)	C(5)	90.2(2)	C(5)	C(6)	C(7)	116.5(5)
Br(10)	Br(8)	Br(7)	179.43(5)	C(5)	C(4)	Br(2)	106.3(4)
C(8)	C(7)	C(6)	115.2(5)	C(3)	C(4)	Br(2)	108.9(4)
C(3)	C(2)	C(1)	116.1(5)	C(3)	C(4)	C(5)	117.5(5)
C(6)	C(5)	Se(1)	111.0(4)	C(7)	C(8)	Br(1)	108.4(4)
C(4)	C(5)	Se(1)	101.8(4)	C(1)	C(8)	Br(1)	105.9(4)
C(4)	C(5)	C(6)	120.1(5)	C(1)	C(8)	C(7)	118.0(5)
C(2)	C(1)	Se(1)	103.0(4)	C(4)	C(3)	C(2)	114.0(5)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6.

Atom	*x*	*y*	*z*	U(eq)
H(7a)	5047(4)	1882(4)	1893(4)	20.6(15)
H(7b)	5086(4)	1031(4)	2605(4)	20.6(15)
H(2a)	5284(3)	4002(4)	2599(4)	22.1(15)
H(2b)	6217(3)	4189(4)	2531(4)	22.1(15)
H(5)	7270(3)	1779(4)	1457(4)	21.2(15)
H(1)	5971(3)	3319(4)	3958(4)	19.9(14)
H(6a)	6449(4)	861(4)	2408(4)	22.1(15)
H(6b)	6059(4)	987(4)	1304(4)	22.1(15)
H(4)	6982(3)	3280(4)	1035(4)	20.2(15)

H(8)	5669(3)	1815(4)	3938(4)	24.6(16)
H(3a)	5301(4)	3001(4)	1233(4)	22.1(15)
H(3b)	5714(4)	3897(4)	882(4)	22.1(15)

Table 1 Crystal data and structure refinement for 7.

Identification code	1
Empirical formula	$C_{16}H_{24}Br_6Se_3$
Formula weight	932.67
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.660(3)
b/Å	11.291(4)
c/Å	13.427(5)
α/°	90
β/°	91.695(7)
γ/°	90
Volume/Å^3	1160.8(7)
Z	2
ρ_{calc}g/cm^3	2.6682
μ/mm^{-1}	15.080
F(000)	861.2
Crystal size/mm^3	0.4 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.72 to 49.98
Index ranges	$-10 \leq h \leq 7$, $-14 \leq k \leq 14$, $-11 \leq l \leq 17$
Reflections collected	4482
Independent reflections	1998 [R_{int} = 0.0797, R_{sigma} = 0.1728]
Data/restraints/parameters	1998/0/114
Goodness-of-fit on F^2	0.905
Final R indexes [I>=2σ (I)]	R_1 = 0.0540, wR_2 = 0.0966
Final R indexes [all data]	R_1 = 0.1050, wR_2 = 0.1115
Largest diff. peak/hole / e Å^{-3}	2.08/-2.03

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 7. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Br(1)	7028.2(19)	11757.8(13)	4247.5(11)	29.5(4)
Br(3)	1341.1(17)	15319.4(12)	3286.9(10)	24.5(4)
Br(2)	416.7(18)	10830.3(12)	6959.8(11)	29.7(4)
Se(2)	0	15000	5000	18.7(5)

Se(1)	3035.2(17)	14201.4(11)	5688(1)	18.9(3)
C(7)	1799(15)	11437(10)	5082(10)	18(3)
C(6)	2611(15)	12255(10)	4312(11)	22(3)
C(4)	5604(16)	12661(12)	5204(10)	21(3)
C(8)	1202(18)	12052(11)	6007(9)	26(4)
C(1)	2446(15)	12857(10)	6560(10)	17(3)
C(5)	4042(16)	13113(11)	4674(10)	24(3)
C(3)	5445(16)	11860(11)	6106(9)	22(3)
C(2)	4256(15)	12353(12)	6930(10)	23(3)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 7. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	23.8(8)	37.1(9)	28.0(9)	11.9(7)	7.7(6)	2.3(7)
Br(3)	23.8(7)	25.8(8)	24.0(8)	2.0(6)	3.6(6)	-1.5(7)
Br(2)	30.7(9)	27.4(8)	31.7(9)	-2.5(7)	9.6(7)	7.6(7)
Se(2)	17.9(10)	17.8(11)	20.3(11)	1.8(8)	1.5(8)	-0.7(8)
Se(1)	15.8(7)	17.7(7)	23.0(8)	1.7(6)	-1.4(5)	-1.2(6)
C(7)	11(7)	6(7)	38(9)	6(5)	4(6)	8(6)
C(6)	8(7)	15(8)	44(10)	-2(5)	8(6)	1(7)
C(4)	15(8)	29(9)	18(8)	-4(6)	2(6)	9(6)
C(8)	44(10)	16(8)	19(8)	-15(6)	9(7)	-11(6)
C(1)	11(7)	6(7)	35(9)	6(5)	7(6)	4(6)
C(5)	19(8)	16(8)	36(9)	-7(6)	6(6)	3(7)
C(3)	21(8)	19(8)	25(8)	0(6)	-2(6)	-2(7)
C(2)	16(8)	32(9)	22(9)	12(6)	10(6)	2(6)

Table 4 Bond Lengths for 7.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br(1)	C(4)	1.991(13)	C(7)	C(8)	1.507(17)
Br(3)	Se(2)	2.5721(15)	C(6)	C(5)	1.531(17)
Br(2)	C(8)	1.986(13)	C(4)	C(5)	1.465(16)
Se(2)	Se(1)	2.6353(15)	C(4)	C(3)	1.520(17)
Se(2)	Se(1)[1]	2.6353(15)	C(8)	C(1)	1.498(16)
Se(1)	C(1)	1.978(12)	C(1)	C(2)	1.565(16)
Se(1)	C(5)	2.006(13)	C(3)	C(2)	1.556(16)
C(7)	C(6)	1.531(16)			

[1]-X,3-Y,1-Z

Table 5 Bond Angles for 7.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Br(3)[1]	Se(2)	Br(3)	180.0	C(3)	C(4)	C(5)	120.7(11)
Se(1)[1]	Se(2)	Br(3)	90.58(4)	C(7)	C(8)	Br(2)	108.4(8)
Se(1)[1]	Se(2)	Br(3)[1]	89.42(4)	C(1)	C(8)	Br(2)	107.6(8)
Se(1)	Se(2)	Br(3)	89.42(4)	C(1)	C(8)	C(7)	119.0(11)
Se(1)	Se(2)	Br(3)[1]	90.58(4)	C(8)	C(1)	Se(1)	109.0(9)
Se(1)[1]	Se(2)	Se(1)	180.0	C(2)	C(1)	Se(1)	104.6(8)
C(1)	Se(1)	Se(2)[1]	104.8(3)	C(2)	C(1)	C(8)	118.8(11)
C(5)	Se(1)	Se(2)[1]	109.0(4)	C(6)	C(5)	Se(1)	108.5(8)
C(5)	Se(1)	C(1)	91.7(5)	C(4)	C(5)	Se(1)	102.0(9)
C(8)	C(7)	C(6)	114.7(10)	C(4)	C(5)	C(6)	120.0(11)
C(5)	C(6)	C(7)	118.0(12)	C(2)	C(3)	C(4)	114.5(10)
C(5)	C(4)	Br(1)	108.7(9)	C(3)	C(2)	C(1)	115.9(11)
C(3)	C(4)	Br(1)	105.5(8)				

[1]-X,3-Y,1-Z

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 7.

Atom	*x*	*y*	*z*	U(eq)
H(7a)	786(15)	11027(10)	4763(10)	22(4)
H(7b)	2668(15)	10825(10)	5279(10)	22(4)
H(6a)	3102(15)	11752(10)	3786(11)	27(4)
H(6b)	1658(15)	12728(10)	3997(11)	27(4)
H(4)	6311(16)	13364(12)	5423(10)	25(4)
H(8)	154(18)	12536(11)	5810(9)	32(4)
H(1)	1839(15)	13179(10)	7151(10)	21(4)
H(5)	4418(16)	13596(11)	4094(10)	29(4)
H(3a)	4977(16)	11085(11)	5881(9)	27(4)
H(3b)	6627(16)	11722(11)	6402(9)	27(4)
H(2a)	4899(15)	12990(12)	7291(10)	28(4)
H(2b)	4046(15)	11711(12)	7414(10)	28(4)