[I] Structure data of λ-$(BETS)_2GaBr_{2.0}Cl_{2.0}$ at room temperature.

Crystal data and experimental details of λ-$(BETS)_2GaBr_{2.0}Cl_{2.0}$ at room temperature(293K).

chemical formula	$C_{20}H_{16}S_8Se_8GaBr_{2.0}Cl_{2.0}$
temperature	293K
formula weight	1444.94
crystal color, habit	black, needle
crystal dimension / mm	0.10 × 0.10 × 0.70
a / Å	16.347(3)
b / Å	18.661(4)
c / Å	6.621(1)
α / °	98.40(2)
β / °	96.53(2)
γ / °	112.44(1)
V / $Å^3$	1814.8(7)
space group	$P\bar{1}$
Z	2
d_{calc} / g cm^{-3}	2.644
F_{000}	1342.00
μ(MoKα) / cm^{-1}	116.15
diffractometer	Rigaku AFC7R
radiation	MoKα(λ= 0.71069 Å)
scan type	2θ-ω
$2\theta_{max}$ / °	55.1
total reflection (unique)	9077 (8357)
No. observation (I>3.00σ(I))	3578
No. Variables	347
Corrections	Lorentz-polarization
	absorption (trans factors: 0.6888-0.6999)

structure solution	Direct methods (SHELXS86)
refinement	full-matrix least-squares
function minimized	$\sum \omega(\|Fo\| - \|Fc\|)^2$
least-squares weights	$\omega = \frac{1}{\sigma^2(Fo)} = \left[\sigma_c^2(Fo) + \frac{p^2}{4} Fo^2 \right]^{-1}$
R, *R*w	0.044, 0.028
goodnedd of fit	1.76
Maximum peak / $e^-/Å^3$	0.69
Minimum peak / $e^-/Å^3$	-0.75

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Se(1)	0.58611(9)	-0.01647(8)	-0.3142(2)	3.34(3)	1.0000
Se(2)	0.58830(9)	-0.07706(8)	0.1090(2)	3.13(3)	1.0000
Se(3)	0.73914(9)	0.16353(8)	-0.0736(2)	3.15(3)	1.0000
Se(4)	0.74753(9)	0.10634(8)	0.3532(2)	2.95(3)	1.0000
Se(5)	0.13278(9)	0.02545(8)	-0.1855(2)	2.97(3)	1.0000
Se(6)	0.12950(9)	-0.03198(8)	0.2424(2)	2.97(3)	1.0000
Se(7)	0.28661(9)	0.20628(8)	0.0554(2)	2.76(3)	1.0000
Se(8)	0.28315(9)	0.15153(8)	0.4888(2)	2.92(3)	1.0000
Ga(1)	0.20876(8)	0.46456(8)	0.8734(2)	2.83(3)	1.0000
Cl(1)	0.0884(1)	0.4673(1)	0.9971(3)	3.82(7)	1.404(8)
Cl(2)	0.3390(1)	0.5640(1)	1.0582(3)	4.50(5)	1.780(8)
Cl(3)	0.2153(2)	0.3490(1)	0.8910(4)	4.18(8)	1.295(8)
Cl(4)	0.1940(1)	0.4760(1)	0.5350(3)	3.88(6)	1.644(7)
S(1)	0.4490(2)	-0.1746(2)	-0.5602(5)	3.84(9)	1.0000
S(2)	0.4480(2)	-0.2423(2)	-0.0924(5)	3.81(9)	1.0000
S(3)	0.8605(3)	0.3336(2)	0.1211(5)	4.59(9)	1.0000
S(4)	0.8784(2)	0.2715(2)	0.5914(5)	3.93(9)	1.0000
S(5)	-0.0207(2)	-0.1270(2)	-0.4173(5)	4.21(9)	1.0000
S(6)	-0.0281(2)	-0.1905(2)	0.0498(5)	4.38(9)	1.0000
S(7)	0.4225(2)	0.3773(2)	0.2810(5)	3.25(8)	1.0000
S(8)	0.4236(2)	0.3153(2)	0.7200(5)	3.28(8)	1.0000
C(1)	0.6346(7)	0.0086(7)	-0.029(2)	2.4(3)	1.0000
C(2)	0.5093(8)	-0.1233(6)	-0.312(2)	2.7(3)	1.0000
C(3)	0.5112(8)	-0.1473(7)	-0.137(2)	2.7(3)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(4)	0.372(1)	-0.2641(8)	-0.507(2)	6.1(4)	1.0000
C(5)	0.397(1)	-0.2969(9)	-0.350(3)	7.8(5)	1.0000
C(6)	0.6971(7)	0.0804(6)	0.073(2)	2.4(3)	1.0000
C(7)	0.8107(7)	0.2372(7)	0.173(2)	2.4(3)	1.0000
C(8)	0.8162(7)	0.2140(6)	0.348(2)	2.0(3)	1.0000
C(9)	0.9292(8)	0.3904(7)	0.366(2)	3.0(3)	1.0000
C(10)	0.8890(8)	0.3678(7)	0.554(2)	3.4(3)	1.0000
C(11)	0.1774(7)	0.0518(6)	0.102(2)	2.2(3)	1.0000
C(12)	0.0470(7)	-0.0762(7)	-0.176(2)	2.4(3)	1.0000
C(13)	0.0436(7)	-0.0989(6)	0.006(2)	2.6(3)	1.0000
C(14)	-0.0815(10)	-0.2237(8)	-0.379(2)	5.7(4)	1.0000
C(15)	-0.049(1)	-0.2485(8)	-0.205(2)	5.8(5)	1.0000
C(16)	0.2417(7)	0.1237(6)	0.198(2)	2.0(3)	1.0000
C(17)	0.3625(7)	0.2795(6)	0.298(2)	1.9(3)	1.0000
C(18)	0.3589(7)	0.2575(7)	0.480(2)	2.4(3)	1.0000
C(19)	0.3868(7)	0.4206(7)	0.500(2)	3.7(3)	1.0000
C(20)	0.4279(8)	0.4142(6)	0.703(2)	3.4(3)	1.0000
H(1)	0.3200	-0.2537	-0.4638	6.5162	1.0000
H(2)	0.3448	-0.3031	-0.6366	6.5162	1.0000
H(3)	0.4427	-0.3137	-0.4147	7.8972	1.0000
H(4)	0.3482	-0.3457	-0.3548	7.8972	1.0000
H(5)	0.9870	0.3854	0.3803	3.4836	1.0000
H(6)	0.9450	0.4469	0.3709	3.4836	1.0000
H(7)	0.8303	0.3698	0.5340	3.7806	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(8)	0.9246	0.4075	0.6766	3.7806	1.0000
H(9)	-0.1427	-0.2290	-0.3621	6.1705	1.0000
H(10)	-0.0902	-0.2617	-0.5042	6.1705	1.0000
H(11)	0.0062	-0.2512	-0.2382	6.2497	1.0000
H(12)	-0.0908	-0.3024	-0.2126	6.2497	1.0000
H(13)	0.4003	0.4766	0.5013	3.8063	1.0000
H(14)	0.3216	0.3954	0.4884	3.8063	1.0000
H(15)	0.3980	0.4306	0.8115	4.0249	1.0000
H(16)	0.4894	0.4530	0.7364	4.0249	1.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Se(1)	0.0545(10)	0.0264(8)	0.0303(8)	0.0010(7)	0.0006(7)	0.0072(7)
Se(2)	0.0523(10)	0.0283(8)	0.0277(8)	0.0042(7)	0.0079(7)	0.0071(7)
Se(3)	0.0515(9)	0.0264(8)	0.0273(8)	0.0021(7)	-0.0002(7)	0.0059(7)
Se(4)	0.0494(9)	0.0274(8)	0.0271(8)	0.0071(7)	0.0044(7)	0.0066(7)
Se(5)	0.0473(9)	0.0278(8)	0.0258(8)	0.0020(7)	0.0061(7)	0.0071(6)
Se(6)	0.0459(9)	0.0263(8)	0.0275(8)	-0.0001(7)	0.0039(7)	0.0086(6)
Se(7)	0.0410(9)	0.0257(8)	0.0285(8)	0.0019(7)	0.0046(7)	0.0098(6)
Se(8)	0.0416(9)	0.0279(8)	0.0282(8)	-0.0010(7)	0.0050(7)	0.0089(6)
Ga(1)	0.0283(8)	0.0342(9)	0.0421(9)	0.0093(7)	0.0040(6)	0.0096(7)
Cl(1)	0.037(2)	0.072(2)	0.048(2)	0.030(1)	0.020(1)	0.017(1)
Cl(2)	0.033(1)	0.038(1)	0.073(2)	-0.0048(9)	-0.0088(10)	0.001(1)
Cl(3)	0.045(2)	0.034(2)	0.082(2)	0.013(1)	0.010(1)	0.023(1)
Cl(4)	0.055(2)	0.069(2)	0.037(1)	0.037(1)	0.014(1)	0.019(1)
S(1)	0.052(2)	0.036(2)	0.033(2)	-0.004(2)	-0.004(2)	0.004(2)
S(2)	0.055(2)	0.029(2)	0.042(2)	-0.004(2)	0.013(2)	0.008(2)
S(3)	0.078(3)	0.030(2)	0.039(2)	-0.007(2)	0.003(2)	0.010(2)
S(4)	0.062(3)	0.036(2)	0.031(2)	0.003(2)	-0.006(2)	0.003(2)
S(5)	0.058(3)	0.042(2)	0.033(2)	-0.003(2)	-0.007(2)	0.004(2)
S(6)	0.067(3)	0.031(2)	0.040(2)	-0.011(2)	0.014(2)	0.006(2)
S(7)	0.044(2)	0.026(2)	0.040(2)	-0.001(2)	0.007(2)	0.009(2)
S(8)	0.044(2)	0.034(2)	0.034(2)	0.006(2)	-0.003(2)	0.001(2)
C(1)	0.035(8)	0.036(8)	0.025(7)	0.015(7)	0.015(6)	0.010(6)
C(2)	0.037(8)	0.013(7)	0.044(9)	0.003(6)	0.009(7)	0.002(6)
C(3)	0.043(8)	0.028(8)	0.031(8)	0.014(7)	0.004(7)	0.006(7)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(4)	0.09(1)	0.04(1)	0.06(1)	-0.014(9)	0.010(9)	0.020(9)
C(5)	0.08(1)	0.05(1)	0.11(2)	-0.025(9)	-0.03(1)	0.03(1)
C(6)	0.033(7)	0.016(7)	0.036(8)	0.004(6)	0.011(6)	0.002(6)
C(7)	0.026(7)	0.026(8)	0.032(8)	0.007(6)	0.000(6)	-0.001(6)
C(8)	0.030(7)	0.018(7)	0.029(7)	0.009(6)	0.003(6)	0.010(6)
C(9)	0.036(8)	0.031(8)	0.029(7)	0.001(6)	-0.001(6)	-0.001(6)
C(10)	0.053(9)	0.047(9)	0.026(7)	0.020(7)	-0.003(6)	0.000(6)
C(11)	0.048(8)	0.020(7)	0.017(7)	0.016(6)	0.006(6)	0.003(6)
C(12)	0.031(7)	0.023(7)	0.036(8)	0.007(6)	0.014(6)	0.004(6)
C(13)	0.027(7)	0.016(7)	0.046(9)	0.000(6)	0.004(6)	0.005(6)
C(14)	0.09(1)	0.033(9)	0.06(1)	-0.011(8)	-0.003(9)	0.002(8)
C(15)	0.10(1)	0.034(10)	0.07(1)	0.007(9)	0.03(1)	0.003(9)
C(16)	0.042(8)	0.017(7)	0.024(7)	0.016(6)	0.008(6)	0.010(6)
C(17)	0.021(7)	0.020(7)	0.030(7)	0.002(5)	0.012(6)	0.010(6)
C(18)	0.024(7)	0.032(8)	0.035(8)	0.012(6)	0.005(6)	0.003(6)
C(19)	0.030(8)	0.035(8)	0.068(10)	0.007(6)	0.021(7)	0.001(7)
C(20)	0.047(9)	0.021(7)	0.051(9)	0.001(6)	0.021(7)	-0.002(6)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Se(1)	C(1)	1.88(1)	Se(1)	C(2)	1.91(1)
Se(2)	C(1)	1.91(1)	Se(2)	C(3)	1.90(1)
Se(3)	C(6)	1.90(1)	Se(3)	C(7)	1.90(1)
Se(4)	C(6)	1.85(1)	Se(4)	C(8)	1.90(1)
Se(5)	C(11)	1.88(1)	Se(5)	C(12)	1.90(1)
Se(6)	C(11)	1.89(1)	Se(6)	C(13)	1.89(1)
Se(7)	C(16)	1.88(1)	Se(7)	C(17)	1.90(1)
Se(8)	C(16)	1.89(1)	Se(8)	C(18)	1.90(1)
Ga(1)	Cl(1)	2.230(3)	Ga(1)	Cl(2)	2.281(2)
Ga(1)	Cl(3)	2.219(3)	Ga(1)	Cl(4)	2.276(2)
S(1)	C(2)	1.75(1)	S(1)	C(4)	1.78(1)
S(2)	C(3)	1.77(1)	S(2)	C(5)	1.78(2)
S(3)	C(7)	1.77(1)	S(3)	C(9)	1.79(1)
S(4)	C(8)	1.75(1)	S(4)	C(10)	1.80(1)
S(5)	C(12)	1.74(1)	S(5)	C(14)	1.77(1)
S(6)	C(13)	1.75(1)	S(6)	C(15)	1.79(1)
S(7)	C(17)	1.74(1)	S(7)	C(19)	1.82(1)
S(8)	C(18)	1.75(1)	S(8)	C(20)	1.84(1)
C(1)	C(6)	1.35(1)	C(2)	C(3)	1.30(1)
C(4)	C(5)	1.38(2)	C(7)	C(8)	1.30(1)
C(9)	C(10)	1.51(2)	C(11)	C(16)	1.35(1)
C(12)	C(13)	1.34(1)	C(14)	C(15)	1.42(2)
C(17)	C(18)	1.33(1)	C(19)	C(20)	1.48(2)

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
S(1)	H(1)	2.29	S(1)	H(2)	2.29
S(2)	H(3)	2.32	S(2)	H(4)	2.32
S(3)	H(5)	2.31	S(3)	H(6)	2.31
S(4)	H(7)	2.32	S(4)	H(8)	2.31
S(5)	H(9)	2.28	S(5)	H(10)	2.28
S(6)	H(11)	2.31	S(6)	H(12)	2.31
S(7)	H(13)	2.35	S(7)	H(14)	2.35
S(8)	H(15)	2.35	S(8)	H(16)	2.36
C(4)	H(1)	1.00	C(4)	H(2)	0.97
C(4)	H(3)	1.84	C(4)	H(4)	1.89
C(5)	H(1)	1.88	C(5)	H(2)	1.96
C(5)	H(3)	1.02	C(5)	H(4)	0.95
C(9)	H(5)	0.98	C(9)	H(6)	0.98
C(9)	H(7)	2.01	C(9)	H(8)	2.05
C(10)	H(5)	2.03	C(10)	H(6)	2.06
C(10)	H(7)	0.97	C(10)	H(8)	0.97
C(14)	H(9)	0.99	C(14)	H(10)	0.97
C(14)	H(11)	1.89	C(14)	H(12)	1.93
C(15)	H(9)	1.93	C(15)	H(10)	1.96
C(15)	H(11)	0.98	C(15)	H(12)	0.96
C(19)	H(13)	0.98	C(19)	H(14)	0.98
C(19)	H(15)	2.03	C(19)	H(16)	2.00
C(20)	H(13)	2.02	C(20)	H(14)	2.00
C(20)	H(15)	0.99	C(20)	H(16)	0.96

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Se(1)	C(2)	94.1(5)	C(1)	Se(2)	C(3)	93.0(5)
C(6)	Se(3)	C(7)	92.0(5)	C(6)	Se(4)	C(8)	93.5(5)
C(11)	Se(5)	C(12)	93.6(5)	C(11)	Se(6)	C(13)	93.4(5)
C(16)	Se(7)	C(17)	93.5(5)	C(16)	Se(8)	C(18)	92.8(5)
Cl(1)	Ga(1)	Cl(2)	111.87(10)	Cl(1)	Ga(1)	Cl(3)	108.5(1)
Cl(1)	Ga(1)	Cl(4)	109.25(9)	Cl(2)	Ga(1)	Cl(3)	108.97(10)
Cl(2)	Ga(1)	Cl(4)	109.31(9)	Cl(3)	Ga(1)	Cl(4)	108.9(1)
C(2)	S(1)	C(4)	101.6(6)	C(3)	S(2)	C(5)	101.4(6)
C(7)	S(3)	C(9)	102.5(5)	C(8)	S(4)	C(10)	100.0(5)
C(12)	S(5)	C(14)	104.1(6)	C(13)	S(6)	C(15)	98.7(6)
C(17)	S(7)	C(19)	95.4(5)	C(18)	S(8)	C(20)	102.6(6)
Se(1)	C(1)	Se(2)	114.0(6)	Se(1)	C(1)	C(6)	124.4(9)
Se(2)	C(1)	C(6)	121.6(9)	Se(1)	C(2)	S(1)	111.1(6)
Se(1)	C(2)	C(3)	118.5(9)	S(1)	C(2)	C(3)	130.4(10)
Se(2)	C(3)	S(2)	111.9(6)	Se(2)	C(3)	C(2)	120.4(9)
S(2)	C(3)	C(2)	127.6(10)	S(1)	C(4)	C(5)	120(1)
S(2)	C(5)	C(4)	123(1)	Se(3)	C(6)	Se(4)	115.3(5)
Se(3)	C(6)	C(1)	119.4(9)	Se(4)	C(6)	C(1)	125.3(9)
Se(3)	C(7)	S(3)	110.4(6)	Se(3)	C(7)	C(8)	120.3(9)
S(3)	C(7)	C(8)	129.3(9)	Se(4)	C(8)	S(4)	113.5(6)
Se(4)	C(8)	C(7)	118.7(9)	S(4)	C(8)	C(7)	127.8(9)
S(3)	C(9)	C(10)	115.1(8)	S(4)	C(10)	C(9)	113.7(9)
Se(5)	C(11)	Se(6)	114.4(5)	Se(5)	C(11)	C(16)	122.3(8)
Se(6)	C(11)	C(16)	123.2(8)	Se(5)	C(12)	S(5)	112.5(6)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Se(5)	C(12)	C(13)	118.8(9)	S(5)	C(12)	C(13)	128.7(9)
Se(6)	C(13)	S(6)	114.2(7)	Se(6)	C(13)	C(12)	119.1(9)
S(6)	C(13)	C(12)	126.5(9)	S(5)	C(14)	C(15)	119(1)
S(6)	C(15)	C(14)	119(1)	Se(7)	C(16)	Se(8)	115.2(5)
Se(7)	C(16)	C(11)	122.3(8)	Se(8)	C(16)	C(11)	122.2(8)
Se(7)	C(17)	S(7)	118.7(6)	Se(7)	C(17)	C(18)	119.0(8)
S(7)	C(17)	C(18)	121.7(9)	Se(8)	C(18)	S(8)	114.3(6)
Se(8)	C(18)	C(17)	119.4(8)	S(8)	C(18)	C(17)	126.2(9)
S(7)	C(19)	C(20)	113.5(9)	S(8)	C(20)	C(19)	115.2(8)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	S(1)	H(1)	97.6	C(2)	S(1)	H(2)	124.5
C(4)	S(1)	H(1)	24.7	C(4)	S(1)	H(2)	23.8
H(1)	S(1)	H(2)	39.6	C(3)	S(2)	H(3)	96.8
C(3)	S(2)	H(4)	122.6	C(5)	S(2)	H(3)	24.8
C(5)	S(2)	H(4)	22.1	H(3)	S(2)	H(4)	39.1
C(7)	S(3)	H(5)	98.9	C(7)	S(3)	H(6)	124.6
C(9)	S(3)	H(5)	23.5	C(9)	S(3)	H(6)	23.5
H(5)	S(3)	H(6)	39.2	C(8)	S(4)	H(7)	89.8
C(8)	S(4)	H(8)	123.1	C(10)	S(4)	H(7)	23.1
C(10)	S(4)	H(8)	23.1	H(7)	S(4)	H(8)	39.2
C(12)	S(5)	H(9)	107.5	C(12)	S(5)	H(10)	122.7
C(14)	S(5)	H(9)	24.2	C(14)	S(5)	H(10)	23.7
H(9)	S(5)	H(10)	39.8	C(13)	S(6)	H(11)	88.4
C(13)	S(6)	H(12)	121.6	C(15)	S(6)	H(11)	23.5
C(15)	S(6)	H(12)	23.0	H(11)	S(6)	H(12)	39.3
C(17)	S(7)	H(13)	117.5	C(17)	S(7)	H(14)	80.5
C(19)	S(7)	H(13)	22.9	C(19)	S(7)	H(14)	22.8
H(13)	S(7)	H(14)	38.5	C(18)	S(8)	H(15)	112.1
C(18)	S(8)	H(16)	115.6	C(20)	S(8)	H(15)	23.4
C(20)	S(8)	H(16)	22.5	H(15)	S(8)	H(16)	38.5
S(1)	C(4)	H(1)	107.4	S(1)	C(4)	H(2)	108.9
S(1)	C(4)	H(3)	104.7	S(1)	C(4)	H(4)	149.3
C(5)	C(4)	H(1)	103.3	C(5)	C(4)	H(2)	111.5
C(5)	C(4)	H(3)	33.4	C(5)	C(4)	H(4)	28.7

Table 6. Bond Angles(°) (continued)

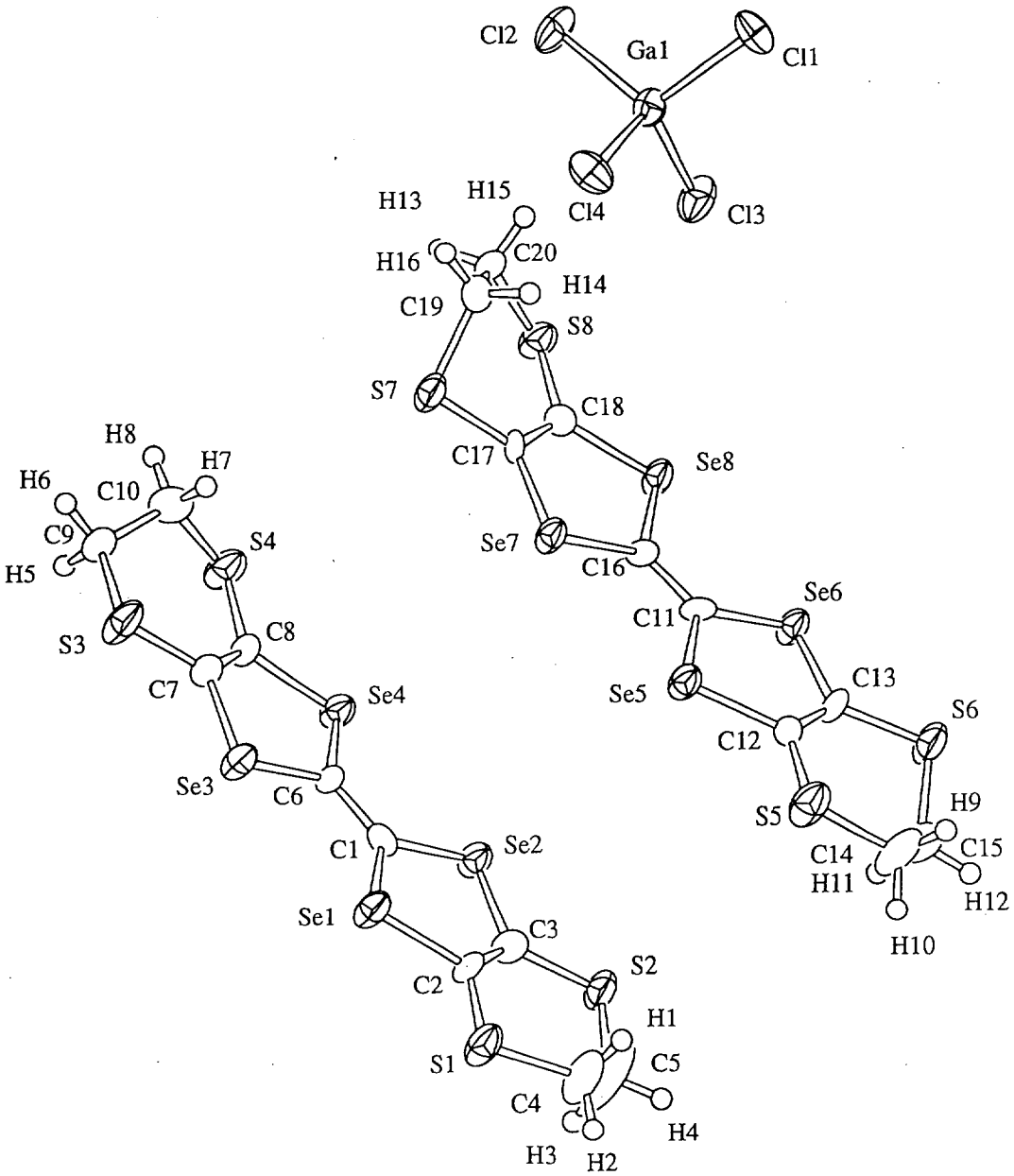
atom	atom	atom	angle	atom	atom	atom	angle
H(1)	C(4)	H(2)	103.4	H(1)	C(4)	H(3)	136.2
H(1)	C(4)	H(4)	90.0	H(2)	C(4)	H(3)	93.4
H(2)	C(4)	H(4)	90.7	H(3)	C(4)	H(4)	49.2
S(2)	C(5)	H(1)	108.4	S(2)	C(5)	H(2)	150.8
S(2)	C(5)	H(3)	108.7	S(2)	C(5)	H(4)	113.0
C(4)	C(5)	H(1)	31.2	C(4)	C(5)	H(2)	27.6
C(4)	C(5)	H(3)	98.8	C(4)	C(5)	H(4)	106.9
H(1)	C(5)	H(2)	47.6	H(1)	C(5)	H(3)	129.6
H(1)	C(5)	H(4)	92.0	H(2)	C(5)	H(3)	85.2
H(2)	C(5)	H(4)	87.2	H(3)	C(5)	H(4)	103.6
S(3)	C(9)	H(5)	109.7	S(3)	C(9)	H(6)	109.7
S(3)	C(9)	H(7)	97.5	S(3)	C(9)	H(8)	140.9
C(10)	C(9)	H(5)	107.5	C(10)	C(9)	H(6)	109.6
C(10)	C(9)	H(7)	27.5	C(10)	C(9)	H(8)	26.5
H(5)	C(9)	H(6)	104.7	H(5)	C(9)	H(7)	134.8
H(5)	C(9)	H(8)	96.5	H(6)	C(9)	H(7)	98.7
H(6)	C(9)	H(8)	90.1	H(7)	C(9)	H(8)	44.9
S(4)	C(10)	H(5)	96.5	S(4)	C(10)	H(6)	139.5
S(4)	C(10)	H(7)	110.2	S(4)	C(10)	H(8)	110.1
C(9)	C(10)	H(5)	27.4	C(9)	C(10)	H(6)	26.7
C(9)	C(10)	H(7)	106.6	C(9)	C(10)	H(8)	109.5
H(5)	C(10)	H(6)	44.6	H(5)	C(10)	H(7)	134.0
H(5)	C(10)	H(8)	98.0	H(6)	C(10)	H(7)	96.3
H(6)	C(10)	H(8)	89.8	H(7)	C(10)	H(8)	106.5

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
S(5)	C(14)	H(9)	108.4	S(5)	C(14)	H(10)	109.2
S(5)	C(14)	H(11)	104.9	S(5)	C(14)	H(12)	147.8
C(15)	C(14)	H(9)	104.8	C(15)	C(14)	H(10)	109.2
C(15)	C(14)	H(11)	30.2	C(15)	C(14)	H(12)	28.5
H(9)	C(14)	H(10)	105.0	H(9)	C(14)	H(11)	134.5
H(9)	C(14)	H(12)	89.4	H(10)	C(14)	H(11)	92.1
H(10)	C(14)	H(12)	90.9	H(11)	C(14)	H(12)	47.8
S(6)	C(15)	H(9)	105.2	S(6)	C(15)	H(10)	147.4
S(6)	C(15)	H(11)	109.9	S(6)	C(15)	H(12)	110.7
C(14)	C(15)	H(9)	29.7	C(14)	C(15)	H(10)	27.7
C(14)	C(15)	H(11)	102.8	C(14)	C(15)	H(12)	106.7
H(9)	C(15)	H(10)	47.0	H(9)	C(15)	H(11)	132.0
H(9)	C(15)	H(12)	90.4	H(10)	C(15)	H(11)	87.7
H(10)	C(15)	H(12)	89.2	H(11)	C(15)	H(12)	106.1
S(7)	C(19)	H(13)	111.0	S(7)	C(19)	H(14)	111.1
S(7)	C(19)	H(15)	140.5	S(7)	C(19)	H(16)	104.5
C(20)	C(19)	H(13)	108.5	C(20)	C(19)	H(14)	107.2
C(20)	C(19)	H(15)	27.5	C(20)	C(19)	H(16)	27.3
H(13)	C(19)	H(14)	105.1	H(13)	C(19)	H(15)	95.7
H(13)	C(19)	H(16)	89.5	H(14)	C(19)	H(15)	88.0
H(14)	C(19)	H(16)	132.7	H(15)	C(19)	H(16)	45.3
S(8)	C(20)	H(13)	142.3	S(8)	C(20)	H(14)	105.6
S(8)	C(20)	H(15)	108.8	S(8)	C(20)	H(16)	110.4
C(19)	C(20)	H(13)	27.4	C(19)	C(20)	H(14)	27.8

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(19)	C(20)	H(15)	108.9	C(19)	C(20)	H(16)	107.8
H(13)	C(20)	H(14)	45.5	H(13)	C(20)	H(15)	96.1
H(13)	C(20)	H(16)	88.8	H(14)	C(20)	H(15)	89.3
H(14)	C(20)	H(16)	133.7	H(15)	C(20)	H(16)	105.3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Se7
C16
Se6
C11
C13
Se5
S6
C12
S5
H9
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H12
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C7
Se4
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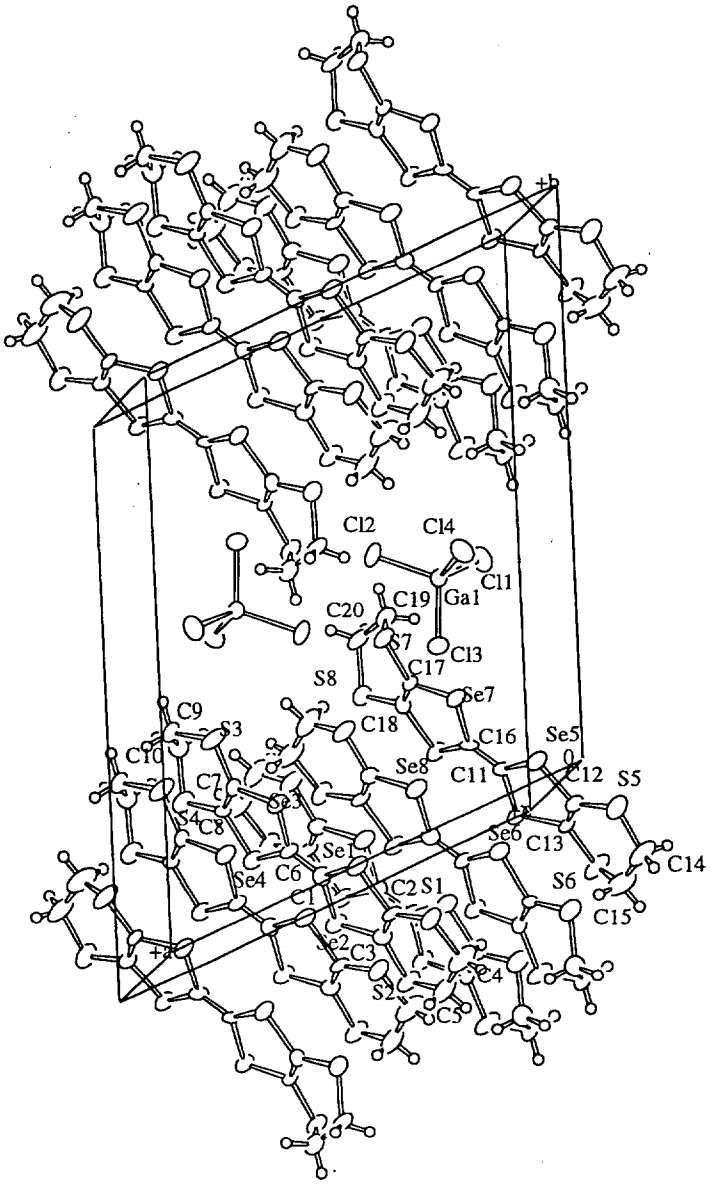
H2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C20
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Se5
C10
C7
Se8
C11
C12
S5
S4
C8
Se3
Se6
C13
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S2
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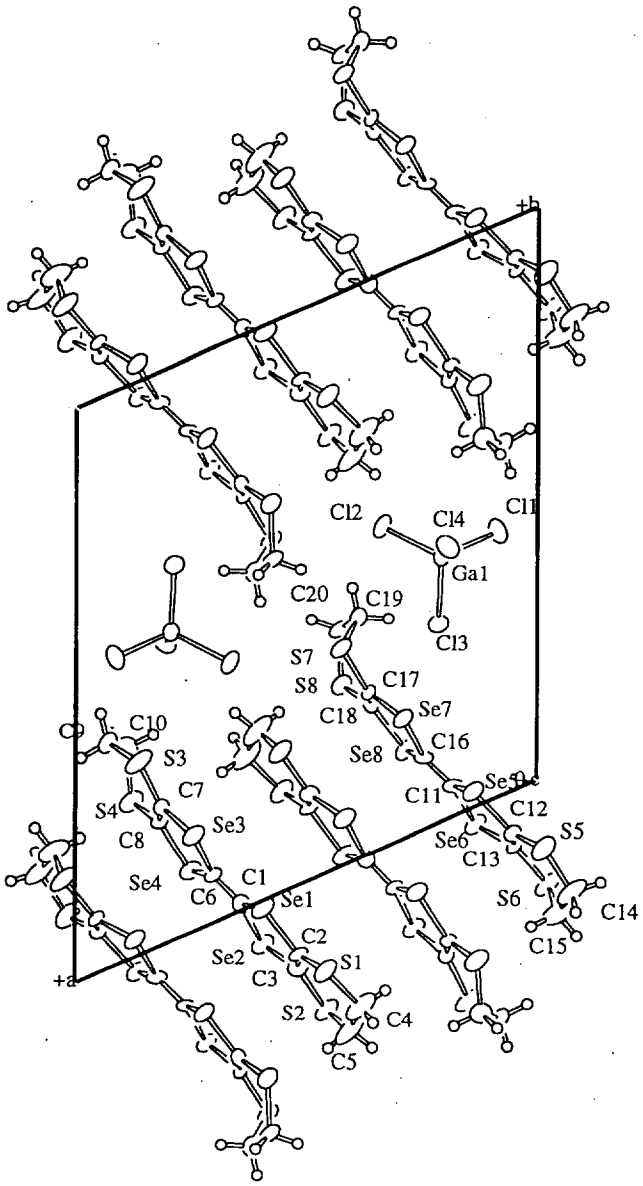


[II] Structure data of λ-$(BETS)_2GaBr_{0.3}Cl_{3.7}$ at 7K.

Crystal data and experimental details of λ-$(BETS)_2GaBr_{0.3}Cl_{3.7}$ at low temperature(7K).

chemical formula	$C_{20}H_{16}S_8Se_8GaBr_{0.3}Cl_{3.7}$
temperature	7K
formula weight	1369.37
crystal color, habit	black, needle
crystal dimension / mm	0.15 × 0.08 × 0.81
a / Å	15.909(4)
b / Å	18.430(5)
c / Å	6.536(2)
α / °	98.67(2)
β / °	96.69(3)
γ / °	111.97(2)
V / $Å^3$	1732(1)
space group	$P\bar{1}$
Z	2
d_{calc} / g cm^{-3}	2.628
F_{000}	1280.80
μ(MoKα) / cm^{-1}	103.43
diffractometer	Mac Science DIP-320
radiation	MoKα(λ= 0.71069 Å)
scan type	-
$2\theta_{max}$ / °	61.0
total reflection	7403
No. observation (I>3.00σ(I))	5199
No. Variables	274
Corrections	-
structure solution	Direct methods (SHELXS86)

refinement	full-matrix least-squares
function minimized	$\sum \omega(\lvert Fo\rvert - \lvert Fc\rvert)^2$
least-squares weights	$\omega = \frac{1}{\sigma^2(Fo)} = \left[\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2\right]^{-1}$
R, *R*w	0.066, 0.077
goodnedd of fit	3.59
Maximum peak / $e^-/Å^3$	2.71
Minimum peak / $e^-/Å^3$	-2.22

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Se(1)	0.58612(8)	-0.01476(8)	-0.3207(2)	1.60(2)	1.0000
Se(2)	0.58900(8)	-0.07797(8)	0.1068(2)	1.55(2)	1.0000
Se(3)	0.74255(8)	0.16556(8)	-0.0810(2)	1.56(2)	1.0000
Se(4)	0.75223(8)	0.10758(8)	0.3530(2)	1.52(2)	1.0000
Se(5)	0.12759(8)	0.02424(8)	-0.1881(2)	1.57(2)	1.0000
Se(6)	0.12541(8)	-0.03376(8)	0.2478(2)	1.55(2)	1.0000
Se(7)	0.28429(8)	0.20710(8)	0.0515(2)	1.55(2)	1.0000
Se(8)	0.28259(8)	0.15037(8)	0.4917(2)	1.54(2)	1.0000
Ga(1)	0.21079(9)	0.46839(9)	0.8767(2)	1.63(3)	1.0000
Cl(1)	0.0892(2)	0.4689(2)	1.0024(5)	1.86(7)	1.03(1)
Cl(2)	0.3395(1)	0.5677(1)	1.0577(4)	1.67(5)	1.32(1)
Cl(3)	0.2199(2)	0.3538(2)	0.8927(5)	1.98(7)	1.05(1)
Cl(4)	0.1953(2)	0.4792(2)	0.5428(4)	1.87(6)	1.17(1)
S(1)	0.4469(2)	-0.1745(2)	-0.5708(5)	1.71(6)	1.0000
S(2)	0.4435(2)	-0.2447(2)	-0.0952(5)	1.78(6)	1.0000
S(3)	0.8627(2)	0.3384(2)	0.1136(5)	1.87(6)	1.0000
S(4)	0.8865(2)	0.2748(2)	0.5915(5)	1.70(6)	1.0000
S(5)	-0.0245(2)	-0.1320(2)	-0.4219(5)	1.78(6)	1.0000
S(6)	-0.0323(2)	-0.1959(2)	0.0550(5)	1.61(6)	1.0000
S(7)	0.4237(2)	0.3798(2)	0.2774(5)	1.59(6)	1.0000
S(8)	0.4280(2)	0.3157(2)	0.7219(5)	1.65(6)	1.0000
C(1)	0.6355(8)	0.0066(7)	-0.030(2)	1.4(2)	1.0000
C(2)	0.5087(8)	-0.1219(7)	-0.322(2)	1.5(2)	1.0000
C(3)	0.5093(8)	-0.1484(8)	-0.143(2)	1.8(2)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(4)	0.3597(9)	-0.2616(8)	-0.509(2)	2.0(2)	1.0000
C(5)	0.4005(9)	-0.3031(8)	-0.358(2)	2.0(2)	1.0000
C(6)	0.6992(7)	0.0826(7)	0.069(2)	1.2(2)	1.0000
C(7)	0.8160(8)	0.2410(7)	0.166(2)	1.2(2)	1.0000
C(8)	0.8226(8)	0.2162(7)	0.347(2)	1.5(2)	1.0000
C(9)	0.9340(8)	0.3960(7)	0.367(2)	1.4(2)	1.0000
C(10)	0.8915(8)	0.3718(7)	0.554(2)	1.6(2)	1.0000
C(11)	0.1730(7)	0.0485(7)	0.103(2)	1.1(2)	1.0000
C(12)	0.0434(8)	-0.0787(7)	-0.180(2)	1.3(2)	1.0000
C(13)	0.0405(8)	-0.1034(7)	0.003(2)	1.5(2)	1.0000
C(14)	-0.0943(8)	-0.2298(7)	-0.380(2)	1.5(2)	1.0000
C(15)	-0.0491(8)	-0.2564(7)	-0.202(2)	1.6(2)	1.0000
C(16)	0.2376(8)	0.1240(7)	0.198(2)	1.5(2)	1.0000
C(17)	0.3616(8)	0.2800(7)	0.300(2)	1.3(2)	1.0000
C(18)	0.3607(8)	0.2558(7)	0.486(2)	1.6(2)	1.0000
C(19)	0.3886(8)	0.4239(7)	0.503(2)	1.5(2)	1.0000
C(20)	0.4316(9)	0.4158(8)	0.712(2)	1.9(2)	1.0000
H(1)	0.3160	-0.2453	-0.4430	2.3975	1.0000
H(2)	0.3265	-0.2992	-0.6367	2.3975	1.0000
H(3)	0.4498	-0.3123	-0.4141	2.3611	1.0000
H(4)	0.3541	-0.3539	-0.3529	2.3611	1.0000
H(5)	0.9915	0.3889	0.3738	1.6784	1.0000
H(6)	0.9478	0.4512	0.3696	1.6784	1.0000
H(7)	0.8302	0.3701	0.5348	1.9282	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(8)	0.9261	0.4109	0.6777	1.9282	1.0000
H(9)	-0.1515	-0.2293	-0.3474	1.7754	1.0000
H(10)	-0.1070	-0.2678	-0.5078	1.7754	1.0000
H(11)	0.0093	-0.2544	-0.2291	1.9339	1.0000
H(12)	-0.0871	-0.3106	-0.1975	1.9339	1.0000
H(13)	0.4049	0.4794	0.5012	1.7710	1.0000
H(14)	0.3231	0.3986	0.4882	1.7710	1.0000
H(15)	0.3999	0.4302	0.8190	2.1586	1.0000
H(16)	0.4943	0.4533	0.7443	2.1586	1.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Se(1)	0.0203(6)	0.0227(7)	0.0140(6)	0.0088(5)	-0.0049(5)	-0.0034(5)
Se(2)	0.0188(6)	0.0211(6)	0.0154(7)	0.0082(5)	-0.0037(5)	-0.0031(5)
Se(3)	0.0189(6)	0.0211(6)	0.0155(7)	0.0081(5)	-0.0046(5)	-0.0036(5)
Se(4)	0.0197(6)	0.0216(6)	0.0137(6)	0.0088(5)	-0.0033(5)	-0.0024(5)
Se(5)	0.0196(6)	0.0224(6)	0.0140(6)	0.0086(5)	-0.0037(5)	-0.0032(5)
Se(6)	0.0183(6)	0.0212(7)	0.0154(7)	0.0078(5)	-0.0042(5)	-0.0037(5)
Se(7)	0.0187(6)	0.0212(7)	0.0150(7)	0.0076(5)	-0.0042(5)	-0.0029(5)
Se(8)	0.0185(6)	0.0212(6)	0.0148(6)	0.0079(5)	-0.0041(5)	-0.0032(5)
Ga(1)	0.0192(7)	0.0239(7)	0.0155(7)	0.0100(6)	-0.0048(6)	-0.0047(6)
Cl(1)	0.021(2)	0.029(2)	0.017(2)	0.012(1)	-0.005(1)	-0.004(1)
Cl(2)	0.017(1)	0.023(1)	0.018(1)	0.0078(9)	-0.0055(9)	-0.0054(10)
Cl(3)	0.022(2)	0.027(2)	0.022(2)	0.011(1)	-0.005(1)	-0.005(1)
Cl(4)	0.022(1)	0.028(2)	0.019(2)	0.013(1)	-0.006(1)	-0.005(1)
S(1)	0.021(1)	0.022(2)	0.016(2)	0.007(1)	-0.007(1)	-0.004(1)
S(2)	0.022(2)	0.022(2)	0.019(2)	0.009(1)	-0.004(1)	-0.004(1)
S(3)	0.025(2)	0.022(2)	0.018(2)	0.008(1)	-0.007(1)	-0.006(1)
S(4)	0.019(1)	0.021(2)	0.020(2)	0.007(1)	-0.006(1)	-0.003(1)
S(5)	0.022(1)	0.020(2)	0.019(2)	0.007(1)	-0.007(1)	-0.006(1)
S(6)	0.020(1)	0.020(2)	0.015(2)	0.004(1)	-0.002(1)	-0.003(1)
S(7)	0.019(1)	0.019(2)	0.018(2)	0.006(1)	-0.003(1)	-0.002(1)
S(8)	0.019(1)	0.022(2)	0.018(2)	0.007(1)	-0.004(1)	-0.003(1)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Se(1)	C(1)	1.90(1)	Se(1)	C(2)	1.89(1)
Se(2)	C(1)	1.86(1)	Se(2)	C(3)	1.92(1)
Se(3)	C(6)	1.89(1)	Se(3)	C(7)	1.91(1)
Se(4)	C(6)	1.87(1)	Se(4)	C(8)	1.90(1)
Se(5)	C(11)	1.89(1)	Se(5)	C(12)	1.88(1)
Se(6)	C(11)	1.87(1)	Se(6)	C(13)	1.92(1)
Se(7)	C(16)	1.88(1)	Se(7)	C(17)	1.91(1)
Se(8)	C(16)	1.90(1)	Se(8)	C(18)	1.88(1)
Ga(1)	Cl(1)	2.179(3)	Ga(1)	Cl(2)	2.236(2)
Ga(1)	Cl(3)	2.188(4)	Ga(1)	Cl(4)	2.218(3)
S(1)	C(2)	1.75(1)	S(1)	C(4)	1.82(1)
S(2)	C(3)	1.79(1)	S(2)	C(5)	1.80(1)
S(3)	C(7)	1.77(1)	S(3)	C(9)	1.83(1)
S(4)	C(8)	1.75(1)	S(4)	C(10)	1.81(1)
S(5)	C(12)	1.74(1)	S(5)	C(14)	1.81(1)
S(6)	C(13)	1.77(1)	S(6)	C(15)	1.80(1)
S(7)	C(17)	1.77(1)	S(7)	C(19)	1.81(1)
S(8)	C(18)	1.74(1)	S(8)	C(20)	1.84(1)
C(1)	C(6)	1.39(2)	C(2)	C(3)	1.33(2)
C(4)	C(5)	1.57(2)	C(7)	C(8)	1.34(2)
C(9)	C(10)	1.51(2)	C(11)	C(16)	1.39(2)
C(12)	C(13)	1.34(2)	C(14)	C(15)	1.54(2)
C(17)	C(18)	1.36(2)	C(19)	C(20)	1.52(2)

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
S(1)	H(1)	2.32	S(1)	H(2)	2.32
S(2)	H(3)	2.29	S(2)	H(4)	2.30
S(3)	H(5)	2.31	S(3)	H(6)	2.31
S(4)	H(7)	2.31	S(4)	H(8)	2.31
S(5)	H(9)	2.30	S(5)	H(10)	2.30
S(6)	H(11)	2.29	S(6)	H(12)	2.29
S(7)	H(13)	2.30	S(7)	H(14)	2.30
S(8)	H(15)	2.33	S(8)	H(16)	2.33
C(4)	H(1)	0.97	C(4)	H(2)	0.96
C(4)	H(3)	2.08	C(4)	H(4)	2.09
C(5)	H(1)	2.08	C(5)	H(2)	2.09
C(5)	H(3)	0.96	C(5)	H(4)	0.96
C(9)	H(5)	0.97	C(9)	H(6)	0.95
C(9)	H(7)	2.02	C(9)	H(8)	2.03
C(10)	H(5)	2.03	C(10)	H(6)	2.04
C(10)	H(7)	0.96	C(10)	H(8)	0.96
C(14)	H(9)	0.96	C(14)	H(10)	0.95
C(14)	H(11)	2.07	C(14)	H(12)	2.07
C(15)	H(9)	2.06	C(15)	H(10)	2.06
C(15)	H(11)	0.95	C(15)	H(12)	0.96
C(19)	H(13)	0.96	C(19)	H(14)	0.96
C(19)	H(15)	2.04	C(19)	H(16)	2.03
C(20)	H(13)	2.05	C(20)	H(14)	2.04
C(20)	H(15)	0.96	C(20)	H(16)	0.96

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Se(1)	C(2)	93.1(5)	C(1)	Se(2)	C(3)	92.9(5)
C(6)	Se(3)	C(7)	92.5(5)	C(6)	Se(4)	C(8)	93.4(5)
C(11)	Se(5)	C(12)	93.0(5)	C(11)	Se(6)	C(13)	92.3(5)
C(16)	Se(7)	C(17)	92.5(5)	C(16)	Se(8)	C(18)	93.5(5)
Cl(1)	Ga(1)	Cl(2)	111.9(1)	Cl(1)	Ga(1)	Cl(3)	108.1(1)
Cl(1)	Ga(1)	Cl(4)	109.3(1)	Cl(2)	Ga(1)	Cl(3)	109.3(1)
Cl(2)	Ga(1)	Cl(4)	109.6(1)	Cl(3)	Ga(1)	Cl(4)	108.6(1)
C(2)	S(1)	C(4)	101.9(6)	C(3)	S(2)	C(5)	101.6(6)
C(7)	S(3)	C(9)	101.5(6)	C(8)	S(4)	C(10)	99.7(6)
C(12)	S(5)	C(14)	106.0(6)	C(13)	S(6)	C(15)	97.7(6)
C(17)	S(7)	C(19)	94.9(6)	C(18)	S(8)	C(20)	104.9(6)
Se(1)	C(1)	Se(2)	115.7(6)	Se(1)	C(1)	C(6)	120.2(9)
Se(2)	C(1)	C(6)	124.0(9)	Se(1)	C(2)	S(1)	112.8(7)
Se(1)	C(2)	C(3)	118.8(9)	S(1)	C(2)	C(3)	128.4(10)
Se(2)	C(3)	S(2)	111.7(7)	Se(2)	C(3)	C(2)	119.4(9)
S(2)	C(3)	C(2)	128.9(10)	S(1)	C(4)	C(5)	113.0(9)
S(2)	C(5)	C(4)	113.2(9)	Se(3)	C(6)	Se(4)	115.8(6)
Se(3)	C(6)	C(1)	121.5(9)	Se(4)	C(6)	C(1)	122.6(9)
Se(3)	C(7)	S(3)	110.6(6)	Se(3)	C(7)	C(8)	119.4(9)
S(3)	C(7)	C(8)	129.9(9)	Se(4)	C(8)	S(4)	114.4(7)
Se(4)	C(8)	C(7)	118.6(9)	S(4)	C(8)	C(7)	126.9(10)
S(3)	C(9)	C(10)	114.4(8)	S(4)	C(10)	C(9)	112.8(9)
Se(5)	C(11)	Se(6)	116.3(6)	Se(5)	C(11)	C(16)	120.2(9)
Se(6)	C(11)	C(16)	123.5(9)	Se(5)	C(12)	S(5)	113.6(7)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle
Se(5)	C(12)	C(13)	119.3(9)
Se(6)	C(13)	S(6)	112.6(7)
S(6)	C(13)	C(12)	128.5(9)
S(6)	C(15)	C(14)	113.9(9)
Se(7)	C(16)	C(11)	123.4(9)
Se(7)	C(17)	S(7)	117.2(7)
S(7)	C(17)	C(18)	122.9(9)
Se(8)	C(18)	C(17)	118.5(9)
S(7)	C(19)	C(20)	113.9(9)
S(5)	C(12)	C(13)	127.0(9)
Se(6)	C(13)	C(12)	118.9(9)
S(5)	C(14)	C(15)	113.8(8)
Se(7)	C(16)	Se(8)	115.7(6)
Se(8)	C(16)	C(11)	120.9(9)
Se(7)	C(17)	C(18)	119.7(9)
Se(8)	C(18)	S(8)	117.2(7)
S(8)	C(18)	C(17)	124.3(10)
S(8)	C(20)	C(19)	114.9(9)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	S(1)	H(1)	93.7	C(2)	S(1)	H(2)	124.5
C(4)	S(1)	H(1)	23.3	C(4)	S(1)	H(2)	22.9
H(1)	S(1)	H(2)	39.1	C(3)	S(2)	H(3)	94.4
C(3)	S(2)	H(4)	124.4	C(5)	S(2)	H(3)	23.2
C(5)	S(2)	H(4)	23.3	H(3)	S(2)	H(4)	39.5
C(7)	S(3)	H(5)	97.1	C(7)	S(3)	H(6)	123.4
C(9)	S(3)	H(5)	23.6	C(9)	S(3)	H(6)	23.0
H(5)	S(3)	H(6)	39.2	C(8)	S(4)	H(7)	88.7
C(8)	S(4)	H(8)	122.7	C(10)	S(4)	H(7)	23.1
C(10)	S(4)	H(8)	23.0	H(7)	S(4)	H(8)	39.3
C(12)	S(5)	H(9)	105.7	C(12)	S(5)	H(10)	125.5
C(14)	S(5)	H(9)	23.3	C(14)	S(5)	H(10)	23.2
H(9)	S(5)	H(10)	39.5	C(13)	S(6)	H(11)	86.3
C(13)	S(6)	H(12)	121.2	C(15)	S(6)	H(11)	23.3
C(15)	S(6)	H(12)	23.6	H(11)	S(6)	H(12)	39.6
C(17)	S(7)	H(13)	117.6	C(17)	S(7)	H(14)	80.1
C(19)	S(7)	H(13)	23.3	C(19)	S(7)	H(14)	23.3
H(13)	S(7)	H(14)	39.4	C(18)	S(8)	H(15)	112.9
C(18)	S(8)	H(16)	118.2	C(20)	S(8)	H(15)	23.1
C(20)	S(8)	H(16)	22.9	H(15)	S(8)	H(16)	38.9
S(1)	C(4)	H(1)	109.0	S(1)	C(4)	H(2)	109.5
S(1)	C(4)	H(3)	95.7	S(1)	C(4)	H(4)	138.0
C(5)	C(4)	H(1)	108.3	C(5)	C(4)	H(2)	109.6
C(5)	C(4)	H(3)	26.0	C(5)	C(4)	H(4)	25.6

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H(1)	C(4)	H(2)	107.3	H(1)	C(4)	H(3)	133.9
H(1)	C(4)	H(4)	98.4	H(2)	C(4)	H(3)	99.8
H(2)	C(4)	H(4)	91.2	H(3)	C(4)	H(4)	43.7
S(2)	C(5)	H(1)	95.7	S(2)	C(5)	H(2)	138.0
S(2)	C(5)	H(3)	108.9	S(2)	C(5)	H(4)	108.8
C(4)	C(5)	H(1)	26.2	C(4)	C(5)	H(2)	25.5
C(4)	C(5)	H(3)	108.2	C(4)	C(5)	H(4)	109.4
H(1)	C(5)	H(2)	43.6	H(1)	C(5)	H(3)	134.1
H(1)	C(5)	H(4)	99.2	H(2)	C(5)	H(3)	98.7
H(2)	C(5)	H(4)	91.1	H(3)	C(5)	H(4)	108.1
S(3)	C(9)	H(5)	107.6	S(3)	C(9)	H(6)	108.4
S(3)	C(9)	H(7)	96.1	S(3)	C(9)	H(8)	139.9
C(10)	C(9)	H(5)	108.5	C(10)	C(9)	H(6)	110.2
C(10)	C(9)	H(7)	26.7	C(10)	C(9)	H(8)	26.3
H(5)	C(9)	H(6)	107.5	H(5)	C(9)	H(7)	134.8
H(5)	C(9)	H(8)	98.9	H(6)	C(9)	H(7)	100.4
H(6)	C(9)	H(8)	91.1	H(7)	C(9)	H(8)	44.9
S(4)	C(10)	H(5)	94.3	S(4)	C(10)	H(6)	137.9
S(4)	C(10)	H(7)	108.9	S(4)	C(10)	H(8)	109.0
C(9)	C(10)	H(5)	26.9	C(9)	C(10)	H(6)	26.0
C(9)	C(10)	H(7)	108.4	C(9)	C(10)	H(8)	109.5
H(5)	C(10)	H(6)	44.8	H(5)	C(10)	H(7)	134.8
H(5)	C(10)	H(8)	99.5	H(6)	C(10)	H(7)	99.0
H(6)	C(10)	H(8)	90.6	H(7)	C(10)	H(8)	108.2

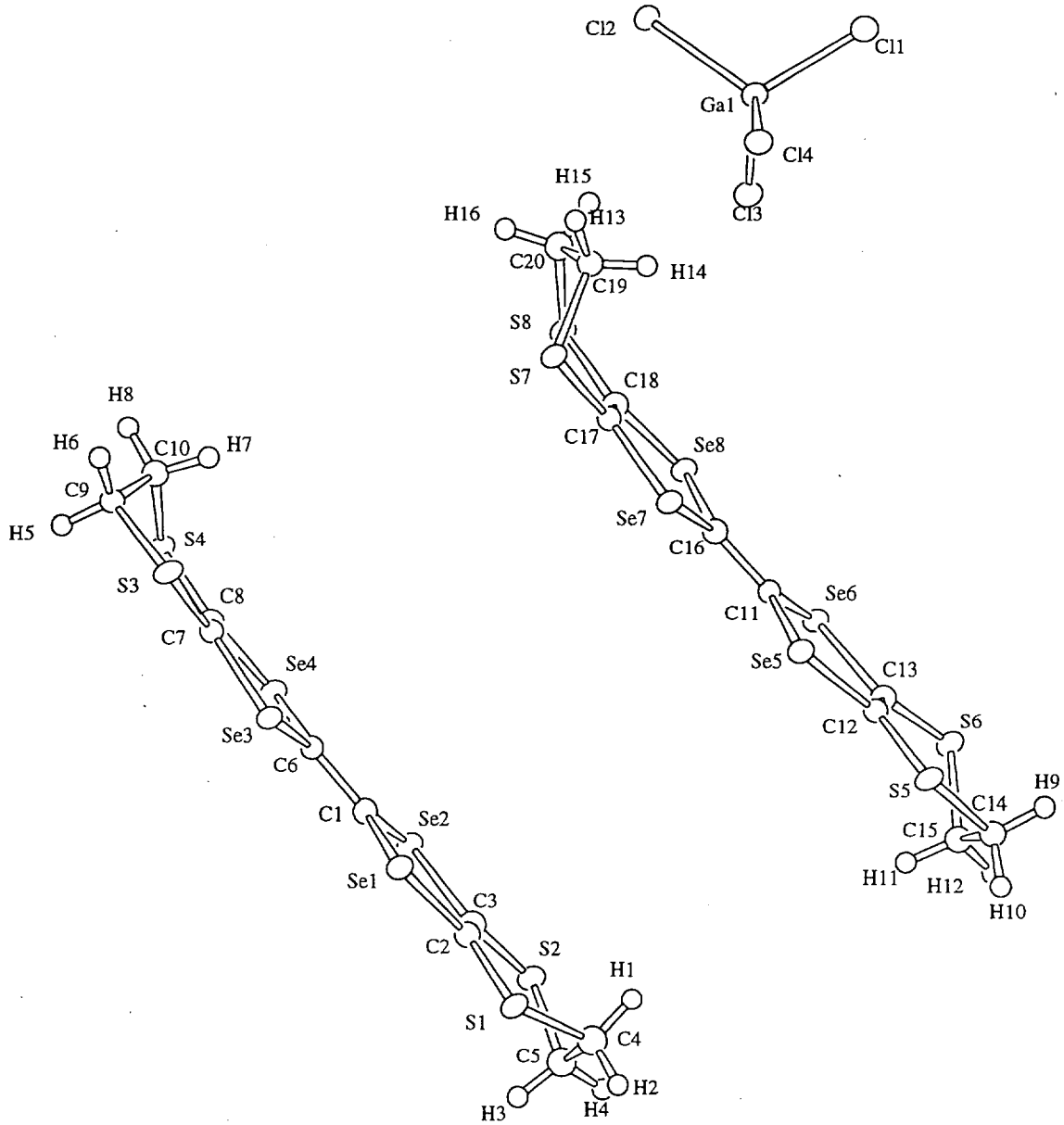
Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle
S(5)	C(14)	H(9)	108.4
S(5)	C(14)	H(11)	98.1
C(15)	C(14)	H(9)	108.5
C(15)	C(14)	H(11)	25.8
H(9)	C(14)	H(10)	108.4
H(9)	C(14)	H(12)	96.2
H(10)	C(14)	H(12)	92.4
S(6)	C(15)	H(9)	97.9
S(6)	C(15)	H(11)	108.2
C(14)	C(15)	H(9)	26.2
C(14)	C(15)	H(11)	109.2
H(9)	C(15)	H(10)	44.2
H(9)	C(15)	H(12)	96.9
H(10)	C(15)	H(12)	92.8
S(7)	C(19)	H(13)	108.2
S(7)	C(19)	H(15)	139.7
C(20)	C(19)	H(13)	109.3
C(20)	C(19)	H(15)	26.6
H(13)	C(19)	H(14)	108.2
H(13)	C(19)	H(16)	90.1
H(14)	C(19)	H(16)	133.9
S(8)	C(20)	H(13)	140.2
S(8)	C(20)	H(15)	108.5
C(19)	C(20)	H(13)	26.2

atom	atom	atom	angle
S(5)	C(14)	H(10)	108.6
S(5)	C(14)	H(12)	139.6
C(15)	C(14)	H(10)	108.9
C(15)	C(14)	H(12)	26.0
H(9)	C(14)	H(11)	134.3
H(10)	C(14)	H(11)	96.9
H(11)	C(14)	H(12)	44.0
S(6)	C(15)	H(10)	139.7
S(6)	C(15)	H(12)	107.8
C(14)	C(15)	H(10)	25.9
C(14)	C(15)	H(12)	109.3
H(9)	C(15)	H(11)	135.4
H(10)	C(15)	H(11)	97.1
H(11)	C(15)	H(12)	108.2
S(7)	C(19)	H(14)	108.3
S(7)	C(19)	H(16)	105.0
C(20)	C(19)	H(14)	108.8
C(20)	C(19)	H(16)	26.5
H(13)	C(19)	H(15)	99.0
H(14)	C(19)	H(15)	89.9
H(15)	C(19)	H(16)	44.8
S(8)	C(20)	H(14)	105.6
S(8)	C(20)	H(16)	108.9
C(19)	C(20)	H(14)	26.4

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(19)	C(20)	H(15)	108.2	C(19)	C(20)	H(16)	108.2
H(13)	C(20)	H(14)	44.6	H(13)	C(20)	H(15)	98.2
H(13)	C(20)	H(16)	89.3	H(14)	C(20)	H(15)	89.6
H(14)	C(20)	H(16)	133.2	H(15)	C(20)	H(16)	107.9



[III] Structure data of λ-$(BETS)_2GaBr_{1.3}Cl_{2.7}$ at 7K.

Crystal data and experimental details of λ-$(BETS)_2GaBr_{1.3}Cl_{2.7}$ at low temperature(7K).

chemical formula	$C_{20}H_{16}S_8Se_8GaBr_{1.3}Cl_{2.7}$
temperature	7K
formula weight	1413.82
crystal color, habit	black, needle
crystal dimension / mm	0.20 × 0.10 × 0.50
a / Å	16.00(1)
b / Å	18.42(1)
c / Å	6.535(5)
α / °	98.79(5)
β / °	95.49(7)
γ / °	112.10(4)
V / $Å^3$	1738(2)
space group	$P\bar{1}$
Z	2
d_{calc} / g cm^{-3}	2.701
F_{000}	1316.80
μ(MoKα) / cm^{-1}	113.74
diffractometer	Mac Science DIP-320
radiation	MoKα(λ= 0.71069 Å)
scan type	-
$2\theta_{max}$ / °	60.6
total reflection	6234
No. observation (I>3.00σ(I))	4636
No. Variables	274
Corrections	-
structure solution	Direct methods (SHELXS86)

refinement	full-matrix least-squares
function minimized	$\sum \omega(\|Fo\| - \|Fc\|)^2$
least-squares weights	$\omega = \frac{1}{\sigma^2(Fo)} = \left[\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2\right]^{-1}$
R, *R*w	0.061, 0.083
goodnedd of fit	4.96
Maximum peak / $e^-/Å^3$	2.30
Minimum peak / $e^-/Å^3$	-1.77

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Se(1)	0.58643(9)	-0.01455(8)	-0.3204(2)	0.71(3)	1.0000
Se(2)	0.58940(9)	-0.07778(8)	0.1069(2)	0.73(3)	1.0000
Se(3)	0.74262(9)	0.16559(8)	-0.0816(2)	0.66(3)	1.0000
Se(4)	0.75222(9)	0.10726(8)	0.3518(2)	0.72(3)	1.0000
Se(5)	0.12844(9)	0.02449(8)	-0.1875(2)	0.70(3)	1.0000
Se(6)	0.12645(9)	-0.03345(8)	0.2483(2)	0.71(3)	1.0000
Se(7)	0.28489(9)	0.20681(8)	0.0514(2)	0.69(3)	1.0000
Se(8)	0.28279(9)	0.15053(8)	0.4916(2)	0.70(3)	1.0000
Ga(1)	0.2098(1)	0.46685(9)	0.8748(3)	0.79(3)	1.0000
Cl(1)	0.0868(2)	0.4669(2)	1.0008(5)	1.16(7)	1.20(1)
Cl(2)	0.3402(1)	0.5682(1)	1.0610(3)	0.43(4)	1.66(1)
Cl(3)	0.2200(2)	0.3521(2)	0.8911(5)	0.86(7)	1.06(1)
Cl(4)	0.1950(1)	0.4783(1)	0.5335(4)	1.03(5)	1.55(1)
S(1)	0.4469(2)	-0.1737(2)	-0.5681(6)	0.87(7)	1.0000
S(2)	0.4449(2)	-0.2441(2)	-0.0964(6)	0.97(7)	1.0000
S(3)	0.8625(2)	0.3383(2)	0.1125(6)	0.82(7)	1.0000
S(4)	0.8851(2)	0.2740(2)	0.5916(6)	0.88(7)	1.0000
S(5)	-0.0239(2)	-0.1309(2)	-0.4217(6)	0.78(7)	1.0000
S(6)	-0.0316(2)	-0.1949(2)	0.0551(6)	0.92(7)	1.0000
S(7)	0.4244(2)	0.3790(2)	0.2759(6)	0.82(7)	1.0000
S(8)	0.4272(2)	0.3157(2)	0.7229(6)	0.88(7)	1.0000
C(1)	0.6381(9)	0.0074(8)	-0.041(2)	0.8(2)	1.0000
C(2)	0.5092(9)	-0.1213(8)	-0.322(2)	0.7(2)	1.0000
C(3)	0.5110(9)	-0.1487(8)	-0.148(2)	0.8(2)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(4)	0.3623(9)	-0.2592(8)	-0.509(2)	0.7(2)	1.0000
C(5)	0.4013(10)	-0.3024(8)	-0.362(2)	1.0(2)	1.0000
C(6)	0.7015(9)	0.0813(8)	0.057(2)	0.8(2)	1.0000
C(7)	0.8165(9)	0.2399(8)	0.159(2)	0.5(2)	1.0000
C(8)	0.8229(9)	0.2157(8)	0.343(2)	0.9(2)	1.0000
C(9)	0.9349(10)	0.3960(8)	0.362(2)	1.0(2)	1.0000
C(10)	0.889(1)	0.3713(9)	0.560(2)	1.2(3)	1.0000
C(11)	0.1767(9)	0.0503(8)	0.097(2)	0.7(2)	1.0000
C(12)	0.0440(9)	-0.0789(8)	-0.181(2)	0.8(2)	1.0000
C(13)	0.0433(9)	-0.1035(8)	0.003(2)	0.7(2)	1.0000
C(14)	-0.0924(10)	-0.2293(8)	-0.378(2)	1.0(2)	1.0000
C(15)	-0.0460(9)	-0.2557(8)	-0.208(2)	0.8(2)	1.0000
C(16)	0.2410(9)	0.1240(8)	0.189(2)	0.9(2)	1.0000
C(17)	0.3636(9)	0.2797(8)	0.292(2)	0.8(2)	1.0000
C(18)	0.3622(9)	0.2567(8)	0.478(2)	0.8(2)	1.0000
C(19)	0.3856(10)	0.4234(8)	0.508(2)	1.1(2)	1.0000
C(20)	0.4300(10)	0.4170(8)	0.716(2)	1.0(2)	1.0000
H(1)	0.3199	-0.2436	-0.4387	0.8470	1.0000
H(2)	0.3292	-0.2967	-0.6363	0.8470	1.0000
H(3)	0.4502	-0.3120	-0.4215	1.1607	1.0000
H(4)	0.3547	-0.3534	-0.3606	1.1607	1.0000
H(5)	0.9916	0.3872	0.3687	1.1735	1.0000
H(6)	0.9512	0.4516	0.3628	1.1735	1.0000
H(7)	0.8270	0.3695	0.5405	1.6106	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(8)	0.9217	0.4105	0.6864	1.6106	1.0000
H(9)	-0.1480	-0.2291	-0.3372	1.2406	1.0000
H(10)	-0.1069	-0.2677	-0.5062	1.2406	1.0000
H(11)	0.0137	-0.2501	-0.2401	1.0141	1.0000
H(12)	-0.0804	-0.3105	-0.2098	1.0141	1.0000
H(13)	0.4002	0.4788	0.5056	1.3342	1.0000
H(14)	0.3209	0.3966	0.4939	1.3342	1.0000
H(15)	0.3991	0.4313	0.8245	1.2293	1.0000
H(16)	0.4924	0.4548	0.7463	1.2293	1.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Se(1)	0.0037(6)	0.0081(7)	0.0101(8)	-0.0012(6)	-0.0020(6)	-0.0016(5)
Se(2)	0.0040(6)	0.0085(7)	0.0107(8)	-0.0008(6)	-0.0023(6)	-0.0008(6)
Se(3)	0.0033(6)	0.0085(7)	0.0086(8)	-0.0017(6)	0.0000(6)	-0.0004(5)
Se(4)	0.0038(6)	0.0074(7)	0.0117(8)	-0.0011(6)	-0.0021(6)	-0.0007(5)
Se(5)	0.0030(6)	0.0095(7)	0.0092(8)	-0.0011(6)	-0.0014(6)	-0.0012(5)
Se(6)	0.0038(6)	0.0079(7)	0.0101(8)	-0.0017(6)	-0.0018(6)	-0.0005(5)
Se(7)	0.0036(6)	0.0074(7)	0.0107(8)	-0.0016(6)	-0.0013(6)	-0.0003(5)
Se(8)	0.0027(6)	0.0085(7)	0.0102(8)	-0.0018(6)	-0.0013(6)	-0.0008(6)
Ga(1)	0.0019(7)	0.0092(8)	0.0139(9)	-0.0012(6)	-0.0029(7)	-0.0003(6)
Cl(1)	0.008(1)	0.019(2)	0.016(2)	0.005(1)	-0.001(1)	0.000(1)
Cl(2)	-0.0016(8)	0.0063(10)	0.006(1)	-0.0036(7)	-0.0017(8)	-0.0023(7)
Cl(3)	0.004(1)	0.012(2)	0.013(2)	0.000(1)	-0.002(1)	0.000(1)
Cl(4)	0.007(1)	0.017(1)	0.013(1)	0.0038(10)	0.001(1)	0.0004(9)
S(1)	0.005(2)	0.011(2)	0.012(2)	-0.001(1)	-0.002(2)	-0.001(1)
S(2)	0.007(2)	0.009(2)	0.016(2)	-0.001(1)	-0.002(2)	-0.002(1)
S(3)	0.007(2)	0.008(2)	0.011(2)	-0.002(1)	0.001(2)	0.001(1)
S(4)	0.006(2)	0.011(2)	0.012(2)	-0.001(1)	-0.003(2)	0.000(1)
S(5)	0.003(1)	0.011(2)	0.008(2)	-0.004(1)	0.000(2)	0.000(1)
S(6)	0.006(2)	0.009(2)	0.013(2)	-0.003(1)	-0.001(2)	-0.001(1)
S(7)	0.006(2)	0.007(2)	0.012(2)	-0.002(1)	-0.001(2)	-0.001(1)
S(8)	0.007(2)	0.008(2)	0.013(2)	0.000(1)	-0.004(2)	-0.002(1)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Se(1)	C(1)	1.84(1)	Se(1)	C(2)	1.89(1)
Se(2)	C(1)	1.92(1)	Se(2)	C(3)	1.94(1)
Se(3)	C(6)	1.85(1)	Se(3)	C(7)	1.87(1)
Se(4)	C(6)	1.92(1)	Se(4)	C(8)	1.90(1)
Se(5)	C(11)	1.86(1)	Se(5)	C(12)	1.89(1)
Se(6)	C(11)	1.92(1)	Se(6)	C(13)	1.91(1)
Se(7)	C(16)	1.83(1)	Se(7)	C(17)	1.88(1)
Se(8)	C(16)	1.94(1)	Se(8)	C(18)	1.91(1)
Ga(1)	Cl(1)	2.205(4)	Ga(1)	Cl(2)	2.280(2)
Ga(1)	Cl(3)	2.196(3)	Ga(1)	Cl(4)	2.266(3)
S(1)	C(2)	1.73(1)	S(1)	C(4)	1.77(1)
S(2)	C(3)	1.78(1)	S(2)	C(5)	1.81(1)
S(3)	C(7)	1.77(1)	S(3)	C(9)	1.82(1)
S(4)	C(8)	1.77(1)	S(4)	C(10)	1.82(1)
S(5)	C(12)	1.73(1)	S(5)	C(14)	1.81(1)
S(6)	C(13)	1.77(1)	S(6)	C(15)	1.84(1)
S(7)	C(17)	1.74(1)	S(7)	C(19)	1.88(2)
S(8)	C(18)	1.77(1)	S(8)	C(20)	1.85(1)
C(1)	C(6)	1.37(2)	C(2)	C(3)	1.31(2)
C(4)	C(5)	1.56(2)	C(7)	C(8)	1.35(2)
C(9)	C(10)	1.59(2)	C(11)	C(16)	1.36(2)
C(12)	C(13)	1.35(2)	C(14)	C(15)	1.51(2)
C(17)	C(18)	1.35(2)	C(19)	C(20)	1.51(2)