Crystal data for **5e**

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{49}H_{32}N_2S_2SeCl_2$
Formula Weight	862.79
Crystal Color, Habit	gold, plate
Crystal Dimensions	0.53 X 0.18 X 0.03 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	4 oscillations @ 3.3 minutes
Detector Position	86.60 mm
Detector Swing Angle	0.00°
Pixel Size	0.100 mm
Lattice Parameters	a = 17.752(2)Å b = 11.020(1) Å c = 21.341(2) Å β = 106.958(3)°
	V = 3993.4(7) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.435 g/cm^3
F_{000}	1760.00
μ(MoKα)	12.17 cm^{-1}

B. Intensity Measurements

Diffractometer	RAXIS-IV

Radiation	MoKα (λ = 0.71070 Å) graphite monochromated
Detector Aperture	300 mm x 300 mm
Data Images	45 exposures @ 21.0 minutes
Oscillation Range	3.0°
Detector Position	86.60 mm
Detector Swing Angle	0.00°
Pixel Size	0.100 mm
$2\theta_{max}$	55.5°
No. of Reflections Measured	Total: 7767
Corrections	Lorentz-polarization Secondary Extinction (coefficient: 6.47400e-07)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.0500
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	4539
No. Variables	626
Reflection/Parameter Ratio	7.25
Residuals: R; Rw	0.070 ; 0.083
Residuals: R1	0.070
No. of Reflections to calc R1	4539
Goodness of Fit Indicator	2.05

Max Shift/Error in Final Cycle	0.30
Maximum peak in Final Diff. Map	0.65 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-1.27 $e^-/\AA^3$

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

atom	x	y	z	B_{eq}
Se(1)	0.55161(3)	-0.21947(5)	0.38820(3)	2.74(1)
Cl(1)	0.4337(1)	0.3982(2)	0.1684(2)	8.56(8)
Cl(2)	0.5631(2)	0.2664(3)	0.2587(2)	9.39(8)
S(1)	0.30509(8)	0.0709(1)	0.21058(7)	2.91(3)
S(2)	0.26502(8)	0.0722(1)	0.34194(7)	2.75(3)
N(1)	0.3437(2)	-0.0359(4)	0.4559(2)	2.33(9)
N(2)	0.4372(2)	-0.0139(4)	0.1859(2)	2.58(9)
C(1)	0.2944(3)	0.1210(5)	0.1313(3)	2.4(1)
C(2)	0.2335(3)	0.2060(5)	0.1129(3)	2.7(1)
C(3)	0.1979(3)	0.2302(5)	0.1617(3)	2.8(1)
C(4)	0.2295(3)	0.1640(5)	0.2179(3)	2.7(1)
C(5)	0.2103(3)	0.1638(5)	0.2790(3)	2.6(1)
C(6)	0.1544(3)	0.2295(5)	0.2986(3)	2.8(1)
C(7)	0.1564(3)	0.2068(5)	0.3623(3)	2.8(1)
C(8)	0.2133(3)	0.1228(5)	0.3949(3)	2.4(1)
C(9)	0.2306(3)	0.0816(5)	0.4608(3)	2.7(1)
C(10)	0.2912(3)	0.0018(5)	0.4893(3)	2.4(1)
C(11)	0.3151(3)	-0.0517(5)	0.5542(3)	2.7(1)
C(12)	0.3783(3)	-0.1209(5)	0.5595(3)	2.6(1)
C(13)	0.3970(3)	-0.1090(5)	0.4971(3)	2.3(1)
C(14)	0.4618(3)	-0.1647(5)	0.4801(3)	2.3(1)
C(15)	0.4840(3)	-0.1275(5)	0.4251(3)	2.4(1)
C(16)	0.4560(3)	-0.0279(5)	0.3837(3)	2.7(1)
C(17)	0.4744(3)	-0.0230(5)	0.3273(3)	2.5(1)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(42)	0.6830(3)	-0.2111(6)	0.2913(3)	3.9(1)
C(43)	0.3189(3)	0.1150(5)	0.0227(3)	2.5(1)
C(44)	0.3610(4)	0.1981(6)	-0.0035(3)	3.6(1)
C(45)	0.3360(4)	0.2258(6)	-0.0697(3)	4.1(1)
C(46)	0.2702(4)	0.1728(7)	-0.1106(3)	4.9(2)
C(47)	0.2270(4)	0.0903(7)	-0.0857(3)	4.6(2)
C(48)	0.2511(3)	0.0633(5)	-0.0185(3)	3.2(1)
C(49)	0.4680(6)	0.304(1)	0.2409(6)	9.5(3)
H(1)	0.218(3)	0.244(5)	0.071(3)	3(1)
H(2)	0.156(3)	0.287(4)	0.157(2)	3(1)
H(3)	0.119(4)	0.284(5)	0.271(3)	3(1)
H(4)	0.122(3)	0.245(5)	0.383(3)	3(1)
H(5)	0.290(3)	-0.039(5)	0.587(3)	3(1)
H(6)	0.406(2)	-0.168(4)	0.596(2)	3.1(8)
H(7)	0.425(4)	0.034(6)	0.395(4)	3(1)
H(8)	0.455(3)	0.041(5)	0.297(3)	2(1)
H(9)	0.573(3)	-0.121(5)	0.130(3)	3(1)
H(10)	0.471(3)	-0.008(5)	0.046(3)	3(1)
H(11)	0.123(3)	-0.030(6)	0.506(3)	4(1)
H(12)	0.044(4)	0.049(7)	0.568(4)	5(1)
H(13)	0.050(4)	0.253(6)	0.595(4)	5(1)
H(14)	0.140(3)	0.378(5)	0.566(3)	4(1)
H(15)	0.219(3)	0.302(5)	0.505(3)	3(1)
H(16)	0.616(3)	-0.202(5)	0.533(3)	3(1)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(18)	0.5228(3)	-0.1146(5)	0.3144(3)	2.7(1)
C(19)	0.5437(3)	-0.1338(5)	0.2563(3)	2.5(1)
C(20)	0.5042(3)	-0.0774(5)	0.1963(3)	2.5(1)
C(21)	0.5272(3)	-0.0821(5)	0.1359(3)	3.2(1)
C(22)	0.4722(3)	-0.0210(5)	0.0899(3)	3.1(1)
C(23)	0.4147(3)	0.0203(5)	0.1217(3)	2.6(1)
C(24)	0.3443(3)	0.0824(5)	0.0932(3)	2.8(1)
C(25)	0.1792(3)	0.1282(5)	0.5001(3)	2.9(1)
C(26)	0.1268(4)	0.0531(6)	0.5181(3)	3.7(1)
C(27)	0.0789(4)	0.1009(7)	0.5546(4)	4.6(2)
C(28)	0.0830(4)	0.2211(7)	0.5711(3)	4.4(2)
C(29)	0.1358(4)	0.2953(6)	0.5533(3)	4.1(2)
C(30)	0.1831(4)	0.2495(5)	0.5175(3)	3.2(1)
C(31)	0.5051(3)	-0.2642(5)	0.5233(3)	2.5(1)
C(32)	0.5871(3)	-0.2641(5)	0.5462(3)	2.9(1)
C(33)	0.6261(4)	-0.3571(6)	0.5883(3)	3.7(1)
C(34)	0.5836(4)	-0.4474(5)	0.6065(4)	4.3(2)
C(35)	0.5031(4)	-0.4469(6)	0.5833(4)	4.3(2)
C(36)	0.4633(4)	-0.3583(5)	0.5420(3)	3.3(1)
C(37)	0.6043(3)	-0.2293(5)	0.2555(3)	2.9(1)
C(38)	0.5831(4)	-0.3341(5)	0.2198(3)	3.9(1)
C(39)	0.6407(5)	-0.4193(7)	0.2191(4)	5.3(2)
C(40)	0.7185(4)	-0.3991(7)	0.2536(3)	5.0(2)
C(41)	0.7397(4)	-0.2959(7)	0.2895(4)	4.9(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(17)	0.682(3)	-0.357(5)	0.604(3)	4(1)
H(18)	0.610(3)	-0.510(5)	0.635(3)	5(1)
H(19)	0.474(4)	-0.510(6)	0.596(3)	5(1)
H(20)	0.407(3)	-0.361(5)	0.526(3)	3(1)
H(21)	0.530(3)	-0.348(5)	0.196(3)	4(1)
H(22)	0.626(3)	-0.492(5)	0.195(3)	6(1)
H(23)	0.757(5)	-0.458(7)	0.252(4)	5(1)
H(24)	0.793(3)	-0.282(5)	0.313(3)	5(1)
H(25)	0.698(4)	-0.140(7)	0.317(4)	4(1)
H(26)	0.407(3)	0.236(5)	0.024(3)	4(1)
H(27)	0.365(4)	0.283(5)	-0.087(3)	4(1)
H(28)	0.254(4)	0.192(6)	-0.156(4)	5(1)
H(29)	0.182(3)	0.053(4)	-0.114(3)	5(1)
H(30)	0.221(3)	0.009(5)	-0.001(3)	3(1)
H(31)	0.4604	0.3478	0.2771	11.3616
H(32)	0.4376	0.2322	0.2343	11.3616

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Se(1)	0.0352(3)	0.0359(3)	0.0335(3)	0.0063(2)	0.0110(2)	0.0050(3)
Cl(1)	0.076(1)	0.081(2)	0.159(3)	0.007(1)	0.019(2)	0.021(2)
Cl(2)	0.095(2)	0.144(2)	0.102(2)	-0.015(2)	0.004(2)	0.051(2)
S(1)	0.0351(7)	0.0462(8)	0.0297(7)	0.0118(6)	0.0102(6)	0.0071(6)
S(2)	0.0338(7)	0.0425(8)	0.0282(7)	0.0084(6)	0.0093(6)	0.0033(6)
N(1)	0.028(2)	0.031(2)	0.030(2)	0.000(2)	0.009(2)	-0.001(2)
N(2)	0.029(2)	0.039(2)	0.029(2)	0.003(2)	0.008(2)	0.003(2)
C(1)	0.029(3)	0.037(3)	0.026(3)	0.002(2)	0.008(2)	-0.001(2)
C(2)	0.040(3)	0.030(3)	0.031(3)	0.002(2)	0.008(2)	0.004(2)
C(3)	0.033(3)	0.038(3)	0.035(3)	0.008(2)	0.007(2)	-0.001(2)
C(4)	0.032(3)	0.040(3)	0.028(3)	0.001(2)	0.007(2)	0.004(2)
C(5)	0.033(3)	0.026(3)	0.039(3)	0.003(2)	0.011(2)	-0.002(2)
C(6)	0.037(3)	0.037(3)	0.036(3)	0.009(2)	0.014(2)	0.006(3)
C(7)	0.036(3)	0.042(3)	0.031(3)	0.005(2)	0.012(2)	0.003(2)
C(8)	0.031(3)	0.029(3)	0.033(3)	0.004(2)	0.009(2)	-0.001(2)
C(9)	0.029(3)	0.044(3)	0.032(3)	-0.002(2)	0.010(2)	-0.002(2)
C(10)	0.030(3)	0.033(3)	0.029(3)	-0.003(2)	0.008(2)	-0.001(2)
C(11)	0.032(3)	0.043(3)	0.029(3)	-0.001(2)	0.010(2)	0.002(2)
C(12)	0.033(3)	0.039(3)	0.025(3)	-0.002(2)	0.005(2)	0.002(2)
C(13)	0.026(2)	0.035(3)	0.024(3)	-0.005(2)	0.004(2)	0.003(2)
C(14)	0.027(2)	0.033(3)	0.026(3)	-0.003(2)	0.005(2)	0.001(2)
C(15)	0.026(2)	0.033(3)	0.026(3)	-0.007(2)	-0.002(2)	0.006(2)
C(16)	0.028(3)	0.034(3)	0.036(3)	-0.006(2)	0.004(2)	0.004(2)
C(17)	0.027(3)	0.040(3)	0.025(3)	0.002(2)	0.006(2)	-0.005(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(18)	0.027(3)	0.044(3)	0.032(3)	-0.001(2)	0.009(2)	-0.009(2)
C(19)	0.028(3)	0.028(3)	0.036(3)	0.001(2)	0.006(2)	0.001(2)
C(20)	0.029(2)	0.039(3)	0.028(3)	0.002(2)	0.012(2)	0.003(2)
C(21)	0.035(3)	0.052(4)	0.037(3)	0.011(3)	0.016(2)	0.004(3)
C(22)	0.041(3)	0.045(3)	0.035(3)	0.006(3)	0.017(3)	0.008(3)
C(23)	0.028(3)	0.042(3)	0.030(3)	-0.001(2)	0.012(2)	0.001(2)
C(24)	0.034(3)	0.035(3)	0.035(3)	0.002(2)	0.007(2)	0.005(2)
C(25)	0.032(3)	0.047(3)	0.032(3)	0.001(2)	0.009(2)	0.001(3)
C(26)	0.041(3)	0.045(3)	0.061(4)	-0.004(3)	0.024(3)	-0.003(3)
C(27)	0.041(3)	0.086(5)	0.055(4)	-0.006(3)	0.027(3)	-0.005(4)
C(28)	0.047(3)	0.081(5)	0.042(4)	0.017(4)	0.014(3)	-0.006(4)
C(29)	0.062(4)	0.048(4)	0.048(4)	0.012(3)	0.022(3)	0.001(3)
C(30)	0.048(3)	0.041(4)	0.038(3)	-0.001(2)	0.020(3)	-0.002(2)
C(31)	0.032(3)	0.035(3)	0.029(3)	0.001(2)	0.008(2)	0.004(2)
C(32)	0.038(3)	0.038(3)	0.031(3)	0.004(2)	0.004(2)	0.005(2)
C(33)	0.044(3)	0.049(4)	0.042(4)	0.011(3)	0.005(3)	0.008(3)
C(34)	0.073(4)	0.027(3)	0.065(4)	0.021(3)	0.022(4)	0.015(3)
C(35)	0.069(4)	0.038(3)	0.059(4)	0.002(3)	0.024(4)	0.015(3)
C(36)	0.046(3)	0.038(3)	0.044(3)	0.001(3)	0.014(3)	0.008(3)
C(37)	0.037(3)	0.038(3)	0.033(3)	0.009(2)	0.009(2)	0.006(3)
C(38)	0.049(4)	0.036(3)	0.058(4)	0.007(3)	0.011(3)	-0.009(3)
C(39)	0.089(5)	0.060(4)	0.061(5)	0.024(4)	0.032(4)	-0.002(4)
C(40)	0.064(4)	0.080(5)	0.046(4)	0.039(4)	0.017(3)	0.013(4)
C(41)	0.043(3)	0.093(5)	0.045(4)	0.026(4)	0.006(3)	-0.003(4)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(42)	0.035(3)	0.074(4)	0.037(3)	0.015(3)	0.008(3)	-0.002(3)
C(43)	0.032(3)	0.034(3)	0.030(3)	0.004(2)	0.011(2)	0.002(2)
C(44)	0.048(3)	0.049(4)	0.042(3)	0.007(3)	0.018(3)	0.008(3)
C(45)	0.064(4)	0.048(4)	0.049(4)	0.021(3)	0.028(3)	0.014(3)
C(46)	0.081(4)	0.080(5)	0.031(3)	0.045(4)	0.025(3)	0.019(3)
C(47)	0.053(4)	0.084(5)	0.033(3)	0.021(4)	0.005(3)	-0.007(3)
C(48)	0.041(3)	0.044(3)	0.035(3)	0.008(3)	0.010(3)	-0.002(3)
C(49)	0.126(7)	0.138(9)	0.129(8)	-0.032(7)	0.088(5)	-0.005(7)

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(Å)

atom	atom	distance	atom	atom	distance
Se(1)	C(15)	1.907(6)	Se(1)	C(18)	1.898(6)
Cl(1)	C(49)	1.81(1)	Cl(2)	C(49)	1.67(1)
S(1)	C(1)	1.737(6)	S(1)	C(4)	1.732(6)
S(2)	C(5)	1.734(5)	S(2)	C(8)	1.742(6)
N(1)	C(10)	1.392(7)	N(1)	C(13)	1.353(6)
N(2)	C(20)	1.341(7)	N(2)	C(23)	1.365(7)
C(1)	C(2)	1.397(7)	C(1)	C(24)	1.432(8)
C(2)	C(3)	1.391(8)	C(3)	C(4)	1.377(8)
C(4)	C(5)	1.441(8)	C(5)	C(6)	1.388(8)
C(6)	C(7)	1.372(8)	C(7)	C(8)	1.398(7)
C(8)	C(9)	1.424(8)	C(9)	C(10)	1.386(7)
C(9)	C(25)	1.498(8)	C(10)	C(11)	1.449(8)
C(11)	C(12)	1.334(8)	C(12)	C(13)	1.469(8)
C(13)	C(14)	1.442(7)	C(14)	C(15)	1.404(8)
C(14)	C(31)	1.493(7)	C(15)	C(16)	1.406(7)
C(16)	C(17)	1.338(8)	C(17)	C(18)	1.404(7)
C(18)	C(19)	1.411(8)	C(19)	C(20)	1.412(7)
C(19)	C(37)	1.509(7)	C(20)	C(21)	1.463(8)
C(21)	C(22)	1.345(8)	C(22)	C(23)	1.453(8)
C(23)	C(24)	1.398(7)	C(24)	C(43)	1.485(8)
C(25)	C(26)	1.381(8)	C(25)	C(30)	1.385(8)
C(26)	C(27)	1.413(9)	C(27)	C(28)	1.37(1)
C(28)	C(29)	1.378(10)	C(29)	C(30)	1.383(9)
C(31)	C(32)	1.393(8)	C(31)	C(36)	1.400(8)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(32)	C(33)	1.406(8)	C(33)	C(34)	1.372(9)
C(34)	C(35)	1.370(10)	C(35)	C(36)	1.366(9)
C(37)	C(38)	1.374(8)	C(37)	C(42)	1.397(8)
C(38)	C(39)	1.391(9)	C(39)	C(40)	1.38(1)
C(40)	C(41)	1.36(1)	C(41)	C(42)	1.383(9)
C(43)	C(44)	1.396(8)	C(43)	C(48)	1.389(8)
C(44)	C(45)	1.386(9)	C(45)	C(46)	1.37(1)
C(46)	C(47)	1.39(1)	C(47)	C(48)	1.403(9)

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C(2)	H(1)	1.02(6)	C(3)	H(2)	1.00(5)
C(6)	H(3)	0.88(6)	C(7)	H(4)	0.89(6)
C(11)	H(5)	0.85(6)	C(12)	H(6)	0.97(4)
C(16)	H(7)	0.89(7)	C(17)	H(8)	0.94(6)
C(21)	H(9)	1.01(5)	C(22)	H(10)	0.97(6)
C(26)	H(11)	1.14(6)	C(27)	H(12)	0.95(7)
C(28)	H(13)	1.09(8)	C(29)	H(14)	0.99(5)
C(30)	H(15)	1.09(5)	C(32)	H(16)	1.07(6)
C(33)	H(17)	1.03(6)	C(34)	H(18)	1.05(6)
C(35)	H(19)	0.80(6)	C(36)	H(20)	1.07(5)
C(38)	H(21)	1.04(5)	C(39)	H(22)	1.11(6)
C(40)	H(23)	1.18(8)	C(41)	H(24)	1.04(5)
C(42)	H(25)	0.95(7)	C(44)	H(26)	0.91(5)
C(45)	H(27)	0.94(6)	C(46)	H(28)	0.88(7)
C(47)	H(29)	1.11(5)	C(48)	H(30)	1.09(6)
C(49)	H(31)	0.95	C(49)	H(32)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(15)	Se(1)	C(18)	88.2(2)	C(1)	S(1)	C(4)	91.9(3)
C(5)	S(2)	C(8)	91.9(3)	C(10)	N(1)	C(13)	106.8(4)
C(20)	N(2)	C(23)	107.1(5)	S(1)	C(1)	C(2)	110.0(4)
S(1)	C(1)	C(24)	123.3(4)	C(2)	C(1)	C(24)	126.6(5)
C(1)	C(2)	C(3)	113.6(5)	C(2)	C(3)	C(4)	113.1(5)
S(1)	C(4)	C(3)	111.3(4)	S(1)	C(4)	C(5)	118.4(4)
C(3)	C(4)	C(5)	130.2(5)	S(2)	C(5)	C(4)	118.3(4)
S(2)	C(5)	C(6)	111.0(4)	C(4)	C(5)	C(6)	130.6(5)
C(5)	C(6)	C(7)	112.9(5)	C(6)	C(7)	C(8)	114.8(5)
S(2)	C(8)	C(7)	109.4(4)	S(2)	C(8)	C(9)	122.4(4)
C(7)	C(8)	C(9)	128.2(5)	C(8)	C(9)	C(10)	123.6(5)
C(8)	C(9)	C(25)	116.9(5)	C(10)	C(9)	C(25)	119.5(5)
N(1)	C(10)	C(9)	120.9(5)	N(1)	C(10)	C(11)	108.3(4)
C(9)	C(10)	C(11)	130.7(5)	C(10)	C(11)	C(12)	108.6(5)
C(11)	C(12)	C(13)	106.1(5)	N(1)	C(13)	C(12)	110.0(5)
N(1)	C(13)	C(14)	123.2(5)	C(12)	C(13)	C(14)	126.8(4)
C(13)	C(14)	C(15)	121.7(5)	C(13)	C(14)	C(31)	117.5(5)
C(15)	C(14)	C(31)	120.8(5)	Se(1)	C(15)	C(14)	123.6(4)
Se(1)	C(15)	C(16)	107.8(4)	C(14)	C(15)	C(16)	128.2(5)
C(15)	C(16)	C(17)	117.5(5)	C(16)	C(17)	C(18)	118.1(5)
Se(1)	C(18)	C(17)	107.9(4)	Se(1)	C(18)	C(19)	124.2(4)
C(17)	C(18)	C(19)	127.7(5)	C(18)	C(19)	C(20)	122.9(5)
C(18)	C(19)	C(37)	119.0(5)	C(20)	C(19)	C(37)	117.7(5)
N(2)	C(20)	C(19)	124.1(5)	N(2)	C(20)	C(21)	109.6(5)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(19)	C(20)	C(21)	126.2(5)	C(20)	C(21)	C(22)	107.1(5)
C(21)	C(22)	C(23)	106.0(5)	N(2)	C(23)	C(22)	110.1(4)
N(2)	C(23)	C(24)	122.3(5)	C(22)	C(23)	C(24)	127.6(5)
C(1)	C(24)	C(23)	121.5(5)	C(1)	C(24)	C(43)	116.7(5)
C(23)	C(24)	C(43)	121.9(5)	C(9)	C(25)	C(26)	121.4(5)
C(9)	C(25)	C(30)	119.5(5)	C(26)	C(25)	C(30)	119.2(6)
C(25)	C(26)	C(27)	119.6(6)	C(26)	C(27)	C(28)	120.5(7)
C(27)	C(28)	C(29)	119.6(7)	C(28)	C(29)	C(30)	120.4(6)
C(25)	C(30)	C(29)	120.7(6)	C(14)	C(31)	C(32)	120.9(5)
C(14)	C(31)	C(36)	119.9(5)	C(32)	C(31)	C(36)	119.2(5)
C(31)	C(32)	C(33)	119.5(6)	C(32)	C(33)	C(34)	120.1(6)
C(33)	C(34)	C(35)	119.8(6)	C(34)	C(35)	C(36)	121.6(6)
C(31)	C(36)	C(35)	119.7(6)	C(19)	C(37)	C(38)	120.8(5)
C(19)	C(37)	C(42)	119.7(5)	C(38)	C(37)	C(42)	119.5(6)
C(37)	C(38)	C(39)	119.4(6)	C(38)	C(39)	C(40)	120.6(7)
C(39)	C(40)	C(41)	120.3(6)	C(40)	C(41)	C(42)	119.7(6)
C(37)	C(42)	C(41)	120.5(6)	C(24)	C(43)	C(44)	121.6(5)
C(24)	C(43)	C(48)	119.5(5)	C(44)	C(43)	C(48)	118.8(5)
C(43)	C(44)	C(45)	120.1(6)	C(44)	C(45)	C(46)	121.1(7)
C(45)	C(46)	C(47)	119.9(6)	C(46)	C(47)	C(48)	119.4(6)
C(43)	C(48)	C(47)	120.6(6)	Cl(1)	C(49)	Cl(2)	113.7(6)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(1)	121(3)	C(3)	C(2)	H(1)	124(3)
C(2)	C(3)	H(2)	119(3)	C(4)	C(3)	H(2)	127(3)
C(5)	C(6)	H(3)	117(4)	C(7)	C(6)	H(3)	129(4)
C(6)	C(7)	H(4)	125(3)	C(8)	C(7)	H(4)	119(3)
C(10)	C(11)	H(5)	116(3)	C(12)	C(11)	H(5)	134(3)
C(11)	C(12)	H(6)	131(2)	C(13)	C(12)	H(6)	122(2)
C(15)	C(16)	H(7)	116(4)	C(17)	C(16)	H(7)	125(4)
C(16)	C(17)	H(8)	122(3)	C(18)	C(17)	H(8)	119(3)
C(20)	C(21)	H(9)	121(3)	C(22)	C(21)	H(9)	130(3)
C(21)	C(22)	H(10)	131(3)	C(23)	C(22)	H(10)	122(3)
C(25)	C(26)	H(11)	119(3)	C(27)	C(26)	H(11)	120(3)
C(26)	C(27)	H(12)	110(4)	C(28)	C(27)	H(12)	129(4)
C(27)	C(28)	H(13)	120(3)	C(29)	C(28)	H(13)	119(3)
C(28)	C(29)	H(14)	122(3)	C(30)	C(29)	H(14)	117(3)
C(25)	C(30)	H(15)	122(2)	C(29)	C(30)	H(15)	116(2)
C(31)	C(32)	H(16)	116(3)	C(33)	C(32)	H(16)	124(3)
C(32)	C(33)	H(17)	118(3)	C(34)	C(33)	H(17)	121(3)
C(33)	C(34)	H(18)	121(3)	C(35)	C(34)	H(18)	117(3)
C(34)	C(35)	H(19)	135(4)	C(36)	C(35)	H(19)	102(4)
C(31)	C(36)	H(20)	119(2)	C(35)	C(36)	H(20)	120(2)
C(37)	C(38)	H(21)	117(3)	C(39)	C(38)	H(21)	122(3)
C(38)	C(39)	H(22)	116(3)	C(40)	C(39)	H(22)	122(3)
C(39)	C(40)	H(23)	120(3)	C(41)	C(40)	H(23)	118(3)
C(40)	C(41)	H(24)	112(3)	C(42)	C(41)	H(24)	127(3)

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(37)	C(42)	H(25)	113(4)	C(41)	C(42)	H(25)	125(4)
C(43)	C(44)	H(26)	121(3)	C(45)	C(44)	H(26)	118(3)
C(44)	C(45)	H(27)	106(4)	C(46)	C(45)	H(27)	132(4)
C(45)	C(46)	H(28)	108(4)	C(47)	C(46)	H(28)	131(4)
C(46)	C(47)	H(29)	119(2)	C(48)	C(47)	H(29)	120(2)
C(43)	C(48)	H(30)	120(2)	C(47)	C(48)	H(30)	118(2)
Cl(1)	C(49)	H(31)	108.3	Cl(1)	C(49)	H(32)	108.3
Cl(2)	C(49)	H(31)	108.4	Cl(2)	C(49)	H(32)	108.4
H(31)	C(49)	H(32)	109.5				

Crystal data for **6b**

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{50}H_{34}N_3Se_2Cl_3$
Formula Weight	941.12
Crystal Color, Habit	green, cubic
Crystal Dimensions	0.50 X 0.25 X 0.20 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 4.0 minutes
Detector Position	86.60 mm
Detector Swing Angle	0.00°
Pixel Size	0.100 mm
Lattice Parameters	a = 17.1534(3)Å b = 9.8246(3) Å c = 25.0922(6) Å β = 106.151(1)°
	V = 4061.8(2) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.539 g/cm^3
F_{000}	1896.00
μ(MoKα)	20.59 cm^{-1}

B. Intensity Measurements

Diffractometer	RAXIS-IV

Radiation	MoKα (λ = 0.71070 Å) graphite monochromated
Detector Aperture	300 mm x 300 mm
Data Images	20 exposures @ 30.0 minutes
Oscillation Range	5.0°
Detector Position	86.60 mm
Detector Swing Angle	0.00°
Pixel Size	0.100 mm
$2\theta_{max}$	55.5°
No. of Reflections Measured	Total: 6826
Corrections	Lorentz-polarization Secondary Extinction (coefficient: 4.11150e-07)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.0700
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	6773
No. Variables	524
Reflection/Parameter Ratio	12.93
Residuals: R; Rw	0.058 ; 0.083
Residuals: R1	0.058
No. of Reflections to calc R1	6773
Goodness of Fit Indicator	1.95

Max Shift/Error in Final Cycle	0.07
Maximum peak in Final Diff. Map	1.76 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-1.59 $e^-/\AA^3$

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

atom	x	y	z	B_{eq}
Se(1)	0.80489(2)	-0.03310(5)	0.04629(2)	2.548(10)
Se(2)	0.84784(3)	0.13514(5)	-0.04430(2)	2.84(1)
Cl(1)	0.65359(8)	-0.4674(2)	-0.04332(6)	4.03(3)
Cl(2)	0.8156(1)	-0.4624(3)	0.0280(1)	8.82(7)
Cl(3)	0.7795(2)	-0.3453(4)	-0.08223(10)	10.62(9)
N(1)	0.7630(2)	0.1967(4)	-0.1421(2)	2.55(8)
N(2)	0.5806(2)	-0.0357(4)	-0.1143(1)	2.07(7)
N(3)	0.6720(2)	-0.1605(4)	0.0455(1)	2.24(7)
C(1)	0.8305(2)	-0.1162(5)	0.1167(2)	2.34(9)
C(2)	0.9132(3)	-0.0872(5)	0.1450(2)	2.54(9)
C(3)	0.9555(3)	-0.0069(5)	0.1178(2)	2.67(9)
C(4)	0.9131(3)	0.0358(5)	0.0643(2)	2.48(9)
C(5)	0.9318(2)	0.1145(5)	0.0227(2)	2.52(9)
C(6)	1.0025(3)	0.1850(5)	0.0197(2)	2.90(10)
C(7)	0.9952(3)	0.2513(5)	-0.0299(2)	2.77(9)
C(8)	0.9188(3)	0.2448(5)	-0.0709(2)	2.57(9)
C(9)	0.8944(2)	0.3012(5)	-0.1240(2)	2.39(9)
C(10)	0.8148(3)	0.2763(5)	-0.1596(2)	2.34(9)
C(11)	0.7764(3)	0.3254(5)	-0.2151(2)	2.79(10)
C(12)	0.7003(3)	0.2715(5)	-0.2306(2)	2.57(9)
C(13)	0.6918(2)	0.1914(5)	-0.1844(2)	2.29(8)
C(14)	0.6241(2)	0.1210(4)	-0.1785(2)	2.18(8)
C(15)	0.6203(2)	0.0794(5)	-0.1249(2)	2.03(8)
C(16)	0.6504(2)	0.1482(4)	-0.0739(2)	2.14(8)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(17)	0.6314(2)	0.0728(5)	-0.0330(2)	2.09(8)
C(18)	0.5877(2)	-0.0433(4)	-0.0577(2)	2.06(8)
C(19)	0.5506(2)	-0.1456(4)	-0.0318(2)	1.99(8)
C(20)	0.5909(2)	-0.1857(4)	0.0226(2)	2.02(8)
C(21)	0.5584(2)	-0.2517(5)	0.0634(2)	2.21(8)
C(22)	0.6209(2)	-0.2653(5)	0.1104(2)	2.19(8)
C(23)	0.6924(2)	-0.2069(4)	0.0981(2)	2.10(8)
C(24)	0.7725(2)	-0.1908(4)	0.1341(2)	2.17(8)
C(25)	0.9506(2)	0.3933(5)	-0.1434(2)	2.56(9)
C(26)	0.9679(3)	0.3678(5)	-0.1940(2)	2.93(10)
C(27)	1.0187(3)	0.4533(6)	-0.2125(2)	3.7(1)
C(28)	1.0534(3)	0.5659(7)	-0.1809(3)	4.2(1)
C(29)	1.0372(3)	0.5926(6)	-0.1308(3)	3.8(1)
C(30)	0.9862(3)	0.5047(5)	-0.1121(2)	3.0(1)
C(31)	0.5527(3)	0.0913(5)	-0.2265(2)	2.39(8)
C(32)	0.5608(3)	0.0376(6)	-0.2762(2)	2.90(10)
C(33)	0.4917(3)	-0.0012(6)	-0.3179(2)	3.5(1)
C(34)	0.4153(3)	0.0160(6)	-0.3109(2)	3.6(1)
C(35)	0.4071(3)	0.0763(6)	-0.2626(2)	3.6(1)
C(36)	0.4749(3)	0.1125(5)	-0.2206(2)	2.79(10)
C(37)	0.5600(3)	-0.1530(5)	-0.1521(2)	3.2(1)
C(38)	0.4695(2)	-0.1974(5)	-0.0615(2)	2.10(8)
C(39)	0.4451(3)	-0.3304(5)	-0.0550(2)	2.38(9)
C(40)	0.3668(3)	-0.3731(5)	-0.0806(2)	2.93(10)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(41)	0.3113(3)	-0.2838(5)	-0.1140(2)	2.97(10)
C(42)	0.3345(3)	-0.1537(5)	-0.1221(2)	2.65(9)
C(43)	0.4134(3)	-0.1095(5)	-0.0967(2)	2.31(9)
C(44)	0.7914(2)	-0.2523(5)	0.1904(2)	2.23(8)
C(45)	0.7744(3)	-0.3882(5)	0.1977(2)	2.62(9)
C(46)	0.7884(3)	-0.4452(6)	0.2501(2)	3.3(1)
C(47)	0.8201(3)	-0.3659(7)	0.2965(2)	4.0(1)
C(48)	0.8396(3)	-0.2314(7)	0.2904(2)	3.7(1)
C(49)	0.8256(3)	-0.1737(5)	0.2377(2)	2.86(10)
C(50)	0.7457(3)	-0.3768(6)	-0.0255(2)	3.8(1)
H(1)	0.9379	-0.1218	0.1811	3.0482
H(2)	1.0104	0.0183	0.1344	3.1985
H(3)	1.0510	0.1865	0.0494	3.4747
H(4)	1.0395	0.2996	-0.0365	3.3241
H(5)	0.7998	0.3841	-0.2365	3.3457
H(6)	0.6606	0.2841	-0.2652	3.0846
H(7)	0.6790	0.2322	-0.0687	2.5682
H(8)	0.6453	0.0951	0.0054	2.5020
H(9)	0.5039	-0.2801	0.0583	2.6480
H(10)	0.6185	-0.3048	0.1445	2.6225
H(11)	0.9444	0.2912	-0.2157	3.5135
H(12)	1.0301	0.4354	-0.2468	4.3985
H(13)	1.0883	0.6246	-0.1938	5.0018
H(14)	1.0603	0.6698	-0.1095	4.5792

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(15)	0.9760	0.5216	-0.0774	3.6380
H(16)	0.6131	0.0273	-0.2817	3.4810
H(17)	0.4974	-0.0398	-0.3514	4.1898
H(18)	0.3687	-0.0130	-0.3389	4.3441
H(19)	0.3545	0.0926	-0.2584	4.2629
H(20)	0.4686	0.1520	-0.1875	3.3503
H(21)	0.5326	-0.2196	-0.1366	3.7942
H(22)	0.5257	-0.1240	-0.1869	3.7942
H(23)	0.6083	-0.1910	-0.1573	3.7942
H(24)	0.4828	-0.3924	-0.0326	2.8550
H(25)	0.3509	-0.4636	-0.0753	3.5203
H(26)	0.2574	-0.3130	-0.1313	3.5590
H(27)	0.2966	-0.0932	-0.1451	3.1842
H(28)	0.4293	-0.0197	-0.1032	2.7696
H(29)	0.7528	-0.4435	0.1659	3.1488
H(30)	0.7761	-0.5383	0.2541	3.9769
H(31)	0.8286	-0.4037	0.3325	4.7825
H(32)	0.8627	-0.1776	0.3224	4.4819
H(33)	0.8394	-0.0812	0.2339	3.4320
H(34)	0.7354	-0.2912	-0.0112	4.5947

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Se(1)	0.0248(2)	0.0393(3)	0.0300(2)	-0.0063(2)	0.0031(2)	0.0074(2)
Se(2)	0.0270(2)	0.0452(3)	0.0336(3)	-0.0096(2)	0.0049(2)	0.0087(2)
Cl(1)	0.0410(6)	0.0596(9)	0.0519(8)	-0.0074(6)	0.0120(6)	-0.0035(7)
Cl(2)	0.054(1)	0.099(2)	0.151(2)	-0.007(1)	-0.023(1)	0.040(2)
Cl(3)	0.103(2)	0.244(4)	0.070(1)	-0.094(2)	0.048(1)	-0.029(2)
N(1)	0.031(2)	0.034(2)	0.032(2)	-0.005(2)	0.009(2)	0.002(2)
N(2)	0.030(2)	0.024(2)	0.024(2)	-0.003(1)	0.005(1)	0.001(1)
N(3)	0.026(2)	0.031(2)	0.027(2)	0.000(1)	0.004(1)	0.002(1)
C(1)	0.027(2)	0.027(2)	0.034(2)	0.000(2)	0.007(2)	0.000(2)
C(2)	0.027(2)	0.033(2)	0.033(2)	0.000(2)	0.002(2)	0.003(2)
C(3)	0.029(2)	0.036(3)	0.034(2)	-0.001(2)	0.005(2)	0.003(2)
C(4)	0.029(2)	0.030(2)	0.034(2)	-0.002(2)	0.008(2)	0.001(2)
C(5)	0.025(2)	0.033(3)	0.037(2)	-0.006(2)	0.008(2)	-0.001(2)
C(6)	0.032(2)	0.038(3)	0.040(3)	-0.003(2)	0.011(2)	0.004(2)
C(7)	0.026(2)	0.039(3)	0.038(2)	-0.005(2)	0.005(2)	0.004(2)
C(8)	0.028(2)	0.033(2)	0.037(2)	-0.007(2)	0.010(2)	0.000(2)
C(9)	0.026(2)	0.030(2)	0.037(2)	0.000(2)	0.011(2)	-0.001(2)
C(10)	0.031(2)	0.028(2)	0.031(2)	0.001(2)	0.012(2)	0.004(2)
C(11)	0.031(2)	0.034(3)	0.042(3)	-0.001(2)	0.013(2)	0.011(2)
C(12)	0.032(2)	0.032(2)	0.035(2)	0.000(2)	0.012(2)	0.007(2)
C(13)	0.029(2)	0.028(2)	0.029(2)	-0.001(2)	0.007(2)	0.002(2)
C(14)	0.029(2)	0.028(2)	0.025(2)	0.001(2)	0.007(2)	0.001(2)
C(15)	0.026(2)	0.025(2)	0.026(2)	-0.001(2)	0.007(2)	0.002(2)
C(16)	0.024(2)	0.026(2)	0.030(2)	-0.004(2)	0.007(2)	-0.003(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(17)	0.023(2)	0.030(2)	0.025(2)	0.000(2)	0.004(2)	-0.001(2)
C(18)	0.029(2)	0.025(2)	0.025(2)	0.001(2)	0.009(2)	0.000(2)
C(19)	0.023(2)	0.024(2)	0.029(2)	-0.002(1)	0.007(2)	0.002(2)
C(20)	0.023(2)	0.027(2)	0.027(2)	-0.001(2)	0.005(2)	0.001(2)
C(21)	0.023(2)	0.029(2)	0.031(2)	-0.001(2)	0.006(2)	0.004(2)
C(22)	0.027(2)	0.028(2)	0.029(2)	0.000(2)	0.008(2)	0.003(2)
C(23)	0.028(2)	0.025(2)	0.027(2)	0.003(2)	0.007(2)	0.002(2)
C(24)	0.027(2)	0.025(2)	0.028(2)	-0.001(2)	0.003(2)	-0.002(2)
C(25)	0.026(2)	0.032(3)	0.039(2)	0.004(2)	0.008(2)	0.010(2)
C(26)	0.026(2)	0.045(3)	0.041(3)	0.007(2)	0.010(2)	0.010(2)
C(27)	0.036(2)	0.060(4)	0.047(3)	0.010(2)	0.019(2)	0.019(3)
C(28)	0.027(2)	0.062(4)	0.071(4)	0.003(2)	0.016(2)	0.031(3)
C(29)	0.036(2)	0.040(3)	0.066(4)	-0.009(2)	0.011(2)	0.011(3)
C(30)	0.035(2)	0.036(3)	0.045(3)	-0.002(2)	0.011(2)	0.007(2)
C(31)	0.029(2)	0.032(2)	0.028(2)	-0.002(2)	0.004(2)	0.005(2)
C(32)	0.028(2)	0.050(3)	0.031(2)	0.001(2)	0.007(2)	0.002(2)
C(33)	0.048(3)	0.052(3)	0.026(2)	0.000(2)	0.000(2)	-0.004(2)
C(34)	0.041(3)	0.051(3)	0.039(3)	-0.008(2)	-0.001(2)	0.004(2)
C(35)	0.034(2)	0.051(3)	0.047(3)	0.000(2)	0.005(2)	0.012(3)
C(36)	0.029(2)	0.043(3)	0.035(2)	0.001(2)	0.011(2)	0.006(2)
C(37)	0.052(3)	0.032(3)	0.036(3)	-0.002(2)	0.013(2)	-0.004(2)
C(38)	0.028(2)	0.028(2)	0.025(2)	0.000(2)	0.009(2)	-0.001(2)
C(39)	0.031(2)	0.025(2)	0.031(2)	0.001(2)	0.004(2)	0.001(2)
C(40)	0.039(2)	0.033(3)	0.039(3)	-0.009(2)	0.009(2)	-0.005(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(41)	0.025(2)	0.041(3)	0.042(3)	-0.006(2)	0.002(2)	-0.008(2)
C(42)	0.026(2)	0.040(3)	0.030(2)	0.002(2)	0.000(2)	-0.006(2)
C(43)	0.031(2)	0.029(2)	0.027(2)	0.000(2)	0.007(2)	-0.001(2)
C(44)	0.028(2)	0.026(2)	0.030(2)	-0.002(2)	0.006(2)	0.001(2)
C(45)	0.028(2)	0.035(3)	0.033(2)	-0.007(2)	0.002(2)	0.004(2)
C(46)	0.031(2)	0.043(3)	0.050(3)	0.001(2)	0.007(2)	0.019(2)
C(47)	0.034(2)	0.082(5)	0.033(3)	-0.001(3)	0.005(2)	0.017(3)
C(48)	0.042(3)	0.070(4)	0.028(2)	-0.011(3)	0.006(2)	-0.006(2)
C(49)	0.042(2)	0.033(3)	0.033(2)	-0.006(2)	0.008(2)	-0.006(2)
C(50)	0.041(3)	0.052(3)	0.051(3)	0.000(2)	0.012(2)	-0.006(3)

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)	1.883(5)	Se(1)	C(4)	1.907(4)
Se(2)	C(5)	1.895(4)	Se(2)	C(8)	1.881(4)
Cl(1)	C(50)	1.759(6)	Cl(2)	C(50)	1.748(6)
Cl(3)	C(50)	1.708(6)	N(1)	C(10)	1.346(5)
N(1)	C(13)	1.378(5)	N(2)	C(15)	1.383(5)
N(2)	C(18)	1.395(5)	N(2)	C(37)	1.471(6)
N(3)	C(20)	1.372(5)	N(3)	C(23)	1.347(5)
C(1)	C(2)	1.427(6)	C(1)	C(24)	1.401(6)
C(2)	C(3)	1.374(7)	C(3)	C(4)	1.401(6)
C(4)	C(5)	1.408(6)	C(5)	C(6)	1.416(6)
C(6)	C(7)	1.379(7)	C(7)	C(8)	1.424(6)
C(8)	C(9)	1.396(6)	C(9)	C(10)	1.430(6)
C(9)	C(25)	1.499(6)	C(10)	C(11)	1.447(6)
C(11)	C(12)	1.362(6)	C(12)	C(13)	1.443(6)
C(13)	C(14)	1.394(6)	C(14)	C(15)	1.425(6)
C(14)	C(31)	1.489(6)	C(15)	C(16)	1.411(6)
C(16)	C(17)	1.378(6)	C(17)	C(18)	1.409(6)
C(18)	C(19)	1.438(6)	C(19)	C(20)	1.403(6)
C(19)	C(38)	1.475(6)	C(20)	C(21)	1.447(6)
C(21)	C(22)	1.363(6)	C(22)	C(23)	1.462(6)
C(23)	C(24)	1.428(6)	C(24)	C(44)	1.487(6)
C(25)	C(26)	1.405(7)	C(25)	C(30)	1.386(7)
C(26)	C(27)	1.381(7)	C(27)	C(28)	1.394(9)
C(28)	C(29)	1.387(9)	C(29)	C(30)	1.400(7)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(31)	C(32)	1.395(7)	C(31)	C(36)	1.399(6)
C(32)	C(33)	1.398(7)	C(33)	C(34)	1.379(8)
C(34)	C(35)	1.392(8)	C(35)	C(36)	1.380(7)
C(38)	C(39)	1.395(6)	C(38)	C(43)	1.407(6)
C(39)	C(40)	1.383(6)	C(40)	C(41)	1.391(7)
C(41)	C(42)	1.370(7)	C(42)	C(43)	1.395(6)
C(44)	C(45)	1.389(6)	C(44)	C(49)	1.400(6)
C(45)	C(46)	1.389(7)	C(46)	C(47)	1.380(8)
C(47)	C(48)	1.382(9)	C(48)	C(49)	1.398(7)

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(2)	H(1)	0.95	C(3)	H(2)	0.95
C(6)	H(3)	0.95	C(7)	H(4)	0.95
C(11)	H(5)	0.95	C(12)	H(6)	0.95
C(16)	H(7)	0.95	C(17)	H(8)	0.95
C(21)	H(9)	0.95	C(22)	H(10)	0.95
C(26)	H(11)	0.95	C(27)	H(12)	0.95
C(28)	H(13)	0.95	C(29)	H(14)	0.95
C(30)	H(15)	0.95	C(32)	H(16)	0.95
C(33)	H(17)	0.95	C(34)	H(18)	0.95
C(35)	H(19)	0.95	C(36)	H(20)	0.95
C(37)	H(21)	0.95	C(37)	H(22)	0.95
C(37)	H(23)	0.95	C(39)	H(24)	0.95
C(40)	H(25)	0.95	C(41)	H(26)	0.95
C(42)	H(27)	0.95	C(43)	H(28)	0.95
C(45)	H(29)	0.95	C(46)	H(30)	0.95
C(47)	H(31)	0.95	C(48)	H(32)	0.95
C(49)	H(33)	0.95	C(50)	H(34)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Se(1)	C(4)	88.5(2)	C(5)	Se(2)	C(8)	88.2(2)
C(10)	N(1)	C(13)	107.1(4)	C(15)	N(2)	C(18)	109.3(3)
C(15)	N(2)	C(37)	124.1(4)	C(18)	N(2)	C(37)	123.5(4)
C(20)	N(3)	C(23)	107.8(3)	Se(1)	C(1)	C(2)	108.7(3)
Se(1)	C(1)	C(24)	121.3(3)	C(2)	C(1)	C(24)	130.0(4)
C(1)	C(2)	C(3)	117.2(4)	C(2)	C(3)	C(4)	116.1(4)
Se(1)	C(4)	C(3)	109.5(3)	Se(1)	C(4)	C(5)	115.3(3)
C(3)	C(4)	C(5)	135.2(4)	Se(2)	C(5)	C(4)	116.3(3)
Se(2)	C(5)	C(6)	110.6(3)	C(4)	C(5)	C(6)	133.2(4)
C(5)	C(6)	C(7)	114.5(4)	C(6)	C(7)	C(8)	117.7(4)
Se(2)	C(8)	C(7)	109.0(3)	Se(2)	C(8)	C(9)	121.0(3)
C(7)	C(8)	C(9)	130.0(4)	C(8)	C(9)	C(10)	120.6(4)
C(8)	C(9)	C(25)	120.0(4)	C(10)	C(9)	C(25)	119.4(4)
N(1)	C(10)	C(9)	119.9(4)	N(1)	C(10)	C(11)	110.1(4)
C(9)	C(10)	C(11)	130.0(4)	C(10)	C(11)	C(12)	106.8(4)
C(11)	C(12)	C(13)	106.5(4)	N(1)	C(13)	C(12)	109.4(4)
N(1)	C(13)	C(14)	121.5(4)	C(12)	C(13)	C(14)	129.0(4)
C(13)	C(14)	C(15)	120.0(4)	C(13)	C(14)	C(31)	122.2(4)
C(15)	C(14)	C(31)	117.7(4)	N(2)	C(15)	C(14)	124.7(4)
N(2)	C(15)	C(16)	107.1(4)	C(14)	C(15)	C(16)	128.1(4)
C(15)	C(16)	C(17)	108.4(4)	C(16)	C(17)	C(18)	108.3(4)
N(2)	C(18)	C(17)	106.9(4)	N(2)	C(18)	C(19)	125.0(4)
C(17)	C(18)	C(19)	127.9(4)	C(18)	C(19)	C(20)	118.4(4)
C(18)	C(19)	C(38)	119.1(4)	C(20)	C(19)	C(38)	122.4(4)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(3)	C(20)	C(19)	121.6(4)	N(3)	C(20)	C(21)	109.3(3)
C(19)	C(20)	C(21)	129.1(4)	C(20)	C(21)	C(22)	106.9(3)
C(21)	C(22)	C(23)	106.4(4)	N(3)	C(23)	C(22)	109.6(3)
N(3)	C(23)	C(24)	121.6(4)	C(22)	C(23)	C(24)	128.7(4)
C(1)	C(24)	C(23)	120.2(4)	C(1)	C(24)	C(44)	121.6(4)
C(23)	C(24)	C(44)	118.2(4)	C(9)	C(25)	C(26)	120.1(4)
C(9)	C(25)	C(30)	121.0(4)	C(26)	C(25)	C(30)	118.9(4)
C(25)	C(26)	C(27)	120.4(5)	C(26)	C(27)	C(28)	120.1(5)
C(27)	C(28)	C(29)	120.2(5)	C(28)	C(29)	C(30)	119.3(5)
C(25)	C(30)	C(29)	121.0(5)	C(14)	C(31)	C(32)	122.3(4)
C(14)	C(31)	C(36)	118.7(4)	C(32)	C(31)	C(36)	119.0(4)
C(31)	C(32)	C(33)	119.9(4)	C(32)	C(33)	C(34)	120.5(5)
C(33)	C(34)	C(35)	119.5(5)	C(34)	C(35)	C(36)	120.4(5)
C(31)	C(36)	C(35)	120.5(5)	C(19)	C(38)	C(39)	122.4(4)
C(19)	C(38)	C(43)	119.3(4)	C(39)	C(38)	C(43)	118.3(4)
C(38)	C(39)	C(40)	120.9(4)	C(39)	C(40)	C(41)	120.1(4)
C(40)	C(41)	C(42)	120.0(4)	C(41)	C(42)	C(43)	120.5(4)
C(38)	C(43)	C(42)	120.1(4)	C(24)	C(44)	C(45)	121.1(4)
C(24)	C(44)	C(49)	120.6(4)	C(45)	C(44)	C(49)	118.3(4)
C(44)	C(45)	C(46)	121.6(4)	C(45)	C(46)	C(47)	119.7(5)
C(46)	C(47)	C(48)	119.8(5)	C(47)	C(48)	C(49)	120.6(5)
C(44)	C(49)	C(48)	119.9(5)	Cl(1)	C(50)	Cl(2)	109.1(3)
Cl(1)	C(50)	Cl(3)	111.7(3)	Cl(2)	C(50)	Cl(3)	114.1(3)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(1)	121.4	C(3)	C(2)	H(1)	121.4
C(2)	C(3)	H(2)	121.9	C(4)	C(3)	H(2)	122.0
C(5)	C(6)	H(3)	122.7	C(7)	C(6)	H(3)	122.8
C(6)	C(7)	H(4)	121.1	C(8)	C(7)	H(4)	121.1
C(10)	C(11)	H(5)	126.5	C(12)	C(11)	H(5)	126.7
C(11)	C(12)	H(6)	126.6	C(13)	C(12)	H(6)	126.8
C(15)	C(16)	H(7)	125.8	C(17)	C(16)	H(7)	125.8
C(16)	C(17)	H(8)	125.8	C(18)	C(17)	H(8)	125.9
C(20)	C(21)	H(9)	126.6	C(22)	C(21)	H(9)	126.5
C(21)	C(22)	H(10)	126.8	C(23)	C(22)	H(10)	126.8
C(25)	C(26)	H(11)	119.8	C(27)	C(26)	H(11)	119.8
C(26)	C(27)	H(12)	119.9	C(28)	C(27)	H(12)	119.9
C(27)	C(28)	H(13)	120.0	C(29)	C(28)	H(13)	119.8
C(28)	C(29)	H(14)	120.3	C(30)	C(29)	H(14)	120.4
C(25)	C(30)	H(15)	119.5	C(29)	C(30)	H(15)	119.5
C(31)	C(32)	H(16)	120.1	C(33)	C(32)	H(16)	120.0
C(32)	C(33)	H(17)	119.8	C(34)	C(33)	H(17)	119.7
C(33)	C(34)	H(18)	120.3	C(35)	C(34)	H(18)	120.2
C(34)	C(35)	H(19)	119.8	C(36)	C(35)	H(19)	119.7
C(31)	C(36)	H(20)	119.8	C(35)	C(36)	H(20)	119.7
N(2)	C(37)	H(21)	109.4	N(2)	C(37)	H(22)	109.4
N(2)	C(37)	H(23)	109.4	H(21)	C(37)	H(22)	109.6
H(21)	C(37)	H(23)	109.5	H(22)	C(37)	H(23)	109.5
C(38)	C(39)	H(24)	119.5	C(40)	C(39)	H(24)	119.6

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(39)	C(40)	H(25)	119.9	C(41)	C(40)	H(25)	120.0
C(40)	C(41)	H(26)	120.0	C(42)	C(41)	H(26)	120.0
C(41)	C(42)	H(27)	119.7	C(43)	C(42)	H(27)	119.8
C(38)	C(43)	H(28)	119.9	C(42)	C(43)	H(28)	120.0
C(44)	C(45)	H(29)	119.2	C(46)	C(45)	H(29)	119.2
C(45)	C(46)	H(30)	120.1	C(47)	C(46)	H(30)	120.2
C(46)	C(47)	H(31)	120.1	C(48)	C(47)	H(31)	120.1
C(47)	C(48)	H(32)	119.7	C(49)	C(48)	H(32)	119.7
C(44)	C(49)	H(33)	120.0	C(48)	C(49)	H(33)	120.0
Cl(1)	C(50)	H(34)	107.2	Cl(2)	C(50)	H(34)	107.2
Cl(3)	C(50)	H(34)	107.3				