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Table I. Crystallographic Data for $C_{36}H_{58}BrIn$ and $C_{30}H_{39}InSe_2$.

formula	$C_{36}H_{58}BrIn$ (1)	$C_{30}H_{39}InSe_2$ (2)
formula weight	685.55	672.35
space group	*Fdd*2	$P2_1/n$
a, Å	14.968(1)	11.103(2)
b, Å	82.54(2)	18.375(1)
c, Å	11.596(2)	14.951(2)
β, deg	---	102.99(1)
V, Å^3	14326(5)	2972.3(9)
Z	16	4
cryst color	colorless	colorless
D(calc), g cm^{-3}	1.271	1.503
μ(MoKα), cm^{-1}	17.96	32.59
temp, K	298(2)	298(2)
radiation	MoKα (λ = 0.71073 Å)	
R(*F*), %	4.12[a]	4.53[a]
$R(wF^2)$, %	9.41[a]	9.37[a]

[a] Quantity minimized = $R(wF^2) = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[(wF_o^2)^2]^{1/2}$; $R = \Sigma\Delta/\Sigma(F_o)$, $\Delta = |(F_o-F_c)|$

Table 1. Crystal data and structure refinement for 1.

Identification code	wells14a
Empirical formula	$C_{36}H_{58}BrIn$
Formula weight	685.55
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Fdd2
Unit cell dimensions	a = 14.968(1) Å alpha = 90° b = 82.54(2) Å beta = 90° c = 11.596(2) Å gamma = 90°
Volume, Z	14326(5) $Å^3$, 16
Density (calculated)	1.271 g/cm^3
Absorption coefficient	1.796 mm^{-1}
F(000)	5728
Crystal size	0.40 x 0.40 x 0.15 mm
Crystal color	Colorless Thin Plate
θ range for data collection	2.24 to 23.49°
Limiting indices	$-1 \le h \le 16$, $-1 \le k \le 92$, $-1 \le l \le 12$
Reflections collected	3273
Independent reflections	2990 (R_{int} = 0.0361)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2990 / 1 / 343
Goodness-of-fit on F^2	1.285
Final R indices [I>2σ(I)]	R1 = 0.0412, wR2 = 0.0941
R indices (all data)	R1 = 0.0503, wR2 = 0.0963
Absolute structure parameter	0.00
Largest diff. peak and hole	0.510 and −0.624 $eÅ^{-3}$

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

	x	y	z	U(eq)
In	8788.1(4)	731.3(1)	9249.2(5)	49(1)
Br	7560.4(9)	879.9(2)	8151(1)	86(1)
C(1)	9670(6)	948(1)	11145(8)	41(2)
C(2)	9754(6)	1017(1)	12208(9)	50(3)
C(3)	9194(5)	985(1)	13114(9)	44(2)
C(4)	8519(6)	875(1)	12925(9)	47(2)
C(5)	8411(5)	794(1)	11879(9)	37(2)
C(6)	8976(5)	834(1)	10937(8)	38(2)
C(7)	10365(6)	994(1)	10185(9)	54(3)
C(8)	10945(8)	1138(1)	10529(14)	97(4)
C(9)	9947(7)	1023(1)	9010(9)	73(3)
C(10)	11026(6)	849(1)	10064(11)	74(3)
C(11)	9334(6)	1062(1)	14314(9)	53(2)
C(12)	9564(12)	1239(2)	14163(14)	137(6)
C(13)	10037(11)	973(2)	14923(12)	122(6)
C(14)	8512(10)	1056(2)	15041(14)	164(9)
C(15)	7596(5)	677(1)	11790(9)	46(2)
C(16)	7526(7)	573(1)	12885(11)	73(3)
C(17)	6751(5)	778(1)	11632(11)	67(3)
C(18)	7656(7)	558(1)	10778(10)	69(3)
C(19)	8313(6)	241(1)	8738(9)	49(2)
C(20)	7592(6)	164(1)	9250(10)	52(2)
C(21)	6757(6)	216(1)	8885(8)	46(2)
C(22)	6627(5)	337(1)	8130(8)	41(2)
C(23)	7371(6)	411(1)	7642(8)	46(2)
C(24)	8234(6)	362(1)	7921(8)	44(2)
C(25)	9061(6)	444(1)	7420(9)	55(3)
C(26)	9517(6)	544(1)	8340(10)	66(3)
C(27)	9706(6)	318(1)	6985(11)	81(4)
C(28)	8835(7)	554(1)	6355(9)	82(4)
C(29)	7703(7)	30(1)	10103(12)	78(3)
C(30)	7558(18)	-130(2)	9594(16)	236(15)
C(31)	8572(11)	31(2)	10742(20)	213(14)
C(32)	7076(15)	43(3)	11102(18)	216(12)
C(33)	5667(6)	402(1)	7836(10)	58(3)
C(34)	4954(6)	279(1)	8193(15)	102(5)
C(35)	5538(7)	557(2)	8509(15)	119(6)
C(36)	5553(8)	429(2)	6561(11)	111(5)

Table 3. Bond lengths [Å] and angles [°] for 1.

In-C(6)	2.152(9)	In-C(26)	2.166(10)
In-Br	2.5503(14)	C(1)-C(2)	1.362(13)
C(1)-C(6)	1.422(11)	C(1)-C(7)	1.570(12)
C(2)-C(3)	1.370(13)	C(3)-C(4)	1.374(12)
C(3)-C(11)	1.545(13)	C(4)-C(5)	1.392(13)
C(5)-C(6)	1.420(12)	C(5)-C(15)	1.563(11)
C(7)-C(10)	1.557(13)	C(7)-C(9)	1.519(14)
C(7)-C(8)	1.529(13)	C(11)-C(13)	1.47(2)
C(11)-C(12)	1.51(2)	C(11)-C(14)	1.49(2)
C(15)-C(18)	1.534(13)	C(15)-C(16)	1.53(2)
C(15)-C(17)	1.524(11)	C(19)-C(24)	1.381(13)
C(19)-C(20)	1.386(12)	C(20)-C(21)	1.389(12)
C(20)-C(29)	1.493(14)	C(21)-C(22)	1.341(12)
C(22)-C(23)	1.390(12)	C(22)-C(33)	1.573(12)
C(23)-C(24)	1.394(12)	C(24)-C(25)	1.526(12)
C(25)-C(27)	1.508(13)	C(25)-C(28)	1.567(14)
C(25)-C(26)	1.511(13)	C(29)-C(30)	1.46(2)
C(29)-C(32)	1.49(2)	C(29)-C(31)	1.50(2)
C(33)-C(35)	1.51(2)	C(33)-C(36)	1.50(2)
C(33)-C(34)	1.529(14)		

C(6)-In-C(26)	131.2(4)	C(6)-In-Br	111.0(2)
C(26)-In-Br	117.6(3)	C(2)-C(1)-C(6)	119.8(8)
C(2)-C(1)-C(7)	118.7(7)	C(6)-C(1)-C(7)	121.5(8)
C(1)-C(2)-C(3)	123.8(8)	C(4)-C(3)-C(2)	117.0(8)
C(4)-C(3)-C(11)	121.1(9)	C(2)-C(3)-C(11)	121.8(8)
C(5)-C(4)-C(3)	122.7(9)	C(4)-C(5)-C(6)	119.3(7)
C(4)-C(5)-C(15)	116.4(8)	C(6)-C(5)-C(15)	123.9(8)
C(1)-C(6)-C(5)	117.2(8)	C(1)-C(6)-In	120.7(6)
C(5)-C(6)-In	122.1(6)	C(10)-C(7)-C(9)	107.6(9)
C(10)-C(7)-C(1)	107.6(8)	C(9)-C(7)-C(1)	113.6(7)
C(10)-C(7)-C(8)	105.1(9)	C(9)-C(7)-C(8)	110.2(10)
C(1)-C(7)-C(8)	112.2(9)	C(13)-C(11)-C(12)	112.1(11)
C(13)-C(11)-C(3)	108.9(8)	C(12)-C(11)-C(3)	109.1(10)
C(13)-C(11)-C(14)	107.6(13)	C(12)-C(11)-C(14)	106.8(12)
C(3)-C(11)-C(14)	112.4(8)	C(18)-C(15)-C(16)	106.3(7)
C(18)-C(15)-C(17)	107.8(9)	C(16)-C(15)-C(17)	110.3(8)
C(18)-C(15)-C(5)	113.7(7)	C(16)-C(15)-C(5)	110.1(8)
C(17)-C(15)-C(5)	108.4(7)	C(24)-C(19)-C(20)	124.0(8)
C(21)-C(20)-C(19)	115.3(8)	C(21)-C(20)-C(29)	122.2(8)
C(19)-C(20)-C(29)	122.5(9)	C(20)-C(21)-C(22)	124.1(8)
C(23)-C(22)-C(21)	118.5(8)	C(23)-C(22)-C(33)	119.5(8)
C(21)-C(22)-C(33)	121.9(8)	C(22)-C(23)-C(24)	121.3(8)
C(19)-C(24)-C(23)	116.8(8)	C(19)-C(24)-C(25)	120.9(8)
C(23)-C(24)-C(25)	122.2(8)	C(24)-C(25)-C(27)	109.8(7)
C(24)-C(25)-C(28)	112.5(8)	C(27)-C(25)-C(28)	105.9(9)
C(24)-C(25)-C(26)	109.8(8)	C(27)-C(25)-C(26)	108.9(9)
C(28)-C(25)-C(26)	109.8(8)	C(25)-C(26)-In	120.4(7)
C(30)-C(29)-C(20)	112.6(11)	C(30)-C(29)-C(32)	106.5(14)
C(20)-C(29)-C(32)	113.0(12)	C(30)-C(29)-C(31)	109.6(14)
C(20)-C(29)-C(31)	114.8(10)	C(32)-C(29)-C(31)	99.3(14)
C(35)-C(33)-C(36)	111.8(11)	C(35)-C(33)-C(22)	107.1(8)
C(36)-C(33)-C(22)	111.5(9)	C(35)-C(33)-C(34)	109.4(10)
C(36)-C(33)-C(34)	106.4(11)	C(22)-C(33)-C(34)	110.6(8)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
In	51(1)	51(1)	45(1)	-5(1)	5(1)	-10(1)
Br	84(1)	90(1)	83(1)	12(1)	-21(1)	-1(1)
C(1)	43(5)	25(5)	57(6)	-3(4)	4(5)	-6(4)
C(2)	39(5)	47(6)	65(6)	-11(5)	-7(5)	-15(4)
C(3)	39(5)	33(5)	62(6)	-13(5)	-7(5)	9(4)
C(4)	44(5)	50(5)	48(5)	2(5)	6(5)	8(4)
C(5)	28(4)	28(4)	54(6)	-1(5)	0(5)	4(3)
C(6)	41(5)	25(4)	46(5)	2(4)	3(4)	0(4)
C(7)	50(5)	51(6)	61(6)	0(5)	10(5)	-18(5)
C(8)	92(8)	90(8)	110(11)	-15(9)	26(9)	-38(7)
C(9)	64(6)	82(8)	72(8)	35(7)	-1(6)	-9(6)
C(10)	54(6)	86(8)	82(8)	-4(7)	20(6)	-6(6)
C(11)	51(5)	61(6)	47(5)	-12(6)	-7(6)	12(4)
C(12)	256(19)	74(8)	81(9)	-27(8)	-18(14)	-24(11)
C(13)	166(14)	119(12)	80(9)	-23(9)	-55(11)	66(11)
C(14)	101(10)	283(24)	108(12)	-123(15)	29(10)	-64(13)
C(15)	42(4)	50(5)	46(5)	-3(5)	9(5)	-4(4)
C(16)	68(6)	66(7)	86(9)	1(7)	7(7)	-13(6)
C(17)	35(5)	92(7)	73(7)	-2(7)	-4(6)	-1(5)
C(18)	72(7)	56(7)	78(8)	-21(6)	17(6)	-38(5)
C(19)	48(5)	46(5)	53(6)	-5(5)	0(5)	0(5)
C(20)	65(6)	34(4)	56(5)	13(5)	-8(6)	-7(4)
C(21)	49(5)	40(5)	50(6)	11(4)	3(4)	-8(4)
C(22)	38(4)	41(5)	45(5)	-10(5)	2(4)	-2(4)
C(23)	66(6)	29(4)	42(5)	1(4)	-3(5)	2(4)
C(24)	53(5)	31(5)	47(5)	-7(4)	3(5)	-8(4)
C(25)	58(6)	51(6)	55(6)	-1(5)	15(5)	-13(5)
C(26)	48(5)	75(7)	74(7)	-24(6)	24(6)	-15(5)
C(27)	70(6)	89(8)	83(9)	-28(7)	25(7)	-21(6)
C(28)	86(8)	102(9)	59(7)	22(7)	17(6)	-16(7)
C(29)	77(7)	67(7)	89(9)	24(7)	-17(7)	-19(6)
C(30)	542(43)	42(7)	123(16)	11(9)	-133(23)	23(16)
C(31)	177(17)	197(20)	264(30)	151(21)	-138(21)	-95(15)
C(32)	255(25)	246(26)	147(17)	136(18)	87(18)	108(21)
C(33)	54(6)	53(6)	69(7)	-10(6)	-13(6)	10(5)
C(34)	42(5)	109(9)	156(13)	34(11)	-11(8)	-8(6)
C(35)	73(8)	105(10)	177(17)	-69(11)	-8(10)	37(8)
C(36)	85(8)	169(14)	79(10)	30(10)	-9(8)	62(9)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

-	x	y	z	U(eq)
H(2A)	10220(6)	1090(1)	12325(9)	60
H(4A)	8119(6)	854(1)	13519(9)	57
H(8A)	10575(8)	1233(1)	10617(14)	146
H(8B)	11383(8)	1158(1)	9941(14)	146
H(8C)	11240(8)	1115(1)	11246(14)	146
H(9A)	9533(7)	1111(1)	9059(9)	109
H(9B)	9636(7)	927(1)	8766(9)	109
H(9C)	10406(7)	1048(1)	8462(9)	109
H(10A)	11295(6)	827(1)	10799(11)	111
H(10B)	11483(6)	876(1)	9517(11)	111
H(10C)	10708(6)	755(1)	9802(11)	111
H(12A)	9080(12)	1294(2)	13783(14)	205
H(12B)	10096(12)	1249(2)	13706(14)	205
H(12C)	9663(12)	1288(2)	14905(14)	205
H(13A)	9871(11)	861(2)	14986(12)	183
H(13B)	10114(11)	1018(2)	15680(12)	183
H(13C)	10587(11)	982(2)	14501(12)	183
H(14A)	8046(10)	1117(2)	14681(14)	246
H(14B)	8638(10)	1100(2)	15789(14)	246
H(14C)	8322(10)	945(2)	15121(14)	246
H(16A)	7470(7)	643(1)	13545(11)	110
H(16B)	8054(7)	508(1)	12961(11)	110
H(16C)	7011(7)	504(1)	12834(11)	110
H(17A)	6695(5)	853(1)	12260(11)	100
H(17B)	6240(5)	707(1)	11617(11)	100
H(17C)	6787(5)	836(1)	10919(11)	100
H(18A)	7689(7)	617(1)	10067(10)	103
H(18B)	7136(7)	490(1)	10771(10)	103
H(18C)	8180(7)	492(1)	10862(10)	103
H(19A)	8885(6)	209(1)	8958(9)	59
H(21A)	6256(6)	164(1)	9184(8)	55
H(23A)	7290(6)	495(1)	7120(8)	55
H(26A)	10032(6)	595(1)	7986(10)	79
H(26B)	9743(6)	469(1)	8915(10)	79
H(27A)	10219(6)	370(1)	6657(11)	121
H(27B)	9419(6)	253(1)	6408(11)	121
H(27C)	9891(6)	250(1)	7615(11)	121
H(28A)	9373(7)	602(1)	6068(9)	123
H(28B)	8424(7)	637(1)	6584(9)	123
H(28C)	8569(7)	489(1)	5760(9)	123
H(30A)	7616(18)	-212(2)	10180(16)	353
H(30B)	7993(18)	-149(2)	9000(16)	353
H(30C)	6969(18)	-135(2)	9268(16)	353
H(31A)	8676(11)	137(2)	11055(20)	319
H(31B)	9048(11)	4(2)	10223(20)	319
H(31C)	8550(11)	-46(2)	11357(20)	319
H(32A)	7179(15)	143(3)	11500(18)	324
H(32B)	7175(15)	-46(3)	11620(18)	324

H(32C)	6471(15)	40(3)	10827(18)	324
H(34A)	5039(6)	181(1)	7770(15)	153
H(34B)	4372(6)	323(1)	8029(15)	153
H(34C)	5004(6)	258(1)	9004(15)	153
H(35A)	5598(7)	535(2)	9318(15)	178
H(35B)	4954(7)	600(2)	8357(15)	178
H(35C)	5982(7)	634(2)	8279(15)	178
H(36A)	5623(8)	327(2)	6164(11)	167
H(36B)	5997(8)	504(2)	6293(11)	167
H(36C)	4969(8)	471(2)	6412(11)	167

Table 6. Crystal data and structure refinement for 2.

Identification code	wells16
Empirical formula	$C_{30}H_{39}InSe_2$
Formula weight	672.35
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Crystal color	Colorless block
Unit cell dimensions	a = 11.103(2) Å alpha = 90° b = 18.375(1) Å beta = 102.99(1)° c = 14.951(2) Å gamma = 90°
Volume, Z	2972.2(7) $Å^3$, 4
Density (calculated)	1.503 Mg/m^3
Absorption coefficient	3.259 mm^{-1}
F(000)	1344
Crystal size	0.30 x 0.20 x 0.20 mm
θ range for data collection	2.18 to 22.50°
Limiting indices	$-11 \le h \le 11$, $-1 \le k \le 19$, $-1 \le l \le 15$
Reflections collected	4671
Independent reflections	3838 (R_{int} = 0.0525)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3831 / 0 / 296
Goodness-of-fit on F^2	1.132
Final R indices [I>2σ(I)]	R1 = 0.0468, wR2 = 0.0966
R indices (all data)	R1 = 0.0859, wR2 = 0.1098
Largest diff. peak and hole	0.700 and -0.511 $eÅ^{-3}$

Table 7. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 2. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
In	4435.7(5)	1457.9(3)	3393.7(4)	48(1)
Se(1)	6384(1)	1551(1)	4643(1)	72(1)
Se(2)	2788(1)	2008(1)	4135(1)	80(1)
C(1)	4007(7)	1084(4)	1990(5)	39(2)
C(2)	4162(7)	1551(4)	1279(5)	40(2)
C(3)	3755(7)	1313(4)	385(5)	50(2)
C(4)	3142(7)	664(4)	157(5)	45(2)
C(5)	3038(7)	214(4)	868(6)	50(2)
C(6)	3449(7)	393(4)	1779(5)	39(2)
C(7)	3252(8)	-167(4)	2491(6)	50(2)
C(8)	3106(11)	-938(5)	2120(7)	107(4)
C(9)	2091(8)	24(6)	2857(7)	91(3)
C(10)	4366(9)	-202(5)	3320(7)	99(4)
C(11)	4846(8)	2282(4)	1456(6)	54(2)
C(12)	4951(10)	2658(6)	573(7)	104(4)
C(13)	4157(10)	2800(5)	1966(8)	101(4)
C(14)	6172(9)	2161(5)	1982(7)	86(3)
C(15)	2639(9)	445(6)	-868(6)	71(3)
C(16)	1235(16)	283(10)	-1021(11)	80(5)
C(16')	1448(25)	791(15)	-1247(18)	82(8)
C(17)	3326(16)	-175(10)	-1121(11)	81(5)
C(17')	2569(28)	-446(16)	-916(19)	99(9)

C(18)	2949(17)	1071(10)	-1550(12)	89(5)
C(18')	3645(28)	532(17)	-1425(20)	109(10)
C(19)	3922(9)	2141(5)	6051(7)	69(3)
C(20)	4702(13)	2461(8)	6821(7)	97(4)
C(21)	5436(10)	3041(7)	6718(9)	98(4)
C(22)	5363(11)	3313(6)	5869(9)	96(4)
C(23)	4597(9)	3016(5)	5110(7)	72(3)
C(24)	3869(8)	2424(5)	5197(6)	56(2)
C(25)	7507(8)	156(6)	4459(6)	62(2)
C(26)	8372(9)	-309(5)	4275(6)	67(3)
C(27)	9217(9)	-57(6)	3800(6)	72(3)
C(28)	9200(8)	648(6)	3552(6)	71(3)
C(29)	8313(9)	1119(5)	3750(6)	65(3)
C(30)	7463(8)	885(5)	4225(5)	53(2)

Table 8. Bond lengths [Å] and angles [°] for 7.

In-C(1)	2.157(7)	In-Se(1)	2.5260(12)
In-Se(2)	2.5508(11)	Se(1)-C(30)	1.913(8)
Se(2)-C(24)	1.921(9)	C(1)-C(2)	1.406(9)
C(1)-C(6)	1.417(10)	C(2)-C(3)	1.382(10)
C(2)-C(11)	1.536(10)	C(3)-C(4)	1.378(10)
C(4)-C(5)	1.371(10)	C(4)-C(15)	1.560(10)
C(5)-C(6)	1.377(10)	C(6)-C(7)	1.532(10)
C(7)-C(8)	1.516(11)	C(7)-C(10)	1.543(11)
C(7)-C(9)	1.550(10)	C(11)-C(12)	1.518(11)
C(11)-C(14)	1.522(11)	C(11)-C(13)	1.527(11)
C(15)-C(16')	1.46(3)	C(15)-C(17)	1.47(2)
C(15)-C(16)	1.55(2)	C(15)-C(18')	1.54(3)
C(15)-C(18)	1.63(2)	C(15)-C(17')	1.64(3)
C(16)-C(16')	1.04(3)	C(16)-C(17')	1.98(3)
C(16')-C(18)	1.89(3)	C(17)-C(17')	1.08(3)
C(17)-C(18')	1.45(3)	C(18)-C(18')	1.25(3)
C(19)-C(24)	1.369(11)	C(19)-C(20)	1.405(14)
C(20)-C(21)	1.371(14)	C(21)-C(22)	1.348(14)
C(22)-C(23)	1.370(13)	C(23)-C(24)	1.378(11)
C(25)-C(26)	1.359(11)	C(25)-C(30)	1.382(11)
C(26)-C(27)	1.378(12)	C(27)-C(28)	1.346(12)
C(28)-C(29)	1.392(11)	C(29)-C(30)	1.371(11)

C(1)-In-Se(1)	134.9(2)	C(1)-In-Se(2)	121.7(2)
Se(1)-In-Se(2)	103.35(4)	C(30)-Se(1)-In	102.1(2)
C(24)-Se(2)-In	98.1(2)	C(2)-C(1)-C(6)	120.0(7)
C(2)-C(1)-In	120.2(5)	C(6)-C(1)-In	119.4(5)
C(3)-C(2)-C(1)	117.9(7)	C(3)-C(2)-C(11)	119.1(7)
C(1)-C(2)-C(11)	122.9(7)	C(4)-C(3)-C(2)	123.4(7)
C(5)-C(4)-C(3)	116.9(7)	C(5)-C(4)-C(15)	122.1(8)
C(3)-C(4)-C(15)	120.9(8)	C(4)-C(5)-C(6)	123.8(7)
C(5)-C(6)-C(1)	117.7(7)	C(5)-C(6)-C(7)	117.4(7)
C(1)-C(6)-C(7)	124.9(7)	C(8)-C(7)-C(6)	113.2(7)
C(8)-C(7)-C(10)	104.9(8)	C(6)-C(7)-C(10)	111.8(6)
C(8)-C(7)-C(9)	108.2(8)	C(6)-C(7)-C(9)	110.6(7)
C(10)-C(7)-C(9)	107.8(8)	C(12)-C(11)-C(14)	105.1(8)
C(12)-C(11)-C(13)	107.2(8)	C(14)-C(11)-C(13)	111.6(8)
C(12)-C(11)-C(2)	112.3(7)	C(14)-C(11)-C(2)	110.2(7)
C(13)-C(11)-C(2)	110.3(7)	C(16')-C(15)-C(17)	135.6(14)
C(16')-C(15)-C(16)	40.1(10)	C(17)-C(15)-C(16)	112.0(12)
C(16')-C(15)-C(18')	117(2)	C(17)-C(15)-C(18')	57.3(13)
C(16)-C(15)-C(18')	139.8(14)	C(16')-C(15)-C(4)	111.3(12)
C(17)-C(15)-C(4)	111.1(9)	C(16)-C(15)-C(4)	108.7(8)
C(18')-C(15)-C(4)	111.1(13)	C(16')-C(15)-C(18)	75.5(13)
C(17)-C(15)-C(18)	101.1(10)	C(16)-C(15)-C(18)	113.0(11)
C(18')-C(15)-C(18)	46.2(12)	C(4)-C(15)-C(18)	110.8(9)
C(16')-C(15)-C(17')	113(2)	C(17)-C(15)-C(17')	40.1(10)
C(16)-C(15)-C(17')	76.4(13)	C(18')-C(15)-C(17')	96(2)
C(4)-C(15)-C(17')	107.6(12)	C(18)-C(15)-C(17')	133.9(13)
C(16')-C(16)-C(15)	65(2)	C(16')-C(16)-C(17')	115(2)
C(15)-C(16)-C(17')	53.8(11)	C(16)-C(16')-C(15)	75(2)
C(16)-C(16')-C(18)	127(3)	C(15)-C(16')-C(18)	56.2(12)
C(17')-C(17)-C(15)	79(2)	C(17')-C(17)-C(18')	140(3)
C(15)-C(17)-C(18')	64.0(14)	C(17)-C(17')-C(15)	61(2)

C(17)-C(17')-C(16)	106(2)	C(15)-C(17')-C(16)	49.8(10)
C(18')-C(18)-C(15)	64(2)	C(18')-C(18)-C(16')	107(2)
C(15)-C(18)-C(16')	48.3(10)	C(18)-C(18')-C(17)	125(3)
C(18)-C(18')-C(15)	70(2)	C(17)-C(18')-C(15)	58.7(13)
C(24)-C(19)-C(20)	119.7(10)	C(21)-C(20)-C(19)	120.3(10)
C(22)-C(21)-C(20)	118.9(11)	C(21)-C(22)-C(23)	121.8(11)
C(22)-C(23)-C(24)	120.3(10)	C(19)-C(24)-C(23)	119.0(9)
C(19)-C(24)-Se(2)	120.5(8)	C(23)-C(24)-Se(2)	120.5(7)
C(26)-C(25)-C(30)	123.0(9)	C(25)-C(26)-C(27)	119.1(9)
C(28)-C(27)-C(26)	119.8(9)	C(27)-C(28)-C(29)	120.4(9)
C(30)-C(29)-C(28)	121.1(9)	C(29)-C(30)-C(25)	116.5(8)
C(29)-C(30)-Se(1)	121.5(7)	C(25)-C(30)-Se(1)	121.7(7)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
In	51(1)	53(1)	39(1)	-5(1)	10(1)	1(1)
Se(1)	63(1)	99(1)	48(1)	-24(1)	0(1)	21(1)
Se(2)	51(1)	120(1)	70(1)	-36(1)	13(1)	4(1)
C(1)	37(5)	41(4)	40(5)	-4(4)	11(4)	1(4)
C(2)	37(5)	43(5)	44(5)	-1(4)	14(4)	4(4)
C(3)	49(5)	63(6)	38(5)	9(4)	12(4)	-1(5)
C(4)	36(5)	55(6)	41(5)	-13(5)	3(4)	6(5)
C(5)	43(5)	47(5)	61(6)	-4(5)	10(5)	-7(4)
C(6)	39(5)	46(5)	34(5)	-11(4)	10(4)	1(4)
C(7)	53(6)	41(5)	58(6)	4(4)	14(5)	-11(5)
C(8)	174(12)	59(7)	105(9)	4(6)	72(9)	-22(7)
C(9)	81(7)	98(8)	115(9)	19(7)	63(7)	6(6)
C(10)	80(8)	89(7)	107(9)	50(7)	-24(7)	-24(7)
C(11)	51(6)	49(5)	60(6)	7(5)	6(5)	-12(5)
C(12)	130(10)	99(8)	75(7)	38(7)	8(7)	-46(8)
C(13)	120(9)	53(6)	146(11)	-20(7)	61(9)	-1(6)
C(14)	74(7)	80(7)	101(8)	8(7)	10(7)	-32(6)
C(15)	64(7)	105(8)	45(5)	-27(6)	10(5)	6(6)
C(19)	74(7)	75(7)	63(7)	-2(6)	24(6)	2(6)
C(20)	123(11)	116(10)	51(7)	15(7)	19(7)	30(9)
C(21)	70(8)	112(10)	101(11)	-43(9)	-4(8)	3(8)
C(22)	113(10)	83(8)	89(9)	-26(8)	17(8)	-23(7)
C(23)	76(7)	73(7)	70(7)	5(6)	22(6)	-1(6)
C(24)	52(6)	66(6)	56(6)	-13(5)	26(5)	5(5)
C(25)	45(6)	81(7)	60(6)	1(6)	11(5)	1(6)
C(26)	63(7)	67(6)	68(7)	0(5)	8(6)	10(6)
C(27)	62(7)	83(8)	66(7)	-16(6)	4(6)	20(6)
C(28)	52(7)	100(8)	61(6)	-7(6)	15(5)	1(6)
C(29)	66(7)	60(6)	62(6)	-4(5)	-1(6)	7(6)
C(30)	52(6)	64(6)	44(5)	-9(5)	12(5)	2(5)

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

	x	y	z	U(eq)
H(3A)	3902(7)	1605(4)	-87(5)	60
H(5A)	2668(7)	-238(4)	725(6)	61
H(8A)	2985(11)	-1264(5)	2594(7)	160
H(8B)	3836(11)	-1076(5)	1918(7)	160
H(8C)	2403(11)	-961(5)	1611(7)	160
H(9A)	2165(8)	511(6)	3096(7)	137
H(9B)	2019(8)	-310(6)	3336(7)	137
H(9C)	1369(8)	-10(6)	2366(7)	137
H(10A)	4514(9)	273(5)	3592(7)	149
H(10B)	5085(9)	-360(5)	3118(7)	149
H(10C)	4192(9)	-539(5)	3765(7)	149
H(12A)	4139(10)	2751(6)	205(7)	156
H(12B)	5396(10)	2351(6)	239(7)	156
H(12C)	5384(10)	3111(6)	716(7)	156
H(13A)	4073(10)	2578(5)	2530(8)	152
H(13B)	3352(10)	2900(5)	1591(8)	152
H(13C)	4613(10)	3246(5)	2097(8)	152
H(14A)	6173(9)	1923(5)	2554(7)	130
H(14B)	6585(9)	2622(5)	2101(7)	130
H(14C)	6596(9)	1863(5)	1624(7)	130
H(19A)	3444(9)	1739(5)	6122(7)	83
H(20A)	4721(13)	2279(8)	7405(7)	116
H(21A)	5975(10)	3243(7)	7223(9)	117
H(22A)	5846(11)	3713(6)	5798(9)	115
H(23A)	4568(9)	3214(5)	4533(7)	87
H(25A)	6918(8)	-24(6)	4756(6)	75
H(26A)	8393(9)	-791(5)	4467(6)	81
H(27A)	9797(9)	-373(6)	3652(6)	86
H(28A)	9785(8)	821(6)	3246(6)	85
H(29A)	8297(9)	1601(5)	3557(6)	78