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Table 1. Crystal data and structure refinement for BRIN.

Identification code	BRIN
Empirical formula	$C_{28}H_{40}Br_2In_2O_4$
Formula weight	830.06
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system	triclinic
Space group	P(-1) [No. 2]
Unit cell dimensions	a = 9.430(2) Å α = 85.23(2)° b = 9.765(2) Å β = 84.91(1)° c = 17.130(3) Å γ = 79.40(2)°
Volume	1540.7(5) Å^3
Z	2
Density (calculated)	1.789 Mg/m^3
Absorption coefficient	4.07 mm^{-1}
F(000)	816
Crystal size	0.2 x 0.25 x 0.56 mm
θ range for data collection	3.09 to 25.98°
Index ranges	$-11 \le h \le 11$, $-11 \le k \le 12$, $0 \le \ell \le 21$
Reflections collected	6032
Independent reflections	6032 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6023 / 0 / 325
Goodness-of-fit on F^2	1.028
Final R indices [I>2σ(I)]	R1 = 0.0325, wR2 = 0.0710
R indices (all data)	R1 = 0.0623, wR2 = 0.0819
Largest diff. peak and hole	0.753 and -1.050 eÅ^{-3}

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [$Å^2$] for BRIN. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
In(1)	0.04915(3)	0.14932(3)	0.45677(2)	0.02515(9)
In(2)	0.42735(4)	0.67470(4)	0.98954(2)	0.03616(10)
Br(1)	0.08797(6)	0.35264(5)	0.35914(3)	0.03975(13)
Br(2)	0.30338(8)	0.92466(6)	0.96167(4)	0.0654(2)
C(01)	0.1719(4)	-0.0471(4)	0.4217(2)	0.0231(9)
C(02)	0.1223(4)	-0.1719(4)	0.4505(2)	0.0240(9)
C(03)	0.1888(5)	-0.2983(5)	0.4203(3)	0.0296(10)
C(04)	0.3010(5)	-0.3029(5)	0.3613(3)	0.0353(11)
C(05)	0.3493(5)	-0.1815(5)	0.3334(3)	0.0334(10)
C(06)	0.2849(5)	-0.0561(5)	0.3637(3)	0.0292(10)
C(07)	0.5624(5)	0.6055(5)	1.0851(3)	0.0341(10)
C(08)	0.6229(5)	0.4639(5)	1.0916(3)	0.0335(10)
C(09)	0.7156(6)	0.4144(6)	1.1513(3)	0.0429(12)
C(010)	0.7467(6)	0.5037(6)	1.2038(3)	0.0478(13)
C(011)	0.6859(6)	0.6423(6)	1.1970(3)	0.0447(13)
C(012)	0.5955(5)	0.6938(5)	1.1387(3)	0.0388(11)
O(1)	0.2234(3)	0.2133(3)	0.5345(2)	0.0326(7)
C(11)	0.3727(5)	0.2020(6)	0.5040(3)	0.0451(13)
C(12)	0.4066(5)	0.3458(5)	0.5041(3)	0.0395(11)
C(13)	0.3145(5)	0.4034(5)	0.5749(3)	0.0420(12)
C(14)	0.1799(5)	0.3420(5)	0.5735(3)	0.0373(11)
O(2)	-0.1368(3)	0.1006(4)	0.3738(2)	0.0399(8)
C(21)	-0.2833(5)	0.1654(7)	0.3814(4)	0.056(2)
C(22)	-0.3558(6)	0.1248(8)	0.3157(4)	0.066(2)
C(23)	-0.2457(7)	0.0167(7)	0.2759(4)	0.067(2)
C(24)	-0.1064(6)	0.0459(8)	0.2981(3)	0.065(2)
O(3)	0.2142(4)	0.6363(4)	1.0797(2)	0.0552(10)
C(31)	0.2134(7)	0.6351(8)	1.1629(3)	0.074(2)
C(32)	0.0774(7)	0.7139(9)	1.1925(4)	0.085(2)
C(33)	0.0078(7)	0.7868(7)	1.1223(4)	0.073(2)
C(34)	0.0693(6)	0.6919(8)	1.0595(4)	0.071(2)
O(4)	0.6399(4)	0.7206(4)	0.9079(2)	0.0562(10)
C(41)	0.6353(7)	0.8010(8)	0.8343(4)	0.073(2)
C(42)	0.7539(8)	0.8864(8)	0.8338(4)	0.075(2)
C(43)	0.8646(7)	0.7900(8)	0.8781(4)	0.067(2)
C(44)	0.7767(6)	0.7212(6)	0.9406(3)	0.0494(14)

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

In(1)-C(01)	2.153(4)	In(1)-C(02)#1	2.157(4)
In(1)-O(1)	2.407(3)	In(1)-O(2)	2.492(3)
In(1)-Br(1)	2.5471(8)	In(2)-C(07)	2.156(4)
In(2)-C(08)#2	2.162(5)	In(2)-O(4)	2.428(4)
In(2)-O(3)	2.488(4)	In(2)-Br(2)	2.5332(9)
C(01)-C(06)	1.386(6)	C(01)-C(02)	1.421(6)
C(02)-C(03)	1.397(6)	C(02)-In(1)#1	2.157(4)
C(03)-C(04)	1.393(6)	C(03)-H(03)	0.96
C(04)-C(05)	1.382(7)	C(04)-H(04)	0.96
C(05)-C(06)	1.385(6)	C(05)-H(05)	0.96
C(06)-H(06)	0.96	C(07)-C(08)	1.396(7)
C(07)-C(012)	1.405(6)	C(08)-C(09)	1.405(6)
C(08)-In(2)#2	2.162(5)	C(09)-C(010)	1.390(7)
C(09)-H(09)	0.96	C(010)-C(011)	1.369(8)
C(010)-H(010)	0.96	C(011)-C(012)	1.377(7)
C(011)-H(011)	0.96	C(012)-H(012)	0.96
O(1)-C(11)	1.444(5)	O(1)-C(14)	1.449(5)
C(11)-C(12)	1.498(7)	C(11)-H(111)	0.96
C(11)-H(112)	0.96	C(12)-C(13)	1.513(7)
C(12)-H(121)	0.96	C(12)-H(122)	0.96
C(13)-C(14)	1.504(6)	C(13)-H(131)	0.96
C(13)-H(132)	0.96	C(14)-H(141)	0.96
C(14)-H(142)	0.96	O(2)-C(21)	1.409(6)
O(2)-C(24)	1.431(6)	C(21)-C(22)	1.487(7)
C(21)-H(211)	0.96	C(21)-H(212)	0.96
C(22)-C(23)	1.500(9)	C(22)-H(221)	0.96
C(22)-H(222)	0.96	C(23)-C(24)	1.483(8)
C(23)-H(231)	0.96	C(23)-H(232)	0.96
C(24)-H(241)	0.96	C(24)-H(242)	0.96
O(3)-C(31)	1.426(6)	O(3)-C(34)	1.437(6)
C(31)-C(32)	1.443(9)	C(31)-H(311)	0.96
C(31)-H(312)	0.96	C(32)-C(33)	1.489(9)
C(32)-H(321)	0.96	C(32)-H(322)	0.96
C(33)-C(34)	1.489(9)	C(33)-H(331)	0.96
C(33)-H(332)	0.96	C(34)-H(341)	0.96
C(34)-H(342)	0.96	O(4)-C(41)	1.431(7)
O(4)-C(44)	1.454(6)	C(41)-C(42)	1.513(9)
C(41)-H(411)	0.96	C(41)-H(412)	0.96
C(42)-C(43)	1.489(9)	C(42)-H(421)	0.96
C(42)-H(422)	0.96	C(43)-C(44)	1.487(8)
C(43)-H(431)	0.96	C(43)-H(432)	0.96
C(44)-H(441)	0.96	C(44)-H(442)	0.96

C(01)-In(1)-C(02)#1	124.7(2)	C(01)-In(1)-O(1)	98.29(13)
C(02)#1-In(1)-O(1)	94.06(13)	C(01)-In(1)-O(2)	85.07(13)
C(02)#1-In(1)-O(2)	85.73(13)	O(1)-In(1)-O(2)	176.01(11)
C(01)-In(1)-Br(1)	112.69(11)	C(02)#1-In(1)-Br(1)	121.39(11)
O(1)-In(1)-Br(1)	88.29(8)	O(2)-In(1)-Br(1)	88.43(9)
C(07)-In(2)-C(08)#2	123.5(2)	C(07)-In(2)-O(4)	89.1(2)
C(08)#2-In(2)-O(4)	92.6(2)	C(07)-In(2)-O(3)	88.6(2)
C(08)#2-In(2)-O(3)	91.1(2)	O(4)-In(2)-O(3)	176.34(13)
C(07)-In(2)-Br(2)	124.24(13)	C(08)#2-In(2)-Br(2)	112.25(12)
O(4)-In(2)-Br(2)	90.15(10)	O(3)-In(2)-Br(2)	88.87(10)
C(06)-C(01)-C(02)	118.1(4)	C(06)-C(01)-In(1)	122.6(3)
C(02)-C(01)-In(1)	118.7(3)	C(03)-C(02)-C(01)	119.4(4)
C(03)-C(02)-In(1)#1	125.0(3)	C(01)-C(02)-In(1)#1	115.6(3)
C(04)-C(03)-C(02)	120.8(4)	C(04)-C(03)-H(03)	119.8(3)
C(02)-C(03)-H(03)	119.4(3)	C(05)-C(04)-C(03)	119.7(4)
C(05)-C(04)-H(04)	119.7(3)	C(03)-C(04)-H(04)	120.5(3)
C(04)-C(05)-C(06)	119.8(4)	C(04)-C(05)-H(05)	120.3(3)

C(06)-C(05)-H(05)	119.9(3)	C(05)-C(06)-C(01)	122.2(4)
C(05)-C(06)-H(06)	118.8(3)	C(01)-C(06)-H(06)	119.0(2)
C(08)-C(07)-C(012)	119.0(4)	C(08)-C(07)-In(2)	116.6(3)
C(012)-C(07)-In(2)	124.3(4)	C(07)-C(08)-C(09)	118.8(4)
C(07)-C(08)-In(2)#2	119.8(3)	C(09)-C(08)-In(2)#2	121.3(4)
C(010)-C(09)-C(08)	121.2(5)	C(010)-C(09)-H(09)	119.8(3)
C(08)-C(09)-H(09)	119.1(3)	C(011)-C(010)-C(09)	119.4(5)
C(011)-C(010)-H(010)	120.2(3)	C(09)-C(010)-H(010)	120.4(3)
C(010)-C(011)-C(012)	120.7(5)	C(010)-C(011)-H(011)	119.7(3)
C(012)-C(011)-H(011)	119.6(3)	C(011)-C(012)-C(07)	120.9(5)
C(011)-C(012)-H(012)	120.1(3)	C(07)-C(012)-H(012)	119.0(3)
C(11)-O(1)-C(14)	109.2(3)	C(11)-O(1)-In(1)	119.9(3)
C(14)-O(1)-In(1)	116.7(3)	O(1)-C(11)-C(12)	105.4(4)
O(1)-C(11)-H(111)	110.7(3)	C(12)-C(11)-H(111)	111.4(3)
O(1)-C(11)-H(112)	110.6(3)	C(12)-C(11)-H(112)	110.0(3)
H(111)-C(11)-H(112)	108.8	C(11)-C(12)-C(13)	102.8(4)
C(11)-C(12)-H(121)	110.5(3)	C(13)-C(12)-H(121)	110.5(3)
C(11)-C(12)-H(122)	111.7(3)	C(13)-C(12)-H(122)	112.0(3)
H(121)-C(12)-H(122)	109.2	C(14)-C(13)-C(12)	102.6(4)
C(14)-C(13)-H(131)	111.8(3)	C(12)-C(13)-H(131)	111.8(3)
C(14)-C(13)-H(132)	110.9(3)	C(12)-C(13)-H(132)	110.4(3)
H(131)-C(13)-H(132)	109.2	O(1)-C(14)-C(13)	106.3(4)
O(1)-C(14)-H(141)	110.7(2)	C(13)-C(14)-H(141)	110.8(3)
O(1)-C(14)-H(142)	110.1(2)	C(13)-C(14)-H(142)	110.1(3)
H(141)-C(14)-H(142)	108.7	C(21)-O(2)-C(24)	108.6(4)
C(21)-O(2)-In(1)	123.3(3)	C(24)-O(2)-In(1)	124.8(3)
O(2)-C(21)-C(22)	107.7(5)	O(2)-C(21)-H(211)	110.6(3)
C(22)-C(21)-H(211)	111.2(4)	O(2)-C(21)-H(212)	109.8(3)
C(22)-C(21)-H(212)	109.0(4)	H(211)-C(21)-H(212)	108.7
C(21)-C(22)-C(23)	105.5(5)	C(21)-C(22)-H(221)	109.7(4)
C(23)-C(22)-H(221)	109.8(4)	C(21)-C(22)-H(222)	112.1(3)
C(23)-C(22)-H(222)	111.0(4)	H(221)-C(22)-H(222)	108.7
C(24)-C(23)-C(22)	103.1(5)	C(24)-C(23)-H(231)	111.9(4)
C(22)-C(23)-H(231)	111.9(3)	C(24)-C(23)-H(232)	110.3(4)
C(22)-C(23)-H(232)	110.5(4)	H(231)-C(23)-H(232)	109.1
O(2)-C(24)-C(23)	105.8(5)	O(2)-C(24)-H(241)	111.1(3)
C(23)-C(24)-H(241)	111.4(4)	O(2)-C(24)-H(242)	109.7(3)
C(23)-C(24)-H(242)	109.9(4)	H(241)-C(24)-H(242)	108.9
C(31)-O(3)-C(34)	107.1(4)	C(31)-O(3)-In(2)	122.8(4)
C(34)-O(3)-In(2)	121.2(4)	O(3)-C(31)-C(32)	108.5(5)
O(3)-C(31)-H(311)	109.0(4)	C(32)-C(31)-H(311)	108.9(5)
O(3)-C(31)-H(312)	110.3(4)	C(32)-C(31)-H(312)	111.9(5)
H(311)-C(31)-H(312)	108.3	C(31)-C(32)-C(33)	105.7(6)
C(31)-C(32)-H(321)	111.6(4)	C(33)-C(32)-H(321)	111.5(5)
C(31)-C(32)-H(322)	109.1(5)	C(33)-C(32)-H(322)	109.9(4)
H(321)-C(32)-H(322)	109.0	C(32)-C(33)-C(34)	102.4(5)
C(32)-C(33)-H(331)	110.3(5)	C(34)-C(33)-H(331)	110.6(4)
C(32)-C(33)-H(332)	112.4(4)	C(34)-C(33)-H(332)	111.9(3)
H(331)-C(33)-H(332)	109.2	O(3)-C(34)-C(33)	104.6(5)
O(3)-C(34)-H(341)	110.6(4)	C(33)-C(34)-H(341)	110.2(4)
O(3)-C(34)-H(342)	111.0(3)	C(33)-C(34)-H(342)	111.3(4)
H(341)-C(34)-H(342)	109.0	C(41)-O(4)-C(44)	109.3(4)
C(41)-O(4)-In(2)	124.3(3)	C(44)-O(4)-In(2)	122.0(3)
O(4)-C(41)-C(42)	104.9(5)	O(4)-C(41)-H(411)	110.2(3)
C(42)-C(41)-H(411)	110.7(4)	O(4)-C(41)-H(412)	111.2(4)
C(42)-C(41)-H(412)	110.9(4)	H(411)-C(41)-H(412)	109.0
C(43)-C(42)-C(41)	102.1(6)	C(43)-C(42)-H(421)	110.9(4)
C(41)-C(42)-H(421)	111.3(4)	C(43)-C(42)-H(422)	111.8(4)
C(41)-C(42)-H(422)	111.5(4)	H(421)-C(42)-H(422)	109.2
C(44)-C(43)-C(42)	103.4(5)	C(44)-C(43)-H(431)	111.3(3)
C(42)-C(43)-H(431)	111.3(4)	C(44)-C(43)-H(432)	110.6(4)
C(42)-C(43)-H(432)	110.9(4)	H(431)-C(43)-H(432)	109.2
O(4)-C(44)-C(43)	105.6(4)	O(4)-C(44)-H(441)	110.6(3)

C(43)-C(44)-H(441)	111.6(4)	O(4)-C(44)-H(442)	110.0(3)
C(43)-C(44)-H(442)	110.3(4)	H(441)-C(44)-H(442)	108.8

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$Å^2$] for BRIN.

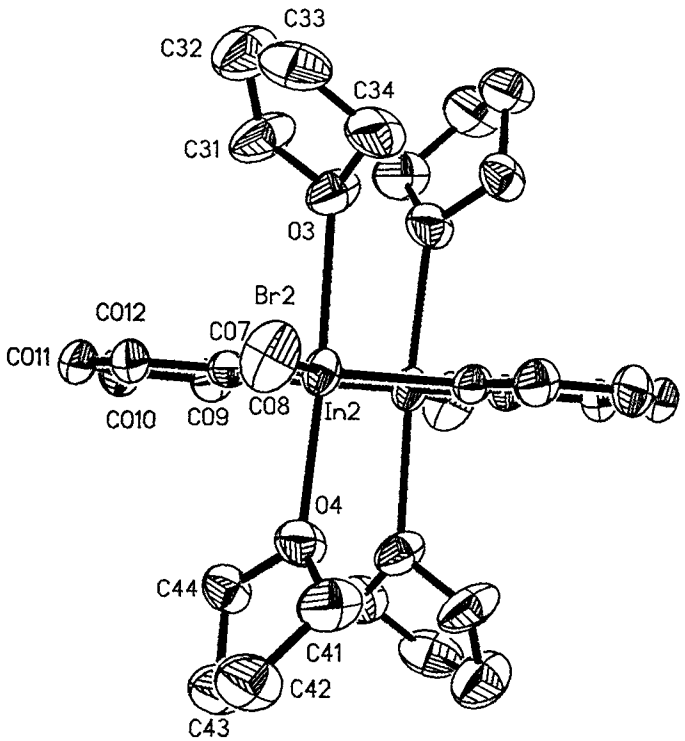
The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
In(1)	0.0215(2)	0.0258(2)	0.0291(2)	-0.00381(12)	0.00352(12)	-0.00851(11)
In(2)	0.0386(2)	0.0372(2)	0.0321(2)	-0.00488(14)	-0.0102(2)	-0.0004(2)
Br(1)	0.0510(3)	0.0342(2)	0.0350(3)	0.0038(2)	0.0003(2)	-0.0145(2)
Br(2)	0.0839(5)	0.0409(3)	0.0646(4)	-0.0021(3)	-0.0149(4)	0.0105(3)
C(01)	0.022(2)	0.026(2)	0.023(2)	-0.005(2)	-0.002(2)	-0.007(2)
C(02)	0.018(2)	0.031(2)	0.025(2)	-0.003(2)	-0.003(2)	-0.007(2)
C(03)	0.025(2)	0.032(2)	0.032(2)	-0.006(2)	-0.004(2)	-0.005(2)
C(04)	0.032(3)	0.039(3)	0.032(3)	-0.010(2)	-0.003(2)	0.006(2)
C(05)	0.024(2)	0.052(3)	0.023(2)	-0.004(2)	0.003(2)	-0.002(2)
C(06)	0.023(2)	0.038(2)	0.027(2)	0.000(2)	0.000(2)	-0.008(2)
C(07)	0.028(2)	0.048(3)	0.027(2)	0.000(2)	-0.003(2)	-0.009(2)
C(08)	0.029(2)	0.046(3)	0.026(2)	-0.002(2)	-0.004(2)	-0.006(2)
C(09)	0.041(3)	0.051(3)	0.036(3)	0.002(2)	-0.009(2)	-0.004(2)
C(010)	0.048(3)	0.063(4)	0.035(3)	0.000(3)	-0.016(2)	-0.013(3)
C(011)	0.043(3)	0.062(3)	0.032(3)	-0.013(2)	-0.004(2)	-0.015(3)
C(012)	0.037(3)	0.044(3)	0.038(3)	-0.009(2)	-0.004(2)	-0.010(2)
O(1)	0.024(2)	0.036(2)	0.040(2)	-0.0071(14)	0.0003(14)	-0.0091(13)
C(11)	0.019(2)	0.056(3)	0.063(4)	-0.018(3)	0.000(2)	-0.009(2)
C(12)	0.030(3)	0.048(3)	0.044(3)	-0.005(2)	-0.003(2)	-0.016(2)
C(13)	0.039(3)	0.045(3)	0.046(3)	-0.015(2)	-0.002(2)	-0.012(2)
C(14)	0.034(3)	0.041(3)	0.039(3)	-0.012(2)	0.003(2)	-0.012(2)
O(2)	0.024(2)	0.057(2)	0.041(2)	-0.021(2)	-0.0024(14)	-0.006(2)
C(21)	0.025(3)	0.080(4)	0.063(4)	-0.021(3)	-0.013(3)	0.003(3)
C(22)	0.033(3)	0.123(6)	0.049(4)	-0.010(4)	-0.011(3)	-0.026(3)
C(23)	0.078(5)	0.082(5)	0.050(4)	-0.019(3)	-0.025(3)	-0.020(4)
C(24)	0.043(3)	0.110(5)	0.041(3)	-0.034(3)	-0.002(3)	0.000(3)
O(3)	0.038(2)	0.087(3)	0.036(2)	-0.007(2)	-0.005(2)	0.005(2)
C(31)	0.058(4)	0.119(6)	0.033(3)	-0.002(3)	-0.002(3)	0.013(4)
C(32)	0.051(4)	0.129(7)	0.067(5)	-0.022(5)	-0.005(3)	0.010(4)
C(33)	0.036(3)	0.073(4)	0.102(6)	0.004(4)	0.007(4)	0.002(3)
C(34)	0.033(3)	0.120(6)	0.061(4)	0.000(4)	-0.017(3)	-0.011(3)
O(4)	0.043(2)	0.087(3)	0.043(2)	0.007(2)	-0.013(2)	-0.022(2)
C(41)	0.049(4)	0.128(6)	0.040(3)	0.013(4)	-0.017(3)	-0.010(4)
C(42)	0.073(5)	0.104(6)	0.050(4)	0.029(4)	-0.015(3)	-0.031(4)
C(43)	0.052(4)	0.100(5)	0.049(4)	0.014(3)	-0.008(3)	-0.022(4)
C(44)	0.041(3)	0.059(3)	0.049(3)	0.006(3)	-0.016(3)	-0.011(3)

Table 5. Hydrogen coordinates and isotropic displacement parameters [Å^2] for BRIN.

	x/a	y/b	z/c	U(eq)
H(03)	0.1568(5)	-0.3829(5)	0.4406(3)	0.044
H(04)	0.3452(5)	-0.3897(5)	0.3400(3)	0.053
H(05)	0.4265(5)	-0.1836(5)	0.2928(3)	0.050
H(06)	0.3199(5)	0.0273(5)	0.3439(3)	0.044
H(09)	0.7572(6)	0.3171(6)	1.1561(3)	0.064
H(010)	0.8107(6)	0.4689(6)	1.2442(3)	0.072
H(011)	0.7061(6)	0.7041(6)	1.2336(3)	0.067
H(012)	0.5544(5)	0.7913(5)	1.1340(3)	0.058
H(111)	0.3856(5)	0.1698(6)	0.4521(3)	0.068
H(112)	0.4346(5)	0.1381(6)	0.5372(3)	0.068
H(121)	0.3780(5)	0.4003(5)	0.4571(3)	0.059
H(122)	0.5077(5)	0.3436(5)	0.5086(3)	0.059
H(131)	0.2938(5)	0.5036(5)	0.5707(3)	0.063
H(132)	0.3620(5)	0.3720(5)	0.6219(3)	0.063
H(141)	0.1387(5)	0.3242(5)	0.6257(3)	0.056
H(142)	0.1095(5)	0.4050(5)	0.5448(3)	0.056
H(211)	-0.2916(5)	0.2648(7)	0.3806(4)	0.084
H(212)	-0.3283(5)	0.1329(7)	0.4302(4)	0.084
H(221)	-0.3811(6)	0.2045(8)	0.2797(4)	0.099
H(222)	-0.4418(6)	0.0887(8)	0.3337(4)	0.099
H(231)	-0.2511(7)	0.0247(7)	0.2201(4)	0.101
H(232)	-0.2585(7)	-0.0753(7)	0.2959(4)	0.101
H(241)	-0.0337(6)	-0.0370(8)	0.2995(3)	0.097
H(242)	-0.0729(6)	0.1144(8)	0.2611(3)	0.097
H(311)	0.2905(7)	0.6791(8)	1.1756(3)	0.111
H(312)	0.2292(7)	0.5409(8)	1.1855(3)	0.111
H(321)	0.0911(7)	0.7788(9)	1.2289(4)	0.127
H(322)	0.0186(7)	0.6508(9)	1.2184(4)	0.127
H(331)	0.0357(7)	0.8764(7)	1.1110(4)	0.110
H(332)	-0.0959(7)	0.7988(7)	1.1288(4)	0.110
H(341)	0.0143(6)	0.6185(8)	1.0594(4)	0.107
H(342)	0.0695(6)	0.7415(8)	1.0088(4)	0.107
H(411)	0.5427(7)	0.8606(8)	0.8309(4)	0.110
H(412)	0.6524(7)	0.7419(8)	0.7913(4)	0.110
H(421)	0.7204(8)	0.9706(8)	0.8602(4)	0.113
H(422)	0.7906(8)	0.9099(8)	0.7813(4)	0.113
H(431)	0.9281(7)	0.8401(8)	0.9000(4)	0.100
H(432)	0.9208(7)	0.7224(8)	0.8449(4)	0.100
H(441)	0.8234(6)	0.6277(6)	0.9548(3)	0.074
H(442)	0.7604(6)	0.7735(6)	0.9864(3)	0.074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C34
C31
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C012
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C010
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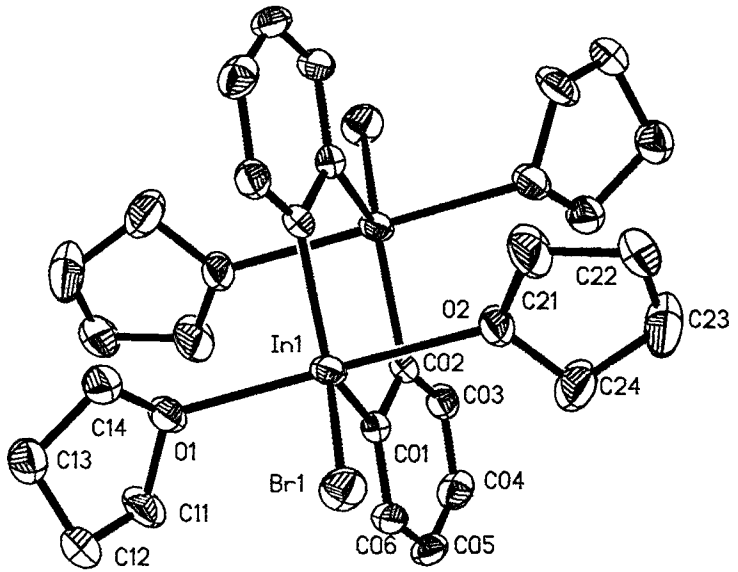
In2
O4
C44
C41
C42
C43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C21
O2
C23
In1
C02
C03
C24
C14
O1
C01
C13
Br1
C04
C11
C06
C05
C12