Table 1. Crystal data and structure refinement for Br-Ph-azain.

Empirical formula	C13 H9 Br N2	
Formula weight	273.13	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 4.0269(12) Å	α= 90°.
	b = 23.489(7) Å	β= 91.527(5)°.
	c = 11.600(4) Å	γ = 90°.
Volume	1096.9(6) $Å^3$	
Z	4	
Density (calculated)	1.654 Mg/m^3	
Absorption coefficient	3.718 mm^{-1}	
F(000)	544	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.73 to 28.38°.	
Index ranges	-5<=h<=5, -30<=k<=28, -15<=l<=14	
Reflections collected	7800	
Independent reflections	2635 [R(int) = 0.0530]	
Completeness to theta = 28.38°	95.3 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2635 / 0 / 181	
Goodness-of-fit on F^2	0.859	
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.1236	
R indices (all data)	R1 = 0.1356, wR2 = 0.1459	
Largest diff. peak and hole	1.365 and -0.359 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Br(1)	2306(2)	3947(1)	2127(1)	62(1)
N(1)	-2967(11)	1541(2)	1321(4)	49(1)
N(2)	-4023(13)	1235(2)	3271(4)	55(1)
C(1)	-3658(16)	1306(3)	238(6)	56(2)
C(2)	-5184(19)	799(3)	339(6)	62(2)
C(3)	-5573(14)	693(2)	1547(5)	53(1)
C(4)	-6961(17)	264(3)	2201(7)	63(2)
C(5)	-6798(18)	322(3)	3373(7)	67(2)
C(6)	-5364(18)	805(3)	3875(6)	65(2)
C(7)	-4155(14)	1161(2)	2133(5)	48(1)
C(8)	-1691(13)	2098(2)	1513(5)	44(1)
C(9)	17(15)	2241(3)	2535(5)	52(2)
C(10)	1168(15)	2786(2)	2707(5)	50(1)
C(11)	714(13)	3195(2)	1863(5)	48(1)
C(12)	-918(15)	3060(3)	839(5)	53(2)
C(13)	-2116(14)	2516(2)	677(5)	50(2)

Table 3. Bond lengths [Å] and angles [°] for Br-Ph-azain.

Br(1)-C(11)	1.899(6)
N(1)-C(7)	1.392(7)
N(1)-C(1)	1.395(7)
N(1)-C(8)	1.421(7)
N(2)-C(7)	1.332(7)
N(2)-C(6)	1.350(8)
C(1)-C(2)	1.346(10)
C(2)-C(3)	1.436(9)
C(3)-C(4)	1.389(8)
C(3)-C(7)	1.405(8)
C(4)-C(5)	1.366(10)
C(5)-C(6)	1.393(9)
C(8)-C(13)	1.387(8)
C(8)-C(9)	1.395(8)
C(9)-C(10)	1.373(8)
C(10)-C(11)	1.382(8)
C(11)-C(12)	1.380(8)
C(12)-C(13)	1.377(8)
C(7)-N(1)-C(1)	106.9(5)
C(7)-N(1)-C(8)	127.9(5)
C(1)-N(1)-C(8)	124.7(5)
C(7)-N(2)-C(6)	114.3(5)
C(2)-C(1)-N(1)	110.7(6)
C(1)-C(2)-C(3)	107.4(6)
C(4)-C(3)-C(7)	117.9(6)
C(4)-C(3)-C(2)	135.6(7)
C(7)-C(3)-C(2)	106.5(6)
C(5)-C(4)-C(3)	117.5(7)
C(4)-C(5)-C(6)	120.4(7)
N(2)-C(6)-C(5)	124.0(7)
N(2)-C(7)-N(1)	125.6(5)
N(2)-C(7)-C(3)	125.9(5)
N(1)-C(7)-C(3)	108.5(5)
C(13)-C(8)-C(9)	118.3(5)
C(13)-C(8)-N(1)	120.2(5)
C(9)-C(8)-N(1)	121.5(5)
C(10)-C(9)-C(8)	120.3(6)
C(9)-C(10)-C(11)	120.5(6)
C(12)-C(11)-C(10)	120.0(6)
C(12)-C(11)-Br(1)	120.3(4)
C(10)-C(11)-Br(1)	119.7(4)
C(13)-C(12)-C(11)	119.3(6)
C(12)-C(13)-C(8)	121.6(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Br-Ph-azain. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	78(1)	49(1)	59(1)	-5(1)	7(1)	-4(1)
N(1)	65(3)	41(3)	42(3)	-4(2)	7(2)	2(2)
N(2)	80(3)	48(3)	38(3)	3(2)	8(3)	3(2)
C(1)	73(4)	48(4)	47(4)	-6(3)	6(3)	-2(3)
C(2)	77(5)	56(4)	55(5)	-7(4)	1(4)	2(4)
C(3)	61(4)	47(4)	50(4)	-4(3)	7(3)	6(3)
C(4)	75(5)	43(4)	70(5)	-6(4)	0(4)	2(3)
C(5)	83(5)	51(4)	66(5)	14(4)	15(4)	0(4)
C(6)	90(5)	56(4)	49(4)	6(3)	10(4)	4(4)
C(7)	56(3)	36(3)	52(4)	2(3)	7(3)	10(2)
C(8)	49(3)	43(3)	41(3)	-2(3)	6(3)	6(2)
C(9)	64(4)	48(4)	43(4)	7(3)	8(3)	5(3)
C(10)	62(4)	45(4)	42(3)	-1(3)	-3(3)	1(3)
C(11)	55(3)	40(3)	48(3)	-2(3)	4(3)	3(3)
C(12)	70(4)	45(4)	43(4)	9(3)	2(3)	4(3)
C(13)	67(4)	47(4)	37(3)	-4(3)	-3(3)	0(3)

Table 5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for Br-Ph-azain.

	x	y	z	U(eq)
H(1)	-2900(120)	1480(20)	-410(50)	46(16)
H(2)	-6020(160)	620(30)	-120(60)	70(30)
H(4)	-7830(160)	-20(30)	1880(60)	80(20)
H(5)	-7750(120)	100(20)	3820(40)	43(15)
H(6)	-5340(140)	860(20)	4660(50)	61(18)
H(9)	180(110)	2000(20)	3110(50)	46(16)
H(10)	2080(110)	2881(19)	3440(40)	40(14)
H(12)	-1450(120)	3280(20)	240(50)	49(16)
H(13)	-3050(130)	2440(20)	-40(50)	58(17)

Table 1. Crystal data and structure refinement for **1**.

Empirical formula	$C_{39} H_{27} N_6 P$	
Formula weight	610.64	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P $2_1/c$	
Unit cell dimensions	a = 13.784(3) Å	α= 90°.
	b = 24.096(5) Å	β= 93.043(5)°.
	c = 9.2284(18) Å	γ = 90°.
Volume	3060.7(10) $Å^3$	
Z	4	
Density (calculated)	1.325 Mg/m^3	
Absorption coefficient	0.130 mm^{-1}	
F(000)	1272	
Crystal size	0.2 x 0.1 x 0.05 mm^3	
Theta range for data collection	1.69 to 28.63°.	
Index ranges	-18<=h<=18, -32<=k<=31, -11<=l<=12	
Reflections collected	22026	
Independent reflections	7260 [R(int) = 0.1714]	
Completeness to theta = 28.63°	92.2 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7260 / 0 / 416	
Goodness-of-fit on F^2	0.779	
Final R indices [I>2sigma(I)]	R1 = 0.0630, wR2 = 0.0759	
R indices (all data)	R1 = 0.3247, wR2 = 0.1104	
Extinction coefficient	0.00032(15)	
Largest diff. peak and hole	0.205 and -0.225 $e.Å^{-3}$	

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)
P(1)	223(1)	3294(1)	34(1)	56(1)
N(1)	-2401(3)	1510(2)	-2607(5)	60(1)
N(2)	-1928(3)	694(2)	-1237(5)	71(1)
N(3)	3958(3)	2977(2)	-3044(4)	51(1)
N(4)	4754(3)	3852(2)	-2601(5)	96(2)
N(5)	-1367(3)	5419(2)	-2615(4)	56(1)
N(6)	-3024(4)	5366(2)	-1927(4)	69(1)
C(1)	-619(3)	2786(2)	-788(5)	51(1)
C(2)	-1344(4)	2886(2)	-1791(6)	83(2)
C(3)	-1958(4)	2472(3)	-2357(6)	85(2)
C(4)	-1806(4)	1928(2)	-1954(6)	52(1)
C(5)	-1102(4)	1825(2)	-905(6)	74(2)
C(6)	-517(3)	2244(2)	-343(5)	73(2)
C(7)	-3052(5)	1583(3)	-3778(7)	104(2)
C(8)	-3520(4)	1116(3)	-4135(7)	115(3)
C(9)	-3177(4)	694(3)	-3201(7)	69(2)
C(10)	-3338(4)	131(3)	-3024(7)	84(2)
C(11)	-2803(5)	-139(2)	-1952(7)	85(2)
C(12)	-2127(4)	155(3)	-1100(6)	86(2)
C(13)	-2458(4)	942(3)	-2265(6)	55(2)
C(14)	1320(3)	3171(2)	-946(5)	43(1)
C(15)	1419(3)	2772(2)	-2041(5)	56(2)
C(16)	2284(4)	2717(2)	-2702(5)	56(2)
C(17)	3073(4)	3047(2)	-2319(5)	48(1)
C(18)	2998(3)	3441(2)	-1251(5)	57(2)
C(19)	2123(4)	3496(2)	-598(5)	61(2)
C(20)	4184(4)	2517(2)	-3859(5)	73(2)
C(21)	5044(4)	2594(2)	-4490(6)	87(2)
C(22)	5390(4)	3124(2)	-4087(6)	67(2)
C(23)	6198(4)	3438(3)	-4356(6)	88(2)
C(24)	6269(5)	3948(3)	-3760(8)	122(3)
C(25)	5541(5)	4146(2)	-2911(7)	134(3)
C(26)	4709(4)	3361(3)	-3158(5)	58(2)
C(27)	-217(3)	3936(2)	-825(5)	50(1)
C(28)	30(3)	4128(2)	-2161(5)	66(2)
C(29)	-354(3)	4608(2)	-2767(5)	66(2)
C(30)	-988(3)	4924(2)	-2003(6)	50(1)
C(31)	-1245(3)	4745(2)	-670(5)	60(2)
C(32)	-849(3)	4263(2)	-92(5)	60(2)
C(33)	-855(4)	5785(2)	-3451(5)	67(2)
C(34)	-1443(5)	6190(2)	-3972(5)	76(2)
C(35)	-2375(5)	6095(2)	-3475(6)	62(2)
C(36)	-3281(5)	6349(2)	-3593(6)	82(2)
C(37)	-4039(4)	6117(3)	-2928(6)	91(2)
C(38)	-3875(4)	5638(2)	-2108(6)	85(2)
C(39)	-2323(5)	5609(2)	-2628(5)	59(2)

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

P(1)-C(1)	1.824(5)
P(1)-C(27)	1.826(4)
P(1)-C(14)	1.827(4)
N(1)-C(7)	1.379(6)
N(1)-C(13)	1.408(6)
N(1)-C(4)	1.413(5)
N(2)-C(13)	1.311(5)
N(2)-C(12)	1.335(5)
N(3)-C(20)	1.384(5)
N(3)-C(26)	1.397(5)
N(3)-C(17)	1.432(5)
N(4)-C(26)	1.291(5)
N(4)-C(25)	1.339(6)
N(5)-C(33)	1.390(5)
N(5)-C(39)	1.394(5)
N(5)-C(30)	1.408(5)
N(6)-C(39)	1.327(5)
N(6)-C(38)	1.347(5)
C(1)-C(2)	1.348(6)
C(1)-C(6)	1.374(5)
C(2)-C(3)	1.390(6)
C(3)-C(4)	1.375(6)
C(4)-C(5)	1.357(5)
C(5)-C(6)	1.377(5)
C(7)-C(8)	1.329(6)
C(8)-C(9)	1.400(7)
C(9)-C(10)	1.385(6)
C(9)-C(13)	1.413(6)
C(10)-C(11)	1.365(6)
C(11)-C(12)	1.382(6)
C(14)-C(19)	1.380(5)
C(14)-C(15)	1.407(5)
C(15)-C(16)	1.374(5)
C(16)-C(17)	1.380(5)
C(17)-C(18)	1.375(5)
C(18)-C(19)	1.383(5)
C(20)-C(21)	1.361(5)
C(21)-C(22)	1.407(6)
C(22)-C(23)	1.379(6)
C(22)-C(26)	1.424(6)
C(23)-C(24)	1.347(6)
C(24)-C(25)	1.390(7)
C(27)-C(28)	1.376(5)
C(27)-C(32)	1.379(5)
C(28)-C(29)	1.379(5)
C(29)-C(30)	1.381(5)
C(30)-C(31)	1.367(5)
C(31)-C(32)	1.379(5)
C(33)-C(34)	1.340(5)
C(34)-C(35)	1.405(6)
C(35)-C(36)	1.388(6)
C(35)-C(39)	1.409(6)
C(36)-C(37)	1.361(6)
C(37)-C(38)	1.391(6)
C(1)-P(1)-C(27)	101.5(2)
C(1)-P(1)-C(14)	102.1(2)

C(27)-P(1)-C(14)	100.75(19)
C(7)-N(1)-C(13)	104.9(5)
C(7)-N(1)-C(4)	125.6(5)
C(13)-N(1)-C(4)	129.4(5)
C(13)-N(2)-C(12)	113.8(6)
C(20)-N(3)-C(26)	107.5(4)
C(20)-N(3)-C(17)	124.8(4)
C(26)-N(3)-C(17)	127.6(4)
C(26)-N(4)-C(25)	115.0(5)
C(33)-N(5)-C(39)	107.2(4)
C(33)-N(5)-C(30)	124.9(5)
C(39)-N(5)-C(30)	127.7(4)
C(39)-N(6)-C(38)	112.1(5)
C(2)-C(1)-C(6)	115.8(5)
C(2)-C(1)-P(1)	126.7(4)
C(6)-C(1)-P(1)	117.5(4)
C(1)-C(2)-C(3)	123.0(5)
C(4)-C(3)-C(2)	120.1(5)
C(5)-C(4)-C(3)	117.4(5)
C(5)-C(4)-N(1)	123.3(5)
C(3)-C(4)-N(1)	119.2(5)
C(4)-C(5)-C(6)	121.1(5)
C(1)-C(6)-C(5)	122.5(5)
C(8)-C(7)-N(1)	112.0(6)
C(7)-C(8)-C(9)	108.6(6)
C(10)-C(9)-C(8)	137.2(7)
C(10)-C(9)-C(13)	117.0(6)
C(8)-C(9)-C(13)	105.7(6)
C(11)-C(10)-C(9)	117.9(6)
C(10)-C(11)-C(12)	119.4(6)
N(2)-C(12)-C(11)	125.4(6)
N(2)-C(13)-N(1)	124.8(6)
N(2)-C(13)-C(9)	126.5(6)
N(1)-C(13)-C(9)	108.7(6)
C(19)-C(14)-C(15)	116.6(4)
C(19)-C(14)-P(1)	117.9(4)
C(15)-C(14)-P(1)	125.5(4)
C(16)-C(15)-C(14)	120.3(4)
C(15)-C(16)-C(17)	121.4(5)
C(18)-C(17)-C(16)	119.6(4)
C(18)-C(17)-N(3)	121.0(5)
C(16)-C(17)-N(3)	119.4(5)
C(17)-C(18)-C(19)	118.6(5)
C(14)-C(19)-C(18)	123.5(4)
C(21)-C(20)-N(3)	110.5(5)
C(20)-C(21)-C(22)	107.6(5)
C(23)-C(22)-C(21)	135.8(6)
C(23)-C(22)-C(26)	116.9(6)
C(21)-C(22)-C(26)	107.3(5)
C(24)-C(23)-C(22)	117.9(6)
C(23)-C(24)-C(25)	120.3(7)
N(4)-C(25)-C(24)	123.7(6)
N(4)-C(26)-N(3)	126.7(5)
N(4)-C(26)-C(22)	126.0(6)
N(3)-C(26)-C(22)	107.2(5)
C(28)-C(27)-C(32)	116.1(4)
C(28)-C(27)-P(1)	125.6(4)
C(32)-C(27)-P(1)	118.3(4)
C(27)-C(28)-C(29)	122.6(4)

C(28)-C(29)-C(30)	119.7(5)
C(31)-C(30)-C(29)	119.0(5)
C(31)-C(30)-N(5)	121.4(5)
C(29)-C(30)-N(5)	119.6(5)
C(30)-C(31)-C(32)	120.0(5)
C(31)-C(32)-C(27)	122.6(4)
C(34)-C(33)-N(5)	110.1(5)
C(33)-C(34)-C(35)	108.2(5)
C(36)-C(35)-C(34)	137.5(6)
C(36)-C(35)-C(39)	115.4(6)
C(34)-C(35)-C(39)	107.2(5)
C(37)-C(36)-C(35)	119.5(6)
C(36)-C(37)-C(38)	118.6(6)
N(6)-C(38)-C(37)	126.0(5)
N(6)-C(39)-N(5)	124.3(5)
N(6)-C(39)-C(35)	128.4(6)
N(5)-C(39)-C(35)	107.3(5)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	65(1)	45(1)	58(1)	3(1)	9(1)	5(1)
N(1)	53(3)	65(4)	61(4)	6(3)	-6(2)	2(3)
N(2)	91(4)	55(4)	66(4)	4(3)	2(3)	-14(3)
N(3)	52(3)	41(3)	61(3)	-3(2)	5(2)	-3(2)
N(4)	97(4)	67(4)	129(4)	-19(4)	38(3)	-34(3)
N(5)	64(3)	38(3)	66(3)	9(2)	8(3)	2(3)
N(6)	60(3)	62(3)	86(4)	-2(3)	1(3)	5(3)
C(1)	60(4)	42(4)	52(4)	13(3)	-2(3)	6(3)
C(2)	85(5)	53(4)	109(6)	39(4)	-23(4)	-14(4)
C(3)	72(5)	65(4)	115(5)	31(4)	-33(3)	-14(4)
C(4)	44(4)	57(4)	55(4)	5(3)	4(3)	-1(3)
C(5)	82(5)	49(4)	87(5)	14(4)	-28(4)	5(4)
C(6)	67(4)	57(4)	93(5)	15(4)	-22(3)	9(4)
C(7)	92(5)	87(6)	127(6)	12(5)	-51(4)	-11(5)
C(8)	95(6)	104(6)	140(7)	29(6)	-64(4)	-9(5)
C(9)	56(4)	67(5)	83(5)	-5(4)	-9(3)	-12(4)
C(10)	74(5)	67(5)	111(6)	-21(4)	9(4)	-21(4)
C(11)	101(6)	58(5)	96(6)	-7(4)	4(4)	-19(4)
C(12)	103(6)	67(5)	87(5)	4(4)	-2(4)	-17(4)
C(13)	45(4)	59(5)	60(5)	-1(4)	9(3)	-1(4)
C(14)	42(3)	34(3)	51(4)	1(3)	-2(3)	-1(3)
C(15)	59(4)	50(4)	60(4)	-15(3)	4(3)	-4(3)
C(16)	63(4)	48(4)	55(4)	-15(3)	-2(3)	-6(3)
C(17)	61(4)	44(4)	38(4)	2(3)	5(3)	4(3)
C(18)	61(4)	46(4)	63(4)	-5(3)	6(3)	-14(3)
C(19)	66(4)	44(4)	73(4)	-18(3)	8(3)	-4(3)
C(20)	78(4)	46(4)	96(5)	-19(3)	6(3)	12(3)
C(21)	64(5)	95(5)	106(5)	-5(4)	26(4)	27(4)
C(22)	60(4)	75(5)	67(4)	10(4)	5(3)	2(4)
C(23)	68(5)	109(6)	90(5)	12(5)	26(4)	-2(5)
C(24)	103(6)	123(7)	145(7)	-2(6)	41(5)	-39(6)
C(25)	139(7)	102(6)	166(7)	-47(5)	72(5)	-57(5)
C(26)	52(4)	70(4)	52(4)	12(4)	5(3)	1(4)
C(27)	58(4)	44(3)	48(4)	5(3)	13(3)	7(3)

C(28)	79(4)	60(4)	61(4)	4(3)	18(3)	28(3)
C(29)	78(4)	61(4)	61(4)	16(3)	25(3)	26(3)
C(30)	50(4)	36(3)	63(4)	5(3)	-1(3)	4(3)
C(31)	67(4)	60(4)	55(4)	5(3)	13(3)	13(3)
C(32)	65(4)	64(4)	53(4)	10(3)	23(3)	10(3)
C(33)	73(4)	53(4)	75(4)	9(3)	23(3)	-11(4)
C(34)	105(6)	48(4)	76(5)	14(3)	9(4)	11(4)
C(35)	70(5)	46(4)	69(4)	0(3)	-13(4)	10(4)
C(36)	105(6)	58(4)	80(5)	1(4)	-20(4)	17(4)
C(37)	84(6)	86(6)	100(6)	2(4)	-15(4)	30(4)
C(38)	62(5)	68(5)	124(6)	7(4)	8(4)	9(4)
C(39)	85(5)	29(4)	63(4)	-8(3)	2(4)	6(4)

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

	x	y	z	U(eq)
H(2B)	-1439	3247	-2119	100
H(3A)	-2471	2564	-3008	102
H(5A)	-1014	1465	-559	89
H(6B)	-35	2157	363	87
H(7A)	-3152	1918	-4261	124
H(8A)	-3997	1077	-4880	138
H(10A)	-3795	-58	-3615	101
H(11A)	-2894	-516	-1797	102
H(12A)	-1782	-39	-371	103
H(15A)	896	2544	-2318	67
H(16A)	2338	2451	-3423	67
H(18A)	3525	3666	-974	68
H(19A)	2074	3766	114	73
H(20A)	3802	2200	-3961	88
H(21A)	5347	2342	-5080	105
H(23A)	6679	3302	-4930	106
H(24A)	6807	4168	-3918	147
H(25A)	5604	4504	-2538	160
H(28A)	472	3926	-2675	79
H(29A)	-187	4718	-3687	79
H(31A)	-1686	4947	-155	72
H(32A)	-1015	4154	830	72
H(33A)	-198	5755	-3624	80
H(34A)	-1266	6482	-4560	91
H(36A)	-3368	6675	-4122	98
H(37A)	-4655	6275	-3020	109
H(38A)	-4401	5493	-1643	102

Table 1. Crystal data and structure refinement for **2**.

Empirical formula	$C_{39}H_{27}N_6Sb$	
Formula weight	701.42	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P $\bar{1}$	
Unit cell dimensions	a = 9.958(9) Å	α= 113.802(12)°.
	b = 13.178(12) Å	β= 93.512(15)°.
	c = 13.772(12) Å	γ = 102.154(16)°.
Volume	1595(2) Å^3	
Z	2	
Density (calculated)	1.461 Mg/m^3	
Absorption coefficient	0.903 mm^{-1}	
F(000)	708	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	1.64 to 28.39°.	
Index ranges	-12<=h<=13, -15<=k<=16, -18<=l<=17	
Reflections collected	10561	
Independent reflections	7093 [R(int) = 0.0672]	
Completeness to theta = 28.39°	88.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7093 / 0 / 415	
Goodness-of-fit on F^2	0.805	
Final R indices [I>2sigma(I)]	R1 = 0.0817, wR2 = 0.1762	
R indices (all data)	R1 = 0.2151, wR2 = 0.2133	
Largest diff. peak and hole	1.820 and -1.590 e.Å^{-3}	

Table 2. 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)
Sb(1)	-3165(1)	673(1)	-1116(1)	56(1)
N(1)	-2346(8)	-40(7)	3180(7)	55(2)
N(3)	2578(9)	4597(8)	419(8)	72(3)
C(37)	-2659(9)	-816(9)	-2180(8)	55(3)
C(23)	-2790(10)	1073(9)	2219(8)	55(3)
N(2)	-3560(9)	1266(8)	4334(8)	68(3)
N(5)	-1948(9)	-3892(7)	-4543(7)	56(2)
C(28)	1385(10)	3643(9)	71(8)	54(3)
C(26)	-2848(10)	-697(9)	263(8)	57(3)
C(25)	-3005(8)	305(8)	276(8)	48(3)
C(22)	-2599(9)	56(9)	2193(8)	50(3)
C(38)	-1328(10)	-949(9)	-2344(9)	68(3)
C(32)	-201(10)	2127(9)	274(8)	56(3)
N(6)	-374(10)	-3131(8)	-5464(8)	67(3)
C(33)	1041(9)	3008(9)	632(8)	55(3)
C(7)	-2840(11)	467(9)	4112(8)	54(3)
C(39)	-1071(10)	-1931(9)	-3118(9)	68(3)
C(27)	-2675(10)	-833(9)	1205(10)	64(3)
C(34)	-2187(10)	-2876(9)	-3776(8)	56(3)
C(24)	-3017(9)	1185(9)	1253(9)	56(3)
C(35)	-3495(10)	-2762(9)	-3644(9)	69(3)
N(4)	4030(11)	4151(11)	1597(10)	115(4)
C(29)	527(11)	3360(9)	-916(9)	67(3)
C(17)	-1349(11)	-5201(11)	-5986(10)	63(3)
C(16)	-2275(12)	-5775(10)	-5539(10)	72(3)
C(31)	-1100(10)	1884(8)	-647(8)	53(3)
C(30)	-718(10)	2489(9)	-1237(8)	65(3)
C(3)	-2432(12)	23(11)	4844(11)	66(3)
C(21)	-1148(11)	-4004(10)	-5320(10)	60(3)
C(36)	-3764(10)	-1784(10)	-2875(9)	73(3)
C(1)	-1638(11)	-799(10)	3316(11)	73(3)
C(18)	-636(15)	-5469(12)	-6832(10)	83(4)
C(9)	3984(13)	6322(10)	694(13)	112(5)
C(20)	293(13)	-3455(12)	-6304(12)	82(4)
C(14)	3775(11)	4840(11)	1194(10)	76(3)
C(15)	-2642(12)	-4995(11)	-4718(10)	77(3)
C(8)	2742(12)	5515(11)	178(11)	93(4)
C(2)	-1688(12)	-755(10)	4289(11)	74(3)
C(12)	6138(18)	5630(20)	2541(15)	163(9)
C(11)	5864(14)	6278(13)	2074(12)	111(5)
C(4)	-2878(15)	427(12)	5826(11)	91(4)
C(6)	-3988(12)	1594(11)	5301(11)	85(4)
C(19)	211(14)	-4594(14)	-7011(10)	86(4)
C(10)	4629(13)	5888(12)	1343(11)	93(4)
C(13)	5236(15)	4549(18)	2280(14)	159(8)
C(5)	-3652(15)	1220(13)	6059(11)	95(4)

Table 3. Bond lengths [Å] and angles [°] for **2**.

Sb(1)-C(37)	2.107(11)
Sb(1)-C(25)	2.163(10)
Sb(1)-C(31)	2.194(10)
N(1)-C(7)	1.364(12)
N(1)-C(1)	1.401(12)
N(1)-C(22)	1.428(12)
N(3)-C(8)	1.360(13)
N(3)-C(28)	1.427(12)
N(3)-C(14)	1.439(13)
C(37)-C(38)	1.393(13)
C(37)-C(36)	1.431(13)
C(23)-C(22)	1.379(13)
C(23)-C(24)	1.407(13)
N(2)-C(7)	1.341(13)
N(2)-C(6)	1.350(13)
N(5)-C(21)	1.353(13)
N(5)-C(15)	1.386(13)
N(5)-C(34)	1.410(12)
C(28)-C(33)	1.360(13)
C(28)-C(29)	1.425(14)
C(26)-C(25)	1.356(12)
C(26)-C(27)	1.385(13)
C(25)-C(24)	1.380(13)
C(22)-C(27)	1.376(13)
C(38)-C(39)	1.392(13)
C(32)-C(31)	1.388(13)
C(32)-C(33)	1.407(13)
N(6)-C(20)	1.333(14)
N(6)-C(21)	1.337(13)
C(7)-C(3)	1.432(14)
C(39)-C(34)	1.411(13)
C(34)-C(35)	1.357(13)
C(35)-C(36)	1.390(13)
N(4)-C(14)	1.298(14)
N(4)-C(13)	1.342(15)
C(29)-C(30)	1.405(13)
C(17)-C(18)	1.364(16)
C(17)-C(16)	1.397(15)
C(17)-C(21)	1.431(14)
C(16)-C(15)	1.319(14)
C(31)-C(30)	1.368(13)
C(3)-C(4)	1.378(16)
C(3)-C(2)	1.394(15)
C(1)-C(2)	1.322(14)
C(18)-C(19)	1.396(16)
C(9)-C(8)	1.376(15)
C(9)-C(10)	1.427(18)
C(20)-C(19)	1.402(16)
C(14)-C(10)	1.387(16)
C(12)-C(11)	1.32(2)
C(12)-C(13)	1.41(2)
C(11)-C(10)	1.398(17)
C(4)-C(5)	1.375(17)
C(6)-C(5)	1.374(16)
C(37)-Sb(1)-C(25)	96.0(4)
C(37)-Sb(1)-C(31)	99.2(3)

C(25)-Sb(1)-C(31)	94.9(4)
C(7)-N(1)-C(1)	107.1(10)
C(7)-N(1)-C(22)	128.3(9)
C(1)-N(1)-C(22)	124.3(10)
C(8)-N(3)-C(28)	126.9(10)
C(8)-N(3)-C(14)	106.3(9)
C(28)-N(3)-C(14)	126.4(10)
C(38)-C(37)-C(36)	114.5(10)
C(38)-C(37)-Sb(1)	126.6(8)
C(36)-C(37)-Sb(1)	118.7(7)
C(22)-C(23)-C(24)	119.9(10)
C(7)-N(2)-C(6)	115.3(10)
C(21)-N(5)-C(15)	106.5(9)
C(21)-N(5)-C(34)	128.0(9)
C(15)-N(5)-C(34)	125.1(10)
C(33)-C(28)-C(29)	119.5(9)
C(33)-C(28)-N(3)	123.3(9)
C(29)-C(28)-N(3)	117.2(10)
C(25)-C(26)-C(27)	121.1(10)
C(26)-C(25)-C(24)	118.3(10)
C(26)-C(25)-Sb(1)	125.2(8)
C(24)-C(25)-Sb(1)	116.5(7)
C(27)-C(22)-C(23)	118.1(10)
C(27)-C(22)-N(1)	122.6(10)
C(23)-C(22)-N(1)	119.3(9)
C(39)-C(38)-C(37)	123.6(10)
C(31)-C(32)-C(33)	121.5(9)
C(20)-N(6)-C(21)	114.0(11)
C(28)-C(33)-C(32)	120.0(9)
N(2)-C(7)-N(1)	126.8(10)
N(2)-C(7)-C(3)	124.8(11)
N(1)-C(7)-C(3)	108.3(11)
C(38)-C(39)-C(34)	120.3(9)
C(22)-C(27)-C(26)	121.4(10)
C(35)-C(34)-N(5)	121.6(10)
C(35)-C(34)-C(39)	117.3(10)
N(5)-C(34)-C(39)	121.1(9)
C(25)-C(24)-C(23)	121.0(9)
C(34)-C(35)-C(36)	122.9(10)
C(14)-N(4)-C(13)	114.6(13)
C(30)-C(29)-C(28)	118.7(10)
C(18)-C(17)-C(16)	138.2(13)
C(18)-C(17)-C(21)	116.1(13)
C(16)-C(17)-C(21)	105.8(11)
C(15)-C(16)-C(17)	107.8(11)
C(30)-C(31)-C(32)	118.3(9)
C(30)-C(31)-Sb(1)	119.1(8)
C(32)-C(31)-Sb(1)	122.5(8)
C(31)-C(30)-C(29)	121.8(10)
C(4)-C(3)-C(2)	138.8(12)
C(4)-C(3)-C(7)	116.1(12)
C(2)-C(3)-C(7)	105.1(11)
N(6)-C(21)-N(5)	124.9(11)
N(6)-C(21)-C(17)	126.7(12)
N(5)-C(21)-C(17)	108.3(11)
C(35)-C(36)-C(37)	121.4(9)
C(2)-C(1)-N(1)	109.5(11)
C(17)-C(18)-C(19)	119.8(12)
C(8)-C(9)-C(10)	105.1(12)

N(6)-C(20)-C(19)	125.3(13)
N(4)-C(14)-C(10)	127.7(11)
N(4)-C(14)-N(3)	125.2(11)
C(10)-C(14)-N(3)	106.9(11)
C(16)-C(15)-N(5)	111.6(11)
N(3)-C(8)-C(9)	112.4(11)
C(1)-C(2)-C(3)	110.0(11)
C(11)-C(12)-C(13)	120.8(15)
C(12)-C(11)-C(10)	118.7(15)
C(5)-C(4)-C(3)	120.1(12)
N(2)-C(6)-C(5)	124.2(13)
C(18)-C(19)-C(20)	118.1(12)
C(14)-C(10)-C(11)	115.7(13)
C(14)-C(10)-C(9)	109.1(11)
C(11)-C(10)-C(9)	135.1(14)
N(4)-C(13)-C(12)	122.3(15)
C(6)-C(5)-C(4)	119.3(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sb(1)	48(1)	53(1)	53(1)	14(1)	-11(1)	8(1)
N(1)	46(5)	58(6)	58(6)	23(5)	-5(4)	13(4)
N(3)	60(6)	48(6)	87(7)	17(5)	-12(5)	-1(5)
C(37)	22(5)	87(8)	59(7)	42(6)	-9(5)	3(5)
C(23)	54(6)	53(7)	44(7)	12(6)	-3(5)	8(5)
N(2)	64(6)	84(7)	49(6)	23(6)	1(5)	20(5)
N(5)	59(6)	36(6)	50(6)	1(5)	-4(5)	7(5)
C(28)	44(6)	51(7)	50(7)	11(6)	-5(5)	6(5)
C(26)	56(6)	49(7)	48(7)	4(6)	3(5)	12(5)
C(25)	34(5)	34(6)	58(7)	5(5)	0(5)	4(4)
C(22)	46(6)	51(7)	43(7)	9(6)	1(5)	17(5)
C(38)	54(7)	65(8)	61(8)	13(7)	-25(6)	6(6)
C(32)	58(6)	64(7)	49(7)	30(6)	4(6)	13(6)
N(6)	64(6)	77(7)	62(7)	30(6)	6(5)	23(6)
C(33)	42(6)	59(7)	50(7)	17(6)	-6(5)	2(5)
C(7)	61(7)	52(7)	34(7)	13(6)	-2(5)	-5(6)
C(39)	40(6)	62(8)	83(9)	9(7)	4(6)	22(6)
C(27)	67(7)	45(7)	78(9)	27(7)	1(6)	12(6)
C(34)	46(6)	55(7)	50(7)	11(6)	-10(5)	7(5)
C(24)	51(6)	52(7)	70(8)	32(7)	6(6)	15(5)
C(35)	46(6)	56(8)	74(8)	6(7)	-6(6)	-2(6)
N(4)	73(7)	152(12)	132(11)	99(10)	-41(7)	-12(7)
C(29)	57(7)	71(8)	75(8)	43(7)	-2(6)	-1(6)
C(17)	47(6)	77(9)	52(8)	13(7)	-1(6)	20(6)
C(16)	63(8)	59(8)	73(9)	9(7)	-8(7)	19(7)
C(31)	60(6)	39(6)	48(7)	8(5)	10(6)	9(5)
C(30)	55(6)	68(8)	48(7)	18(6)	-20(5)	-12(6)
C(3)	60(7)	78(9)	60(9)	44(8)	-9(6)	-4(7)
C(21)	53(7)	47(8)	67(8)	15(7)	-12(6)	11(6)
C(36)	41(6)	71(8)	76(9)	8(7)	-5(6)	5(6)
C(1)	63(7)	69(8)	74(10)	22(7)	-10(6)	19(6)
C(18)	94(10)	69(10)	63(9)	10(8)	-26(8)	22(8)
C(9)	68(9)	48(8)	188(16)	36(10)	-9(10)	-13(7)
C(20)	68(8)	87(11)	82(10)	34(9)	-4(8)	8(7)

C(14)	44(6)	76(9)	81(9)	26(8)	-21(6)	-10(6)
C(15)	84(9)	59(9)	81(10)	24(8)	4(7)	19(8)
C(8)	73(8)	71(9)	130(12)	52(9)	-31(8)	1(7)
C(2)	65(8)	75(9)	68(9)	27(7)	-24(7)	8(7)
C(12)	98(13)	220(20)	137(17)	93(16)	-71(11)	-39(14)
C(11)	71(9)	98(12)	108(13)	22(10)	-29(9)	-34(8)
C(4)	113(12)	90(11)	58(10)	44(9)	-25(8)	-13(9)
C(6)	74(8)	104(11)	60(9)	25(8)	3(7)	12(8)
C(19)	95(10)	105(12)	50(8)	14(9)	10(7)	47(9)
C(10)	63(8)	83(10)	101(11)	19(9)	-14(8)	4(8)
C(13)	71(10)	240(20)	187(19)	153(18)	-57(11)	-32(12)
C(5)	94(10)	110(13)	64(10)	40(9)	-3(8)	-8(9)

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

	x	y	z	U(eq)
H(23A)	-2769	1682	2874	66
H(26A)	-2856	-1304	-391	69
H(38A)	-569	-347	-1913	81
H(32A)	-425	1697	664	67
H(33A)	1627	3155	1253	66
H(39A)	-159	-1965	-3202	81
H(27A)	-2609	-1540	1169	77
H(24A)	-3178	1863	1274	67
H(35A)	-4245	-3365	-4088	83
H(29A)	786	3744	-1339	81
H(16A)	-2578	-6566	-5778	86
H(30A)	-1299	2319	-1867	78
H(36A)	-4681	-1758	-2810	87
H(1A)	-1201	-1261	2801	87
H(18A)	-714	-6233	-7288	100
H(9A)	4329	7002	633	135
H(20A)	858	-2879	-6433	99
H(15A)	-3285	-5164	-4308	92
H(8A)	2088	5590	-284	112
H(2A)	-1286	-1182	4562	88
H(12A)	6938	5894	3050	195
H(11A)	6479	6981	2228	133
H(4A)	-2655	161	6331	110
H(6A)	-4545	2107	5464	102
H(19A)	707	-4761	-7582	104
H(13A)	5484	4092	2591	191
H(5A)	-3946	1501	6723	114

Table 1. Crystal data and structure refinement for **3**.

Empirical formula	$C_{39}H_{27}N_6Bi \cdot 0.5Et_2O \cdot 0.2\ C_6H_{14}$
Formula weight	842.41
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 15.354(6) Å α= 109.589(7)°. b = 16.010(6) Å β= 98.344(7)°. c = 18.127(7) Å γ = 114.720(7)°.
Volume	3595(3) Å^3
Z	4
Density (calculated)	1.557 Mg/m^3
Absorption coefficient	4.945 mm^{-1}
F(000)	1668
Crystal size	0.1 x 0.05 x 0.05 mm^3
Theta range for data collection	1.64 to 28.33°.
Index ranges	-20<=h<=19, -21<=k<=21, -22<=l<=23
Reflections collected	26062
Independent reflections	16615 [R(int) = 0.0520]
Completeness to theta = 28.33°	92.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16615 / 0 / 869
Goodness-of-fit on F^2	0.698
Final R indices [I>2sigma(I)]	R1 = 0.0551, wR2 = 0.0764
R indices (all data)	R1 = 0.1863, wR2 = 0.0943
Largest diff. peak and hole	1.805 and -0.840 e.Å^{-3}

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

	x	y	z	U(eq)
Bi(1)	3078(1)	5202(1)	1132(1)	59(1)
Bi(2)	6462(1)	9502(1)	3520(1)	53(1)
N(1)	7848(7)	7621(6)	3280(5)	58(2)
N(2)	8128(7)	6398(6)	3577(5)	83(3)
N(3)	2516(8)	797(7)	-1132(6)	68(3)
N(4)	927(9)	69(8)	-2202(7)	91(3)
N(5)	3890(6)	6836(6)	-1654(5)	64(2)
N(6)	4977(7)	8642(7)	-818(5)	78(3)
N(7)	6025(6)	7283(6)	5963(5)	58(2)
N(8)	7290(8)	8625(7)	7261(6)	92(3)
N(9)	1753(6)	8290(6)	2418(4)	52(2)
N(10)	922(6)	6540(7)	2173(5)	80(3)
N(11)	7660(6)	14070(6)	6067(6)	60(2)
N(12)	7272(6)	14710(6)	5105(5)	73(3)
C(1)	8520(9)	8633(8)	3447(7)	75(3)
C(2)	9464(10)	8983(9)	3897(7)	88(4)
C(3)	9458(10)	8170(10)	4015(7)	80(3)
C(4)	10183(10)	7982(11)	4376(8)	113(5)
C(5)	9870(11)	7039(13)	4340(8)	121(5)
C(6)	8851(11)	6285(10)	3943(8)	119(5)
C(7)	8465(9)	7339(10)	3646(7)	66(3)
C(8)	6822(8)	7036(7)	2785(7)	52(3)
C(9)	6096(9)	6473(7)	3056(6)	63(3)
C(10)	5098(9)	5927(7)	2596(6)	73(3)
C(11)	4712(7)	5956(6)	1816(6)	51(3)
C(12)	5477(8)	6539(7)	1584(6)	54(3)
C(13)	6480(9)	7067(7)	2051(6)	60(3)
C(14)	3200(9)	485(10)	-1014(8)	84(4)
C(15)	2887(12)	-427(11)	-1644(11)	114(5)
C(16)	1967(12)	-722(11)	-2190(10)	91(4)
C(17)	1261(13)	-1519(12)	-2964(11)	124(6)
C(18)	419(14)	-1536(13)	-3313(11)	149(8)
C(19)	279(10)	-734(13)	-2912(10)	123(6)
C(20)	1731(11)	72(9)	-1866(8)	65(3)
C(21)	2668(10)	1787(9)	-586(7)	57(3)
C(22)	1834(8)	1881(8)	-551(6)	68(3)
C(23)	1939(8)	2823(9)	-64(6)	65(3)
C(24)	2933(9)	3701(8)	418(6)	60(3)
C(25)	3706(7)	3523(7)	362(6)	54(3)
C(26)	3618(8)	2600(9)	-124(6)	62(3)
C(27)	3520(8)	6206(8)	-2500(7)	79(3)
C(28)	3785(9)	6755(9)	-2927(7)	95(4)
C(29)	4407(8)	7781(9)	-2342(7)	69(3)
C(30)	4957(9)	8714(10)	-2344(8)	89(4)
C(31)	5476(10)	9565(9)	-1614(9)	110(5)
C(32)	5464(9)	9501(8)	-877(7)	109(5)
C(33)	4450(8)	7845(8)	-1540(7)	54(3)
C(34)	3738(7)	6472(7)	-1025(6)	51(3)
C(35)	3610(7)	7031(7)	-331(6)	58(3)
C(36)	3428(7)	6658(7)	254(6)	59(3)
C(37)	3364(7)	5723(8)	138(6)	57(3)
C(38)	3467(6)	5186(7)	-564(6)	53(3)
C(39)	3647(6)	5548(7)	-1146(5)	54(3)
C(40)	5286(8)	6274(8)	5670(7)	88(4)

C(41)	5375(10)	6048(10)	6328(9)	108(5)
C(42)	6119(10)	6895(10)	7031(9)	84(4)
C(43)	6519(12)	7157(12)	7849(9)	113(5)
C(44)	7301(12)	8099(12)	8352(8)	125(5)
C(45)	7648(10)	8806(8)	8051(8)	118(5)
C(46)	6558(9)	7674(9)	6777(8)	64(3)
C(47)	6131(8)	7825(7)	5458(6)	48(3)
C(48)	5288(7)	7690(7)	4956(6)	59(3)
C(49)	5378(7)	8190(7)	4454(6)	57(3)
C(50)	6333(8)	8826(6)	4452(6)	52(3)
C(51)	7186(7)	8974(7)	4969(6)	57(3)
C(52)	7080(7)	8484(6)	5474(5)	49(3)
C(53)	1385(9)	8955(7)	2423(6)	71(3)
C(54)	364(9)	8489(9)	2194(7)	77(4)
C(55)	46(9)	7479(11)	2062(7)	76(4)
C(56)	-879(10)	6641(11)	1844(7)	97(4)
C(57)	-919(10)	5741(11)	1787(8)	108(5)
C(58)	-11(11)	5732(9)	1962(8)	108(5)
C(59)	894(8)	7370(8)	2192(6)	62(3)
C(60)	2770(8)	8568(7)	2653(6)	43(2)
C(61)	3102(8)	7898(7)	2308(6)	54(3)
C(62)	4099(8)	8157(7)	2550(6)	48(3)
C(63)	4853(7)	9106(7)	3156(6)	55(3)
C(64)	4506(7)	9785(7)	3503(5)	48(3)
C(65)	3519(8)	9529(7)	3252(5)	50(3)
C(66)	8057(8)	14482(9)	6923(7)	81(4)
C(67)	8245(9)	15458(9)	7256(7)	101(4)
C(68)	7984(8)	15689(9)	6603(8)	72(3)
C(69)	8035(8)	16555(8)	6532(8)	91(4)
C(70)	7711(9)	16470(9)	5752(9)	92(4)
C(71)	7351(9)	15577(10)	5072(8)	93(4)
C(72)	7619(8)	14830(8)	5868(7)	59(3)
C(73)	7442(7)	13077(7)	5501(6)	54(3)
C(74)	7375(7)	12816(7)	4695(6)	65(3)
C(75)	7155(7)	11848(7)	4172(6)	65(3)
C(76)	6934(7)	11096(6)	4438(6)	54(3)
C(77)	7036(7)	11356(7)	5257(6)	58(3)
C(78)	7264(7)	12322(7)	5779(6)	68(3)
C(79)	9930(12)	5207(11)	5378(8)	111(5)
C(80)	11148(19)	6346(19)	7304(16)	323(15)
C(81)	10577(13)	5707(13)	6169(11)	164(7)
C(82)	-1380(50)	1920(60)	140(40)	370(40)
C(83)	-890(30)	1330(30)	230(20)	168(14)
C(84)	-621(16)	3415(16)	22(12)	281(12)
C(85)	-164(17)	1229(17)	736(15)	250(10)
C(86)	-1170(30)	2570(30)	-80(20)	162(13)
C(87)	-560(40)	1770(40)	860(30)	260(20)
O(1)	-450(12)	2450(12)	440(10)	246(6)

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

Bi(1)-C(11)	2.202(10)
Bi(1)-C(24)	2.211(11)
Bi(1)-C(37)	2.251(9)
Bi(2)-C(63)	2.209(10)
Bi(2)-C(76)	2.250(9)
Bi(2)-C(50)	2.283(8)
N(1)-C(7)	1.386(11)

N(1)-C(8)	1.399(10)
N(1)-C(1)	1.401(10)
N(2)-C(6)	1.319(12)
N(2)-C(7)	1.324(11)
N(3)-C(14)	1.359(12)
N(3)-C(20)	1.377(12)
N(3)-C(21)	1.456(12)
N(4)-C(20)	1.292(12)
N(4)-C(19)	1.323(14)
N(5)-C(27)	1.386(10)
N(5)-C(33)	1.399(10)
N(5)-C(34)	1.451(10)
N(6)-C(33)	1.306(10)
N(6)-C(32)	1.314(11)
N(7)-C(46)	1.357(11)
N(7)-C(40)	1.377(10)
N(7)-C(47)	1.440(10)
N(8)-C(46)	1.319(11)
N(8)-C(45)	1.341(12)
N(9)-C(59)	1.375(10)
N(9)-C(60)	1.384(10)
N(9)-C(53)	1.397(10)
N(10)-C(59)	1.336(11)
N(10)-C(58)	1.353(12)
N(11)-C(66)	1.384(10)
N(11)-C(72)	1.402(11)
N(11)-C(73)	1.433(10)
N(12)-C(72)	1.324(10)
N(12)-C(71)	1.365(11)
C(1)-C(2)	1.322(11)
C(2)-C(3)	1.384(13)
C(3)-C(7)	1.398(13)
C(3)-C(4)	1.401(14)
C(4)-C(5)	1.352(14)
C(5)-C(6)	1.390(14)
C(8)-C(13)	1.382(11)
C(8)-C(9)	1.382(11)
C(9)-C(10)	1.351(11)
C(10)-C(11)	1.475(11)
C(11)-C(12)	1.385(10)
C(12)-C(13)	1.362(10)
C(14)-C(15)	1.343(14)
C(15)-C(16)	1.386(15)
C(16)-C(17)	1.405(16)
C(16)-C(20)	1.428(15)
C(17)-C(18)	1.339(19)
C(18)-C(19)	1.368(18)
C(21)-C(22)	1.358(12)
C(21)-C(26)	1.360(11)
C(22)-C(23)	1.394(12)
C(23)-C(24)	1.437(11)
C(24)-C(25)	1.341(11)
C(25)-C(26)	1.379(11)
C(27)-C(28)	1.337(11)
C(28)-C(29)	1.400(12)
C(29)-C(30)	1.377(12)
C(29)-C(33)	1.411(11)
C(30)-C(31)	1.349(13)
C(31)-C(32)	1.376(13)

C(34)-C(39)	1.363(11)
C(34)-C(35)	1.374(11)
C(35)-C(36)	1.389(10)
C(36)-C(37)	1.398(11)
C(37)-C(38)	1.351(11)
C(38)-C(39)	1.373(10)
C(40)-C(41)	1.361(12)
C(41)-C(42)	1.375(13)
C(42)-C(43)	1.364(14)
C(42)-C(46)	1.412(12)
C(43)-C(44)	1.339(14)
C(44)-C(45)	1.363(14)
C(47)-C(48)	1.358(10)
C(47)-C(52)	1.385(11)
C(48)-C(49)	1.386(10)
C(49)-C(50)	1.393(11)
C(50)-C(51)	1.372(10)
C(51)-C(52)	1.377(10)
C(53)-C(54)	1.346(11)
C(54)-C(55)	1.399(13)
C(55)-C(56)	1.364(13)
C(55)-C(59)	1.382(13)
C(56)-C(57)	1.385(14)
C(57)-C(58)	1.391(14)
C(60)-C(61)	1.379(11)
C(60)-C(65)	1.380(11)
C(61)-C(62)	1.364(10)
C(62)-C(63)	1.377(10)
C(63)-C(64)	1.408(11)
C(64)-C(65)	1.352(10)
C(66)-C(67)	1.352(12)
C(67)-C(68)	1.407(12)
C(68)-C(72)	1.375(12)
C(68)-C(69)	1.405(13)
C(69)-C(70)	1.370(13)
C(70)-C(71)	1.353(13)
C(73)-C(74)	1.352(11)
C(73)-C(78)	1.402(10)
C(74)-C(75)	1.379(11)
C(75)-C(76)	1.375(10)
C(76)-C(77)	1.365(10)
C(77)-C(78)	1.372(10)
C(79)-C(81)	1.354(17)
C(79)-C(79)#1	1.40(2)
C(80)-C(81)	1.83(2)
C(82)-C(86)	1.18(8)
C(82)-O(1)	1.23(7)
C(83)-C(85)	1.44(4)
C(83)-O(1)	1.51(4)
C(84)-C(86)	1.19(4)
C(85)-C(87)	1.23(6)
C(86)-O(1)	1.47(3)
C(87)-O(1)	1.50(6)

C(11)-Bi(1)-C(24)	94.7(4)
C(11)-Bi(1)-C(37)	93.0(3)
C(24)-Bi(1)-C(37)	93.6(4)
C(63)-Bi(2)-C(76)	91.1(3)
C(63)-Bi(2)-C(50)	94.6(3)

C(76)-Bi(2)-C(50)	95.9(3)
C(7)-N(1)-C(8)	129.9(10)
C(7)-N(1)-C(1)	103.6(9)
C(8)-N(1)-C(1)	126.2(10)
C(6)-N(2)-C(7)	112.7(10)
C(14)-N(3)-C(20)	109.1(11)
C(14)-N(3)-C(21)	123.4(12)
C(20)-N(3)-C(21)	127.3(11)
C(20)-N(4)-C(19)	116.8(14)
C(27)-N(5)-C(33)	107.4(8)
C(27)-N(5)-C(34)	124.4(8)
C(33)-N(5)-C(34)	128.1(8)
C(33)-N(6)-C(32)	112.9(9)
C(46)-N(7)-C(40)	110.5(9)
C(46)-N(7)-C(47)	127.0(9)
C(40)-N(7)-C(47)	122.3(9)
C(46)-N(8)-C(45)	113.7(10)
C(59)-N(9)-C(60)	130.6(9)
C(59)-N(9)-C(53)	104.1(9)
C(60)-N(9)-C(53)	125.2(9)
C(59)-N(10)-C(58)	113.0(10)
C(66)-N(11)-C(72)	107.9(9)
C(66)-N(11)-C(73)	124.6(9)
C(72)-N(11)-C(73)	127.1(9)
C(72)-N(12)-C(71)	113.8(9)
C(2)-C(1)-N(1)	113.6(10)
C(1)-C(2)-C(3)	105.7(11)
C(2)-C(3)-C(7)	108.6(11)
C(2)-C(3)-C(4)	136.3(14)
C(7)-C(3)-C(4)	115.0(13)
C(5)-C(4)-C(3)	118.4(13)
C(4)-C(5)-C(6)	119.8(13)
N(2)-C(6)-C(5)	125.3(12)
N(2)-C(7)-N(1)	122.6(12)
N(2)-C(7)-C(3)	128.7(12)
N(1)-C(7)-C(3)	108.5(11)
C(13)-C(8)-C(9)	117.3(10)
C(13)-C(8)-N(1)	122.0(10)
C(9)-C(8)-N(1)	120.5(10)
C(10)-C(9)-C(8)	121.2(10)
C(9)-C(10)-C(11)	122.6(9)
C(12)-C(11)-C(10)	113.1(9)
C(12)-C(11)-Bi(1)	124.0(7)
C(10)-C(11)-Bi(1)	122.8(7)
C(13)-C(12)-C(11)	123.1(9)
C(12)-C(13)-C(8)	122.6(10)
C(15)-C(14)-N(3)	110.0(13)
C(14)-C(15)-C(16)	107.9(14)
C(15)-C(16)-C(17)	138.8(17)
C(15)-C(16)-C(20)	107.4(14)
C(17)-C(16)-C(20)	113.6(15)
C(18)-C(17)-C(16)	121.2(18)
C(17)-C(18)-C(19)	118.4(18)
N(4)-C(19)-C(18)	124.4(16)
N(4)-C(20)-N(3)	129.0(14)
N(4)-C(20)-C(16)	125.5(14)
N(3)-C(20)-C(16)	105.5(14)
C(22)-C(21)-C(26)	120.7(12)
C(22)-C(21)-N(3)	118.2(12)

C(26)-C(21)-N(3)	121.2(11)
C(21)-C(22)-C(23)	120.4(11)
C(22)-C(23)-C(24)	120.2(10)
C(25)-C(24)-C(23)	114.8(10)
C(25)-C(24)-Bi(1)	125.8(9)
C(23)-C(24)-Bi(1)	119.3(8)
C(24)-C(25)-C(26)	125.8(10)
C(21)-C(26)-C(25)	118.0(10)
C(28)-C(27)-N(5)	111.1(9)
C(27)-C(28)-C(29)	106.7(10)
C(30)-C(29)-C(28)	137.4(11)
C(30)-C(29)-C(33)	113.7(10)
C(28)-C(29)-C(33)	108.9(9)
C(31)-C(30)-C(29)	119.0(10)
C(30)-C(31)-C(32)	120.6(11)
N(6)-C(32)-C(31)	124.3(11)
N(6)-C(33)-N(5)	124.5(9)
N(6)-C(33)-C(29)	129.3(9)
N(5)-C(33)-C(29)	105.8(9)
C(39)-C(34)-C(35)	119.9(9)
C(39)-C(34)-N(5)	120.5(9)
C(35)-C(34)-N(5)	119.4(9)
C(34)-C(35)-C(36)	119.0(9)
C(35)-C(36)-C(37)	120.9(9)
C(38)-C(37)-C(36)	118.1(9)
C(38)-C(37)-Bi(1)	124.2(7)
C(36)-C(37)-Bi(1)	117.7(7)
C(37)-C(38)-C(39)	121.5(9)
C(34)-C(39)-C(38)	120.5(9)
C(41)-C(40)-N(7)	105.6(10)
C(40)-C(41)-C(42)	111.0(12)
C(43)-C(42)-C(41)	138.3(13)
C(43)-C(42)-C(46)	116.0(12)
C(41)-C(42)-C(46)	105.7(12)
C(44)-C(43)-C(42)	119.8(13)
C(43)-C(44)-C(45)	119.5(13)
N(8)-C(45)-C(44)	124.8(12)
N(8)-C(46)-N(7)	126.7(10)
N(8)-C(46)-C(42)	126.0(12)
N(7)-C(46)-C(42)	107.0(11)
C(48)-C(47)-C(52)	119.1(8)
C(48)-C(47)-N(7)	119.6(9)
C(52)-C(47)-N(7)	121.2(9)
C(47)-C(48)-C(49)	120.2(9)
C(48)-C(49)-C(50)	120.3(8)
C(51)-C(50)-C(49)	119.4(8)
C(51)-C(50)-Bi(2)	120.5(7)
C(49)-C(50)-Bi(2)	119.9(7)
C(50)-C(51)-C(52)	119.3(8)
C(51)-C(52)-C(47)	121.5(9)
C(54)-C(53)-N(9)	112.8(9)
C(53)-C(54)-C(55)	105.0(10)
C(56)-C(55)-C(59)	117.7(12)
C(56)-C(55)-C(54)	133.9(13)
C(59)-C(55)-C(54)	108.5(11)
C(55)-C(56)-C(57)	118.7(12)
C(56)-C(57)-C(58)	118.5(12)
N(10)-C(58)-C(57)	124.8(12)
N(10)-C(59)-N(9)	123.1(11)

N(10)-C(59)-C(55)	127.1(11)
N(9)-C(59)-C(55)	109.6(11)
C(61)-C(60)-C(65)	115.4(9)
C(61)-C(60)-N(9)	122.1(9)
C(65)-C(60)-N(9)	122.5(10)
C(62)-C(61)-C(60)	122.5(9)
C(61)-C(62)-C(63)	122.7(10)
C(62)-C(63)-C(64)	114.3(9)
C(62)-C(63)-Bi(2)	121.7(8)
C(64)-C(63)-Bi(2)	124.1(7)
C(65)-C(64)-C(63)	122.7(9)
C(64)-C(65)-C(60)	122.3(9)
C(67)-C(66)-N(11)	108.7(10)
C(66)-C(67)-C(68)	108.2(10)
C(72)-C(68)-C(69)	115.9(11)
C(72)-C(68)-C(67)	107.9(11)
C(69)-C(68)-C(67)	136.2(12)
C(70)-C(69)-C(68)	118.0(11)
C(71)-C(70)-C(69)	120.7(12)
C(70)-C(71)-N(12)	123.7(11)
N(12)-C(72)-C(68)	127.7(10)
N(12)-C(72)-N(11)	125.0(10)
C(68)-C(72)-N(11)	107.3(10)
C(74)-C(73)-C(78)	117.5(9)
C(74)-C(73)-N(11)	123.3(8)
C(78)-C(73)-N(11)	119.2(9)
C(73)-C(74)-C(75)	121.2(9)
C(76)-C(75)-C(74)	121.0(9)
C(77)-C(76)-C(75)	118.5(9)
C(77)-C(76)-Bi(2)	122.6(7)
C(75)-C(76)-Bi(2)	118.9(7)
C(76)-C(77)-C(78)	120.2(8)
C(77)-C(78)-C(73)	121.3(9)
C(81)-C(79)-C(79)#1	131(2)
C(79)-C(81)-C(80)	164.9(17)
C(86)-C(82)-O(1)	75(5)
C(86)-C(82)-C(83)	132(7)
O(1)-C(82)-C(83)	67(4)
C(86)-C(82)-C(87)	129(6)
O(1)-C(82)-C(87)	54(4)
C(83)-C(82)-C(87)	34(3)
C(87)-C(83)-C(85)	57(4)
C(87)-C(83)-C(82)	93(6)
C(85)-C(83)-C(82)	149(5)
C(87)-C(83)-O(1)	70(4)
C(85)-C(83)-O(1)	108(3)
C(82)-C(83)-O(1)	49(3)
C(87)-C(85)-C(83)	44(3)
C(82)-C(86)-C(84)	150(6)
C(82)-C(86)-O(1)	54(4)
C(84)-C(86)-O(1)	99(3)
C(83)-C(87)-C(85)	78(5)
C(83)-C(87)-O(1)	71(4)
C(85)-C(87)-O(1)	121(4)
C(83)-C(87)-C(82)	53(4)
C(85)-C(87)-C(82)	131(5)
O(1)-C(87)-C(82)	42(3)
C(82)-O(1)-C(86)	51(4)
C(82)-O(1)-C(87)	84(5)

C(86)-O(1)-C(87)	134(3)
C(82)-O(1)-C(83)	64(4)
C(86)-O(1)-C(83)	109(3)
C(87)-O(1)-C(83)	40(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Bi(1)	64(1)	59(1)	60(1)	32(1)	25(1)	31(1)
Bi(2)	59(1)	54(1)	56(1)	28(1)	23(1)	33(1)
N(1)	53(6)	58(6)	51(6)	12(5)	14(5)	29(6)
N(2)	93(8)	71(7)	74(7)	40(6)	-4(6)	36(6)
N(3)	71(8)	55(7)	71(8)	23(6)	19(7)	30(7)
N(4)	73(8)	76(8)	82(9)	34(7)	-1(7)	12(7)
N(5)	79(7)	59(6)	36(6)	17(5)	11(5)	25(5)
N(6)	95(8)	57(6)	63(7)	33(5)	16(6)	20(6)
N(7)	75(7)	51(5)	60(6)	35(5)	26(6)	31(5)
N(8)	110(9)	79(7)	57(7)	29(6)	-4(7)	33(7)
N(9)	50(6)	56(6)	62(6)	24(5)	22(5)	36(5)
N(10)	59(7)	63(6)	96(7)	30(6)	12(6)	20(6)
N(11)	84(7)	51(6)	56(7)	26(6)	28(6)	39(6)
N(12)	85(7)	61(6)	76(7)	33(5)	12(6)	42(5)
C(1)	77(9)	50(8)	91(9)	25(7)	22(8)	31(7)
C(2)	75(10)	72(9)	108(11)	29(8)	14(9)	41(8)
C(3)	67(10)	84(10)	66(9)	15(8)	3(8)	39(9)
C(4)	67(10)	107(12)	138(13)	58(11)	10(9)	26(9)
C(5)	81(12)	148(14)	122(12)	72(12)	4(10)	47(11)
C(6)	95(12)	117(12)	129(13)	74(10)	-14(10)	42(10)
C(7)	65(9)	81(9)	69(8)	44(8)	25(7)	42(8)
C(8)	38(7)	47(7)	64(8)	17(6)	11(7)	24(6)
C(9)	85(9)	46(6)	43(7)	19(6)	17(7)	22(6)
C(10)	84(9)	37(6)	53(8)	11(6)	14(7)	2(6)
C(11)	66(8)	28(5)	53(7)	10(5)	34(7)	20(5)
C(12)	60(7)	60(7)	44(7)	24(6)	16(6)	30(6)
C(13)	73(9)	72(8)	64(8)	44(7)	35(7)	45(7)
C(14)	80(10)	59(9)	112(12)	29(9)	31(9)	39(8)
C(15)	89(12)	73(11)	177(16)	34(11)	64(12)	47(10)
C(16)	76(12)	68(10)	115(14)	27(10)	48(11)	29(10)
C(17)	71(12)	96(12)	128(15)	-8(11)	54(12)	16(11)
C(18)	107(15)	93(13)	135(16)	-16(11)	58(14)	0(13)
C(19)	79(11)	110(12)	94(12)	28(10)	-27(10)	5(11)
C(20)	69(10)	42(8)	62(10)	16(7)	21(9)	16(8)
C(21)	77(10)	71(9)	58(8)	44(8)	35(8)	49(9)
C(22)	55(9)	44(7)	65(8)	13(6)	3(7)	5(7)
C(23)	44(8)	74(8)	79(8)	36(7)	23(7)	29(7)
C(24)	61(8)	94(9)	52(7)	44(7)	29(7)	50(8)
C(25)	50(8)	37(6)	62(8)	22(6)	13(6)	11(6)
C(26)	42(8)	63(7)	69(8)	34(7)	11(7)	14(7)
C(27)	100(9)	63(7)	50(8)	22(7)	7(7)	29(7)
C(28)	128(11)	93(9)	60(8)	46(8)	24(8)	46(9)
C(29)	78(9)	73(8)	57(8)	41(7)	20(7)	30(7)
C(30)	106(11)	104(10)	98(11)	78(9)	57(9)	54(9)
C(31)	122(12)	66(9)	124(12)	57(9)	47(11)	19(8)
C(32)	149(12)	59(8)	100(10)	45(8)	41(10)	29(8)

C(33)	64(8)	43(7)	50(8)	21(6)	22(7)	23(6)
C(34)	55(7)	47(7)	37(7)	16(6)	4(6)	20(6)
C(35)	80(8)	52(7)	59(7)	31(6)	31(7)	40(6)
C(36)	80(8)	71(8)	43(7)	32(6)	30(6)	44(6)
C(37)	81(8)	70(8)	48(7)	28(6)	22(7)	59(7)
C(38)	57(7)	54(6)	54(7)	26(6)	22(6)	28(5)
C(39)	65(7)	53(7)	36(6)	6(6)	11(6)	34(6)
C(40)	85(9)	57(8)	90(10)	30(7)	6(8)	18(7)
C(41)	131(13)	108(11)	100(11)	70(10)	20(10)	58(10)
C(42)	98(11)	82(9)	76(10)	49(9)	16(9)	41(8)
C(43)	153(15)	128(13)	97(12)	83(11)	62(11)	70(11)
C(44)	163(16)	124(12)	91(12)	69(11)	32(11)	62(12)
C(45)	144(13)	70(9)	76(10)	26(8)	-5(10)	20(8)
C(46)	81(10)	79(9)	61(9)	46(8)	31(8)	51(8)
C(47)	51(7)	36(6)	58(7)	26(6)	16(7)	21(6)
C(48)	51(7)	66(7)	76(8)	42(7)	31(7)	30(6)
C(49)	48(7)	68(7)	78(8)	46(6)	29(6)	36(6)
C(50)	78(8)	41(6)	48(7)	22(5)	24(7)	37(6)
C(51)	47(7)	65(7)	68(8)	44(6)	20(6)	25(6)
C(52)	56(7)	42(6)	48(7)	16(5)	3(6)	31(6)
C(53)	74(9)	54(7)	81(8)	27(6)	18(8)	35(7)
C(54)	69(9)	78(9)	97(10)	31(8)	30(8)	55(8)
C(55)	27(8)	94(11)	92(10)	38(9)	10(7)	22(8)
C(56)	75(11)	123(12)	105(11)	54(10)	30(9)	58(10)
C(57)	68(10)	122(13)	110(11)	56(10)	20(9)	26(10)
C(58)	75(10)	76(9)	143(13)	55(9)	15(10)	15(9)
C(59)	49(8)	54(8)	78(8)	29(7)	26(7)	20(7)
C(60)	41(7)	49(7)	52(7)	29(6)	21(6)	26(6)
C(61)	59(8)	57(7)	45(7)	23(6)	11(7)	31(7)
C(62)	50(7)	42(6)	56(7)	17(6)	19(6)	30(6)
C(63)	85(8)	22(5)	44(7)	9(5)	21(7)	20(6)
C(64)	52(7)	33(6)	40(6)	15(5)	2(6)	11(6)
C(65)	57(7)	48(7)	46(7)	23(6)	6(6)	28(6)
C(66)	109(10)	72(9)	52(8)	30(7)	14(8)	41(8)
C(67)	168(13)	68(9)	73(9)	28(8)	42(9)	66(9)
C(68)	80(9)	55(8)	76(9)	26(8)	26(8)	31(7)
C(69)	104(10)	61(8)	102(11)	24(8)	44(9)	43(7)
C(70)	124(12)	74(9)	98(11)	49(9)	46(10)	53(9)
C(71)	121(11)	84(9)	99(11)	53(9)	30(9)	66(9)
C(72)	64(8)	47(7)	57(8)	19(7)	21(7)	25(6)
C(73)	81(8)	37(6)	28(6)	12(5)	2(7)	23(6)
C(74)	102(9)	50(7)	55(7)	30(6)	27(7)	41(7)
C(75)	97(8)	53(7)	45(7)	23(6)	18(6)	38(6)
C(76)	65(7)	51(6)	40(6)	19(5)	4(6)	30(6)
C(77)	91(8)	40(6)	56(7)	27(6)	31(7)	37(6)
C(78)	87(8)	63(7)	53(7)	32(6)	22(7)	33(6)

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

	x	y	z	U(eq)
H(1A)	8322	9021	3259	90
H(2B)	10016	9639	4093	106
H(4B)	10863	8492	4635	135
H(5A)	10335	6896	4580	146
H(6B)	8664	5648	3935	143
H(9A)	6297	6471	3564	76

H(10B)	4638	5517	2778	88
H(12B)	5298	6572	1086	65
H(13A)	6954	7463	1869	72
H(14A)	3798	849	-563	101
H(15A)	3228	-796	-1704	137
H(17A)	1380	-2045	-3240	149
H(18A)	-59	-2079	-3815	179
H(19A)	-311	-755	-3155	148
H(22A)	1188	1312	-854	82
H(23A)	1364	2883	-50	78
H(25A)	4359	4071	678	65
H(26A)	4191	2536	-135	75
H(27A)	3139	5495	-2739	95
H(28A)	3592	6504	-3502	114
H(30A)	4970	8758	-2842	107
H(31A)	5847	10199	-1608	132
H(32A)	5823	10108	-388	130
H(35A)	3643	7650	-254	69
H(36A)	3349	7035	730	71
H(38A)	3415	4557	-656	63
H(39A)	3708	5159	-1627	65
H(40A)	4822	5837	5135	106
H(41A)	4986	5406	6304	130
H(43A)	6251	6683	8058	135
H(44A)	7606	8270	8903	149
H(45A)	8171	9463	8421	141
H(48A)	4647	7260	4948	71
H(49A)	4798	8100	4116	68
H(51A)	7829	9402	4979	68
H(52A)	7659	8597	5833	59
H(53A)	1801	9645	2569	85
H(54A)	-43	8776	2135	92
H(56A)	-1472	6674	1735	116
H(57A)	-1538	5155	1636	130
H(58A)	-48	5126	1933	130
H(61A)	2629	7245	1894	65
H(62A)	4278	7672	2295	57
H(64A)	4975	10436	3922	58
H(65A)	3338	10017	3491	60
H(66A)	8176	14144	7219	97
H(67A)	8503	15900	7820	121
H(69A)	8282	17168	7001	109
H(70A)	7738	17033	5689	111
H(71A)	7147	15552	4553	111
H(74A)	7480	13298	4491	79
H(75A)	7157	11700	3630	78
H(77A)	6952	10876	5461	70
H(78A)	7300	12479	6330	81
H(79A)	9701	5670	5323	133
H(79B)	9345	4639	5372	133
H(80A)	11861	6566	7454	485
H(80B)	10823	5877	7525	485
H(80C)	11061	6930	7526	485
H(81A)	11067	6265	6090	196
H(81B)	10848	5247	6088	196
H(84A)	-1001	3643	-245	422
H(84B)	-96	3422	-211	422
H(84C)	-318	3865	606	422

Table 1. Crystal data and structure refinement for **4**.

Empirical formula	$C_{39}H_{27}BiCl_2N_6 \cdot CH_2Cl_2$
Formula weight	944.47
Temperature	294(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$
Unit cell dimensions	a = 11.8115(19) Å α= 117.420(2)°.
	b = 13.789(2) Å β= 100.217(3)°.
	c = 13.898(2) Å γ = 103.054(3)°.
Volume	1850.8(5) Å^3
Z	2
Density (calculated)	1.695 Mg/m^3
Absorption coefficient	5.091 mm^{-1}
F(000)	924
Crystal size	0.4 x 0.3 x 0.3 mm^3
Theta range for data collection	1.72 to 28.32°.
Index ranges	-15<=h<=15, -18<=k<=18, -18<=l<=18
Reflections collected	13318
Independent reflections	8447 [R(int) = 0.0145]
Completeness to theta = 28.32°	91.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8447 / 0 / 453
Goodness-of-fit on F^2	0.982
Final R indices [I>2sigma(I)]	R1 = 0.0285, wR2 = 0.0687
R indices (all data)	R1 = 0.0353, wR2 = 0.0704
Largest diff. peak and hole	1.303 and -1.141 e.Å^{-3}

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

	x	y	z	U(eq)
Bi(1)	-1791(1)	291(1)	678(1)	39(1)
Cl(1)	-3970(1)	-1210(1)	-36(1)	58(1)
Cl(2)	490(1)	1581(1)	1244(1)	46(1)
Cl(3)	3420(5)	-4007(5)	784(5)	197(2)
Cl(3A)	2849(9)	-4026(8)	-1075(8)	155(3)
Cl(4)	3040(4)	-4855(4)	-1619(4)	169(1)
Cl(4A)	3854(11)	-4377(9)	805(9)	169(4)
N(1)	-3165(3)	569(3)	-3820(3)	50(1)
N(2)	-2935(4)	-1174(3)	-5228(3)	61(1)
N(3)	-2848(3)	4601(2)	4427(3)	48(1)
N(4)	-4172(3)	3645(3)	5094(3)	60(1)
N(5)	-20(3)	-2336(3)	3078(3)	49(1)
N(6)	174(4)	-3996(3)	1554(3)	59(1)
C(1)	-2241(3)	330(3)	-916(3)	41(1)
C(2)	-2954(4)	-670(3)	-1962(3)	49(1)
C(3)	-3277(4)	-592(3)	-2919(3)	51(1)
C(4)	-2871(3)	476(3)	-2835(3)	44(1)
C(5)	-2169(4)	1481(3)	-1772(3)	50(1)
C(6)	-1842(4)	1405(3)	-808(3)	49(1)
C(7)	-3454(4)	1478(4)	-3850(4)	60(1)
C(8)	-3687(4)	1294(4)	-4915(4)	68(1)
C(9)	-3547(4)	217(4)	-5627(4)	62(1)
C(10)	-3644(5)	-444(5)	-6778(4)	78(2)
C(11)	-3380(5)	-1457(6)	-7112(4)	84(2)
C(12)	-3032(5)	-1775(5)	-6344(4)	76(1)
C(13)	-3211(4)	-229(4)	-4926(3)	51(1)
C(14)	-2153(3)	1774(3)	1995(3)	42(1)
C(15)	-3333(4)	1634(3)	2077(3)	54(1)
C(16)	-3567(4)	2563(3)	2876(4)	55(1)
C(17)	-2633(4)	3638(3)	3594(3)	45(1)
C(18)	-1473(4)	3771(3)	3506(3)	53(1)
C(19)	-1226(4)	2849(3)	2712(3)	51(1)
C(20)	-2236(4)	5767(3)	4807(4)	59(1)
C(21)	-2482(4)	6476(4)	5735(4)	65(1)
C(22)	-3269(4)	5758(3)	6004(4)	55(1)
C(23)	-3807(5)	5928(4)	6863(4)	67(1)
C(24)	-4504(5)	4973(4)	6800(5)	77(1)
C(25)	-4667(5)	3863(4)	5944(5)	75(1)
C(26)	-3505(3)	4595(3)	5163(3)	47(1)
C(27)	-1119(3)	-682(3)	1408(3)	41(1)
C(28)	-303(4)	-12(3)	2517(3)	44(1)
C(29)	65(4)	-568(3)	3058(3)	47(1)
C(30)	-390(4)	-1775(3)	2498(3)	44(1)
C(31)	-1206(4)	-2435(3)	1381(3)	48(1)
C(32)	-1573(4)	-1891(3)	824(3)	46(1)
C(33)	216(4)	-1890(4)	4249(4)	60(1)
C(34)	616(4)	-2583(4)	4546(4)	64(1)
C(35)	658(4)	-3524(3)	3536(4)	51(1)
C(36)	1000(4)	-4490(4)	3261(4)	62(1)
C(37)	923(5)	-5190(4)	2159(5)	72(1)
C(38)	533(5)	-4927(4)	1324(4)	69(1)
C(39)	256(4)	-3340(3)	2640(3)	47(1)
C(40)	3792(12)	-3557(10)	-12(11)	201(5)

Table 3. Bond lengths [Å] and angles [°] for **4**.

Bi(1)-C(1)	2.212(4)
Bi(1)-C(27)	2.217(3)
Bi(1)-C(14)	2.223(4)
Bi(1)-Cl(1)	2.5861(11)
Bi(1)-Cl(2)	2.6147(10)
Cl(3)-C(40)	1.575(13)
Cl(3A)-C(40)	1.433(13)
Cl(4)-C(40)	1.969(13)
Cl(4A)-C(40)	1.939(17)
N(1)-C(7)	1.388(5)
N(1)-C(13)	1.401(5)
N(1)-C(4)	1.423(5)
N(2)-C(13)	1.309(5)
N(2)-C(12)	1.348(6)
N(3)-C(26)	1.391(5)
N(3)-C(20)	1.393(5)
N(3)-C(17)	1.417(5)
N(4)-C(26)	1.319(5)
N(4)-C(25)	1.350(6)
N(5)-C(39)	1.376(5)
N(5)-C(33)	1.395(5)
N(5)-C(30)	1.428(4)
N(6)-C(39)	1.325(5)
N(6)-C(38)	1.359(5)
C(1)-C(6)	1.376(5)
C(1)-C(2)	1.385(5)
C(2)-C(3)	1.378(5)
C(3)-C(4)	1.383(5)
C(4)-C(5)	1.397(5)
C(5)-C(6)	1.387(5)
C(7)-C(8)	1.344(6)
C(8)-C(9)	1.424(7)
C(9)-C(10)	1.395(7)
C(9)-C(13)	1.418(6)
C(10)-C(11)	1.383(8)
C(11)-C(12)	1.363(8)
C(14)-C(19)	1.381(5)
C(14)-C(15)	1.395(6)
C(15)-C(16)	1.383(5)
C(16)-C(17)	1.385(5)
C(17)-C(18)	1.377(6)
C(18)-C(19)	1.381(5)
C(20)-C(21)	1.344(6)
C(21)-C(22)	1.425(6)
C(22)-C(23)	1.400(6)
C(22)-C(26)	1.405(5)
C(23)-C(24)	1.341(7)
C(24)-C(25)	1.380(6)
C(27)-C(28)	1.385(5)
C(27)-C(32)	1.385(5)
C(28)-C(29)	1.382(5)
C(29)-C(30)	1.385(5)
C(30)-C(31)	1.392(5)
C(31)-C(32)	1.383(5)
C(33)-C(34)	1.343(6)
C(34)-C(35)	1.425(6)

C(35)-C(36)	1.384(6)
C(35)-C(39)	1.405(5)
C(36)-C(37)	1.354(7)
C(37)-C(38)	1.402(6)
C(1)-Bi(1)-C(27)	142.64(13)
C(1)-Bi(1)-C(14)	106.82(13)
C(27)-Bi(1)-C(14)	110.54(13)
C(1)-Bi(1)-Cl(1)	89.56(10)
C(27)-Bi(1)-Cl(1)	87.22(10)
C(14)-Bi(1)-Cl(1)	95.21(10)
C(1)-Bi(1)-Cl(2)	89.71(10)
C(27)-Bi(1)-Cl(2)	88.92(10)
C(14)-Bi(1)-Cl(2)	92.01(10)
Cl(1)-Bi(1)-Cl(2)	172.64(3)
C(7)-N(1)-C(13)	107.8(3)
C(7)-N(1)-C(4)	125.7(4)
C(13)-N(1)-C(4)	126.5(3)
C(13)-N(2)-C(12)	113.8(4)
C(26)-N(3)-C(20)	106.9(3)
C(26)-N(3)-C(17)	127.0(3)
C(20)-N(3)-C(17)	125.0(3)
C(26)-N(4)-C(25)	113.7(4)
C(39)-N(5)-C(33)	107.0(3)
C(39)-N(5)-C(30)	128.2(3)
C(33)-N(5)-C(30)	124.6(3)
C(39)-N(6)-C(38)	114.4(4)
C(6)-C(1)-C(2)	121.6(3)
C(6)-C(1)-Bi(1)	116.8(3)
C(2)-C(1)-Bi(1)	121.5(3)
C(3)-C(2)-C(1)	119.5(3)
C(2)-C(3)-C(4)	120.0(3)
C(3)-C(4)-C(5)	120.0(3)
C(3)-C(4)-N(1)	120.8(3)
C(5)-C(4)-N(1)	119.1(3)
C(6)-C(5)-C(4)	120.1(3)
C(1)-C(6)-C(5)	118.8(3)
C(8)-C(7)-N(1)	110.5(4)
C(7)-C(8)-C(9)	107.7(4)
C(10)-C(9)-C(13)	116.7(5)
C(10)-C(9)-C(8)	136.1(5)
C(13)-C(9)-C(8)	107.2(4)
C(11)-C(10)-C(9)	116.6(5)
C(12)-C(11)-C(10)	121.1(5)
N(2)-C(12)-C(11)	124.6(5)
N(2)-C(13)-N(1)	126.0(4)
N(2)-C(13)-C(9)	127.2(4)
N(1)-C(13)-C(9)	106.8(4)
C(19)-C(14)-C(15)	119.5(3)
C(19)-C(14)-Bi(1)	120.4(3)
C(15)-C(14)-Bi(1)	120.0(3)
C(16)-C(15)-C(14)	120.1(3)
C(15)-C(16)-C(17)	120.1(4)
C(18)-C(17)-C(16)	119.5(4)
C(18)-C(17)-N(3)	119.4(3)
C(16)-C(17)-N(3)	121.2(4)
C(17)-C(18)-C(19)	121.0(3)
C(14)-C(19)-C(18)	119.8(4)
C(21)-C(20)-N(3)	110.5(4)

C(20)-C(21)-C(22)	107.6(4)
C(23)-C(22)-C(26)	116.4(4)
C(23)-C(22)-C(21)	136.8(4)
C(26)-C(22)-C(21)	106.8(4)
C(24)-C(23)-C(22)	117.3(4)
C(23)-C(24)-C(25)	121.8(5)
N(4)-C(25)-C(24)	123.5(5)
N(4)-C(26)-N(3)	124.6(3)
N(4)-C(26)-C(22)	127.2(4)
N(3)-C(26)-C(22)	108.2(3)
C(28)-C(27)-C(32)	122.1(3)
C(28)-C(27)-Bi(1)	116.0(2)
C(32)-C(27)-Bi(1)	121.7(3)
C(29)-C(28)-C(27)	118.8(3)
C(28)-C(29)-C(30)	120.2(3)
C(29)-C(30)-C(31)	120.2(3)
C(29)-C(30)-N(5)	119.5(3)
C(31)-C(30)-N(5)	120.3(3)
C(32)-C(31)-C(30)	120.3(3)
C(31)-C(32)-C(27)	118.4(3)
C(34)-C(33)-N(5)	110.4(4)
C(33)-C(34)-C(35)	107.5(4)
C(36)-C(35)-C(39)	117.0(4)
C(36)-C(35)-C(34)	136.6(4)
C(39)-C(35)-C(34)	106.4(3)
C(37)-C(36)-C(35)	118.3(4)
C(36)-C(37)-C(38)	120.8(4)
N(6)-C(38)-C(37)	122.7(5)
N(6)-C(39)-N(5)	124.6(3)
N(6)-C(39)-C(35)	126.8(4)
N(5)-C(39)-C(35)	108.6(4)
Cl(3A)-C(40)-Cl(3)	115.0(10)
Cl(3A)-C(40)-Cl(4A)	122.4(9)
Cl(3)-C(40)-Cl(4)	108.8(7)
Cl(4A)-C(40)-Cl(4)	102.0(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Bi(1)	46(1)	36(1)	36(1)	20(1)	10(1)	14(1)
Cl(1)	49(1)	52(1)	61(1)	31(1)	5(1)	5(1)
Cl(2)	46(1)	43(1)	47(1)	22(1)	16(1)	15(1)
N(1)	53(2)	54(2)	48(2)	32(2)	12(2)	17(2)
N(2)	65(2)	62(2)	47(2)	25(2)	15(2)	15(2)
N(3)	48(2)	42(2)	53(2)	22(1)	18(2)	18(1)
N(4)	64(2)	54(2)	67(2)	31(2)	32(2)	24(2)
N(5)	62(2)	58(2)	46(2)	35(2)	22(2)	29(2)
N(6)	80(3)	49(2)	61(2)	33(2)	29(2)	31(2)
C(1)	46(2)	41(2)	41(2)	24(2)	13(2)	18(2)
C(2)	58(2)	37(2)	47(2)	23(2)	8(2)	13(2)
C(3)	59(3)	44(2)	36(2)	18(2)	5(2)	12(2)
C(4)	46(2)	49(2)	41(2)	27(2)	12(2)	19(2)
C(5)	58(2)	41(2)	55(2)	30(2)	15(2)	16(2)
C(6)	59(3)	39(2)	38(2)	17(2)	10(2)	13(2)
C(7)	60(3)	61(2)	70(3)	44(2)	15(2)	21(2)
C(8)	65(3)	81(3)	76(3)	60(3)	15(2)	22(2)
C(9)	49(3)	78(3)	59(3)	46(2)	11(2)	7(2)
C(10)	73(3)	106(4)	55(3)	52(3)	19(2)	11(3)
C(11)	75(4)	109(4)	50(3)	36(3)	25(3)	11(3)
C(12)	75(3)	77(3)	60(3)	28(3)	25(3)	16(3)
C(13)	42(2)	62(2)	46(2)	32(2)	10(2)	8(2)
C(14)	45(2)	43(2)	38(2)	22(2)	12(2)	15(2)
C(15)	46(2)	45(2)	56(2)	18(2)	12(2)	12(2)
C(16)	40(2)	51(2)	60(2)	19(2)	14(2)	14(2)
C(17)	45(2)	47(2)	42(2)	22(2)	15(2)	18(2)
C(18)	46(2)	44(2)	51(2)	15(2)	17(2)	8(2)
C(19)	44(2)	48(2)	51(2)	19(2)	19(2)	12(2)
C(20)	56(3)	48(2)	70(3)	30(2)	22(2)	16(2)
C(21)	66(3)	43(2)	73(3)	21(2)	24(2)	21(2)
C(22)	53(2)	50(2)	55(2)	22(2)	17(2)	24(2)
C(23)	74(3)	62(3)	72(3)	30(2)	33(3)	38(2)
C(24)	87(4)	84(3)	77(3)	41(3)	47(3)	43(3)
C(25)	81(4)	65(3)	88(4)	39(3)	47(3)	28(3)
C(26)	42(2)	49(2)	51(2)	24(2)	17(2)	21(2)
C(27)	47(2)	42(2)	42(2)	26(2)	18(2)	20(2)
C(28)	51(2)	38(2)	42(2)	21(2)	13(2)	18(2)
C(29)	53(2)	49(2)	38(2)	21(2)	9(2)	21(2)
C(30)	50(2)	47(2)	45(2)	28(2)	20(2)	24(2)
C(31)	60(3)	38(2)	48(2)	24(2)	17(2)	19(2)
C(32)	55(2)	41(2)	41(2)	22(2)	12(2)	15(2)
C(33)	74(3)	66(2)	48(2)	33(2)	21(2)	30(2)
C(34)	71(3)	77(3)	58(3)	47(2)	16(2)	25(2)
C(35)	44(2)	57(2)	63(3)	43(2)	13(2)	15(2)
C(36)	55(3)	72(3)	84(3)	59(3)	19(2)	24(2)
C(37)	76(3)	64(3)	106(4)	59(3)	33(3)	38(3)
C(38)	90(4)	58(2)	77(3)	40(2)	33(3)	40(3)
C(39)	49(2)	45(2)	57(2)	33(2)	18(2)	18(2)

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

	x	y	z	U(eq)
H(2A)	-3212	-1388	-2017	59
H(3A)	-3769	-1257	-3622	61
H(5A)	-1921	2202	-1712	60
H(6A)	-1362	2068	-100	58
H(7A)	-3482	2125	-3222	72
H(8A)	-3901	1782	-5145	82
H(10A)	-3875	-216	-7294	93
H(11A)	-3440	-1928	-7873	101
H(12A)	-2849	-2456	-6609	91
H(15A)	-3963	914	1593	65
H(16A)	-4353	2467	2932	66
H(18A)	-845	4492	3988	64
H(19A)	-439	2951	2659	62
H(20A)	-1728	6019	4465	70
H(21A)	-2191	7287	6131	78
H(23A)	-3685	6673	7453	81
H(24A)	-4888	5062	7350	93
H(25A)	-5144	3232	5952	90
H(28A)	-8	799	2891	52
H(29A)	619	-131	3800	57
H(31A)	-1506	-3245	1008	58
H(32A)	-2111	-2326	76	55
H(33A)	112	-1209	4754	72
H(34A)	827	-2470	5277	77
H(36A)	1277	-4655	3819	75
H(37A)	1132	-5853	1954	87
H(38A)	519	-5410	581	83