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Supporting Information

Synthesis and Structural Characterization of Two-Coordinate Low-Valent 14-Group Metal Complexes Bearing Bulky Bis(amido)silane Ligands**

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Crystallographic data for **3b, 4, 5a, 5b,** and **6**

S-1. Crystallographic data for **3b**

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

Identification code	110720am
Empirical formula	C40 H52 Ge N2 O Si
Formula weight	677.52
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 10.8195(15) A alpha = 90 deg. b = 18.818(3) A beta = 103.039(2) deg. c = 19.240(3) A gamma = 90 deg.
Volume	3816.1(9) A^3
Z, Calculated density	4, 1.179 Mg/m^3
Absorption coefficient	0.865 mm^-1
F(000)	1440
Crystal size	0.35 x 0.27 x 0.08 mm
Theta range for data collection	1.99 to 25.50 deg.
Limiting indices	-8<=h<=13, -22<=k<=20, -23<=l<=22
Reflections collected / unique	19903 / 7076 [R(int) = 0.0437]
Completeness to theta = 25.50	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9340 and 0.7516
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	7076 / 3 / 414
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1317
R indices (all data)	R1 = 0.0888, wR2 = 0.1495
Largest diff. peak and hole	0.532 and -0.330 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	-604(6)	6238(4)	3766(3)	129(3)
C(2)	-442(4)	5811(2)	3124(2)	69(1)
C(3)	-1292(6)	5147(3)	3000(4)	140(3)
C(4)	922(4)	5614(2)	3170(2)	52(1)
C(5)	1509(5)	5131(2)	3677(2)	65(1)
C(6)	2735(5)	4909(2)	3731(2)	70(1)
C(7)	3394(4)	5173(2)	3261(2)	65(1)
C(8)	2876(4)	5667(2)	2746(2)	51(1)
C(9)	1619(3)	5901(2)	2700(2)	43(1)
C(10)	3658(4)	5904(2)	2223(2)	64(1)
C(11)	4991(5)	6142(3)	2585(3)	102(2)
C(12)	3703(6)	5320(3)	1682(3)	102(2)
C(13)	3267(6)	6945(3)	252(3)	127(2)
C(14)	3075(4)	7515(2)	791(2)	75(1)
C(15)	4260(5)	7973(3)	1011(3)	116(2)
C(16)	1896(4)	7941(2)	506(2)	53(1)
C(17)	1914(4)	8421(2)	-50(2)	65(1)
C(18)	898(5)	8839(2)	-325(2)	65(1)
C(19)	-165(4)	8797(2)	-62(2)	60(1)
C(20)	-249(3)	8321(2)	481(2)	48(1)
C(21)	792(3)	7890(2)	768(2)	43(1)
C(22)	-1444(4)	8307(2)	754(2)	65(1)
C(23)	-2631(5)	8252(4)	142(3)	137(3)
C(24)	-1521(6)	8950(3)	1220(3)	119(2)
C(25)	-296(3)	7708(2)	2608(2)	46(1)
C(26)	-1534(4)	7486(2)	2387(2)	60(1)
C(27)	-2512(4)	7768(3)	2660(3)	81(1)
C(28)	-2233(5)	8290(3)	3165(3)	105(2)
C(29)	-1034(5)	8523(3)	3401(3)	103(2)
C(30)	-62(4)	8231(2)	3127(2)	75(1)
C(31)	2484(3)	7782(2)	2724(2)	41(1)
C(32)	2808(4)	8453(2)	2534(2)	62(1)
C(33)	3784(4)	8836(2)	2945(3)	77(1)

C(34)	4497(4)	8545(2)	3559(3)	72(1)
C(35)	4217(4)	7877(2)	3766(2)	72(1)
C(36)	3217(4)	7501(2)	3346(2)	58(1)
C(37)	7567(10)	6324(6)	321(6)	256(7)
C(38)	6689(11)	5716(7)	116(8)	321(10)
C(39)	7664(16)	5170(6)	343(7)	305(9)
C(40)	7947(13)	5460(7)	1079(5)	262(7)
Ge(1)	771(1)	6381(1)	1187(1)	53(1)
N(1)	722(3)	7375(1)	1307(1)	42(1)
N(2)	1075(3)	6424(1)	2191(2)	45(1)
O(1)	8331(5)	6128(3)	963(3)	150(2)
Si(1)	1013(1)	7340(1)	2225(1)	38(1)

Table 3. Bond lengths [A] and angles [deg] for **3b**.

C(1)-C(2)	1.516(6)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(4)	1.505(5)
C(2)-C(3)	1.537(7)
C(2)-H(2)	0.9800
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-C(5)	1.378(5)
C(4)-C(9)	1.410(5)
C(5)-C(6)	1.372(6)
C(5)-H(5)	0.9300
C(6)-C(7)	1.366(6)
C(6)-H(6)	0.9300
C(7)-C(8)	1.382(5)
C(7)-H(7)	0.9300
C(8)-C(9)	1.413(5)
C(8)-C(10)	1.519(5)
C(9)-N(2)	1.421(4)
C(10)-C(11)	1.521(6)
C(10)-C(12)	1.522(6)
C(10)-H(10)	0.9800
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.539(7)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(16)	1.501(5)
C(14)-C(15)	1.524(7)
C(14)-H(14)	0.9800
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600

C(16)-C(21)	1.400(5)
C(16)-C(17)	1.404(5)
C(17)-C(18)	1.358(6)
C(17)-H(17)	0.9300
C(18)-C(19)	1.360(6)
C(18)-H(18)	0.9300
C(19)-C(20)	1.394(5)
C(19)-H(19)	0.9300
C(20)-C(21)	1.397(5)
C(20)-C(22)	1.501(5)
C(21)-N(1)	1.433(4)
C(22)-C(24)	1.519(7)
C(22)-C(23)	1.537(6)
C(22)-H(22)	0.9800
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(26)	1.376(5)
C(25)-C(30)	1.385(5)
C(25)-Si(1)	1.870(3)
C(26)-C(27)	1.388(6)
C(26)-H(26)	0.9300
C(27)-C(28)	1.366(7)
C(27)-H(27)	0.9300
C(28)-C(29)	1.348(7)
C(28)-H(28)	0.9300
C(29)-C(30)	1.391(6)
C(29)-H(29)	0.9300
C(30)-H(30)	0.9300
C(31)-C(36)	1.383(5)
C(31)-C(32)	1.383(5)
C(31)-Si(1)	1.859(4)
C(32)-C(33)	1.372(6)
C(32)-H(32)	0.9300
C(33)-C(34)	1.370(6)
C(33)-H(33)	0.9300
C(34)-C(35)	1.374(6)
C(34)-H(34)	0.9300
C(35)-C(36)	1.389(5)
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300

C(37)-O(1)	1.372(9)
C(37)-C(38)	1.483(8)
C(37)-H(37A)	0.9700
C(37)-H(37B)	0.9700
C(38)-C(39)	1.467(8)
C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(39)-C(40)	1.483(8)
C(39)-H(39A)	0.9700
C(39)-H(39B)	0.9700
C(40)-O(1)	1.358(9)
C(40)-H(40A)	0.9700
C(40)-H(40B)	0.9700
Ge(1)-N(2)	1.887(3)
Ge(1)-N(1)	1.888(3)
Ge(1)-Si(1)	2.6616(10)
N(1)-Si(1)	1.724(3)
N(2)-Si(1)	1.726(3)

C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(4)-C(2)-C(1)	112.0(4)
C(4)-C(2)-C(3)	110.7(4)
C(1)-C(2)-C(3)	112.4(4)
C(4)-C(2)-H(2)	107.1
C(1)-C(2)-H(2)	107.1
C(3)-C(2)-H(2)	107.1
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(5)-C(4)-C(9)	118.6(4)
C(5)-C(4)-C(2)	119.6(4)
C(9)-C(4)-C(2)	121.8(3)
C(6)-C(5)-C(4)	122.6(4)
C(6)-C(5)-H(5)	118.7
C(4)-C(5)-H(5)	118.7
C(7)-C(6)-C(5)	118.6(4)

C(7)-C(6)-H(6)	120.7
C(5)-C(6)-H(6)	120.7
C(6)-C(7)-C(8)	122.2(4)
C(6)-C(7)-H(7)	118.9
C(8)-C(7)-H(7)	118.9
C(7)-C(8)-C(9)	118.8(4)
C(7)-C(8)-C(10)	118.4(4)
C(9)-C(8)-C(10)	122.7(3)
C(4)-C(9)-C(8)	119.2(3)
C(4)-C(9)-N(2)	120.7(3)
C(8)-C(9)-N(2)	120.1(3)
C(8)-C(10)-C(11)	113.3(4)
C(8)-C(10)-C(12)	110.4(4)
C(11)-C(10)-C(12)	110.7(4)
C(8)-C(10)-H(10)	107.4
C(11)-C(10)-H(10)	107.4
C(12)-C(10)-H(10)	107.4
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(16)-C(14)-C(15)	113.1(4)
C(16)-C(14)-C(13)	111.0(4)
C(15)-C(14)-C(13)	110.4(4)
C(16)-C(14)-H(14)	107.4
C(15)-C(14)-H(14)	107.4
C(13)-C(14)-H(14)	107.4
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5

C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(21)-C(16)-C(17)	118.6(4)
C(21)-C(16)-C(14)	123.7(3)
C(17)-C(16)-C(14)	117.7(4)
C(18)-C(17)-C(16)	121.3(4)
C(18)-C(17)-H(17)	119.3
C(16)-C(17)-H(17)	119.3
C(17)-C(18)-C(19)	119.9(4)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(18)-C(19)-C(20)	121.4(4)
C(18)-C(19)-H(19)	119.3
C(20)-C(19)-H(19)	119.3
C(19)-C(20)-C(21)	119.1(3)
C(19)-C(20)-C(22)	118.7(3)
C(21)-C(20)-C(22)	122.2(3)
C(20)-C(21)-C(16)	119.6(3)
C(20)-C(21)-N(1)	120.6(3)
C(16)-C(21)-N(1)	119.7(3)
C(20)-C(22)-C(24)	111.0(4)
C(20)-C(22)-C(23)	111.7(4)
C(24)-C(22)-C(23)	111.0(5)
C(20)-C(22)-H(22)	107.6
C(24)-C(22)-H(22)	107.6
C(23)-C(22)-H(22)	107.6
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(30)	116.4(3)
C(26)-C(25)-Si(1)	122.5(3)
C(30)-C(25)-Si(1)	121.1(3)
C(25)-C(26)-C(27)	122.6(4)
C(25)-C(26)-H(26)	118.7

C(27)-C(26)-H(26)	118.7
C(28)-C(27)-C(26)	118.6(4)
C(28)-C(27)-H(27)	120.7
C(26)-C(27)-H(27)	120.7
C(29)-C(28)-C(27)	121.1(4)
C(29)-C(28)-H(28)	119.5
C(27)-C(28)-H(28)	119.5
C(28)-C(29)-C(30)	119.7(5)
C(28)-C(29)-H(29)	120.2
C(30)-C(29)-H(29)	120.2
C(25)-C(30)-C(29)	121.6(4)
C(25)-C(30)-H(30)	119.2
C(29)-C(30)-H(30)	119.2
C(36)-C(31)-C(32)	116.7(3)
C(36)-C(31)-Si(1)	122.2(3)
C(32)-C(31)-Si(1)	120.7(3)
C(33)-C(32)-C(31)	122.3(4)
C(33)-C(32)-H(32)	118.8
C(31)-C(32)-H(32)	118.8
C(34)-C(33)-C(32)	119.9(4)
C(34)-C(33)-H(33)	120.1
C(32)-C(33)-H(33)	120.1
C(33)-C(34)-C(35)	119.8(4)
C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1
C(34)-C(35)-C(36)	119.4(4)
C(34)-C(35)-H(35)	120.3
C(36)-C(35)-H(35)	120.3
C(31)-C(36)-C(35)	121.8(4)
C(31)-C(36)-H(36)	119.1
C(35)-C(36)-H(36)	119.1
O(1)-C(37)-C(38)	104.5(7)
O(1)-C(37)-H(37A)	110.8
C(38)-C(37)-H(37A)	110.8
O(1)-C(37)-H(37B)	110.8
C(38)-C(37)-H(37B)	110.8
H(37A)-C(37)-H(37B)	108.9
C(39)-C(38)-C(37)	95.0(9)
C(39)-C(38)-H(38A)	112.7
C(37)-C(38)-H(38A)	112.7
C(39)-C(38)-H(38B)	112.7
C(37)-C(38)-H(38B)	112.7
H(38A)-C(38)-H(38B)	110.2
C(38)-C(39)-C(40)	90.3(9)

C(38)-C(39)-H(39A)	113.6
C(40)-C(39)-H(39A)	113.6
C(38)-C(39)-H(39B)	113.6
C(40)-C(39)-H(39B)	113.6
H(39A)-C(39)-H(39B)	110.9
O(1)-C(40)-C(39)	100.9(8)
O(1)-C(40)-H(40A)	111.6
C(39)-C(40)-H(40A)	111.6
O(1)-C(40)-H(40B)	111.6
C(39)-C(40)-H(40B)	111.6
H(40A)-C(40)-H(40B)	109.4
N(2)-Ge(1)-N(1)	80.47(11)
N(2)-Ge(1)-Si(1)	40.27(8)
N(1)-Ge(1)-Si(1)	40.21(8)
C(21)-N(1)-Si(1)	137.7(2)
C(21)-N(1)-Ge(1)	125.0(2)
Si(1)-N(1)-Ge(1)	94.83(12)
C(9)-N(2)-Si(1)	132.8(2)
C(9)-N(2)-Ge(1)	128.7(2)
Si(1)-N(2)-Ge(1)	94.79(12)
C(40)-O(1)-C(37)	104.6(7)
N(1)-Si(1)-N(2)	89.91(13)
N(1)-Si(1)-C(31)	116.71(14)
N(2)-Si(1)-C(31)	115.45(15)
N(1)-Si(1)-C(25)	114.22(14)
N(2)-Si(1)-C(25)	115.06(15)
C(31)-Si(1)-C(25)	105.50(15)
N(1)-Si(1)-Ge(1)	44.96(9)
N(2)-Si(1)-Ge(1)	44.95(9)
C(31)-Si(1)-Ge(1)	128.23(10)
C(25)-Si(1)-Ge(1)	126.27(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **3b**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	134(6)	190(7)	78(4)	15(4)	54(4)	60(5)
C(2)	71(3)	72(3)	70(3)	21(2)	28(2)	-5(2)
C(3)	87(4)	120(5)	206(8)	39(5)	19(5)	-33(4)
C(4)	70(3)	41(2)	44(2)	0(2)	11(2)	-7(2)
C(5)	96(4)	47(2)	50(2)	6(2)	11(2)	-12(2)
C(6)	101(4)	43(2)	51(2)	8(2)	-9(2)	4(2)
C(7)	75(3)	43(2)	65(3)	-1(2)	-8(2)	11(2)
C(8)	60(2)	37(2)	51(2)	-6(2)	3(2)	2(2)
C(9)	58(2)	30(2)	38(2)	-3(1)	1(2)	0(2)
C(10)	55(2)	63(3)	71(3)	7(2)	10(2)	12(2)
C(11)	70(3)	128(5)	111(4)	-7(4)	26(3)	-12(3)
C(12)	112(4)	116(4)	84(4)	-24(3)	36(3)	8(3)
C(13)	150(6)	112(5)	144(5)	16(4)	83(5)	60(4)
C(14)	63(3)	99(3)	74(3)	26(3)	35(2)	20(3)
C(15)	57(3)	176(6)	116(5)	29(4)	21(3)	5(4)
C(16)	61(2)	59(2)	40(2)	0(2)	14(2)	2(2)
C(17)	77(3)	76(3)	48(2)	3(2)	24(2)	-5(2)
C(18)	84(3)	64(3)	43(2)	12(2)	8(2)	-6(2)
C(19)	69(3)	54(2)	48(2)	13(2)	-5(2)	6(2)
C(20)	53(2)	45(2)	42(2)	4(2)	3(2)	1(2)
C(21)	49(2)	47(2)	30(2)	2(1)	6(2)	2(2)
C(22)	49(2)	67(3)	76(3)	19(2)	10(2)	12(2)
C(23)	52(3)	214(7)	128(5)	65(5)	-10(3)	-10(4)
C(24)	146(5)	70(3)	170(6)	5(4)	97(5)	26(3)
C(25)	47(2)	48(2)	45(2)	-1(2)	17(2)	2(2)
C(26)	53(2)	64(2)	65(3)	0(2)	19(2)	-1(2)
C(27)	46(3)	107(4)	93(4)	3(3)	23(3)	1(3)
C(28)	73(4)	136(5)	122(5)	-30(4)	56(4)	13(4)
C(29)	83(4)	123(5)	114(4)	-57(4)	45(3)	0(3)
C(30)	66(3)	85(3)	81(3)	-26(3)	34(2)	-1(2)
C(31)	42(2)	40(2)	42(2)	3(2)	12(2)	6(2)
C(32)	59(3)	59(2)	64(3)	19(2)	6(2)	-8(2)
C(33)	70(3)	66(3)	92(3)	10(3)	12(3)	-25(2)
C(34)	49(2)	77(3)	89(3)	-18(3)	9(2)	-12(2)

C(35)	72(3)	69(3)	62(3)	-4(2)	-13(2)	2(2)
C(36)	65(3)	46(2)	55(2)	6(2)	-3(2)	-3(2)
C(37)	199(11)	262(14)	246(12)	150(11)	-79(9)	3(9)
C(38)	200(11)	265(15)	390(20)	-175(15)	-159(12)	9(11)
C(39)	450(20)	155(10)	249(14)	-83(10)	-56(15)	74(11)
C(40)	368(18)	245(13)	151(9)	57(9)	14(10)	-153(12)
Ge(1)	66(1)	49(1)	43(1)	-5(1)	8(1)	4(1)
N(1)	49(2)	42(2)	36(2)	2(1)	10(1)	6(1)
N(2)	54(2)	37(2)	43(2)	3(1)	10(1)	1(1)
O(1)	171(5)	122(4)	138(4)	-11(3)	-2(4)	-34(4)
Si(1)	41(1)	38(1)	36(1)	3(1)	9(1)	3(1)

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

	x	y	z	U(eq)
H(1A)	-390	5947	4186	194
H(1B)	-1469	6392	3695	194
H(1C)	-55	6645	3822	194
H(2)	-707	6116	2704	83
H(3A)	-1158	4895	2590	210
H(3B)	-2165	5288	2922	210
H(3C)	-1083	4845	3412	210
H(5)	1056	4949	3994	78
H(6)	3108	4585	4081	83
H(7)	4219	5016	3289	77
H(10)	3225	6312	1960	77
H(11A)	4943	6511	2924	153
H(11B)	5414	6321	2233	153
H(11C)	5457	5746	2828	153
H(12A)	4129	4911	1923	153
H(12B)	4154	5488	1338	153
H(12C)	2854	5192	1444	153
H(13A)	2530	6646	136	191
H(13B)	3996	6662	457	191
H(13C)	3394	7171	-174	191
H(14)	2955	7267	1219	90
H(15A)	4374	8247	609	174
H(15B)	4986	7674	1173	174
H(15C)	4168	8288	1389	174
H(17)	2637	8454	-233	78
H(18)	929	9153	-694	78
H(19)	-850	9091	-248	72
H(22)	-1416	7883	1052	78
H(23A)	-2683	8662	-159	205
H(23B)	-3373	8227	336	205
H(23C)	-2577	7831	-132	205
H(24A)	-797	8957	1615	178
H(24B)	-2282	8925	1395	178
H(24C)	-1531	9376	943	178
H(26)	-1724	7133	2041	72

H(27)	-3340	7606	2502	97
H(28)	-2881	8487	3349	126
H(29)	-858	8878	3746	124
H(30)	764	8392	3296	89
H(32)	2348	8653	2112	74
H(33)	3962	9291	2807	92
H(34)	5168	8800	3834	87
H(35)	4692	7678	4184	86
H(36)	3035	7047	3487	69
H(37A)	8064	6403	-33	307
H(37B)	7102	6755	372	307
H(38A)	6029	5700	384	386
H(38B)	6316	5700	-392	386
H(39A)	8369	5207	110	366
H(39B)	7330	4690	310	366
H(40A)	7198	5465	1277	314
H(40B)	8615	5193	1393	314

Table 6. Torsion angles [deg] for **3b**.

C(1)-C(2)-C(4)-C(5)	68.7(5)
C(3)-C(2)-C(4)-C(5)	-57.6(5)
C(1)-C(2)-C(4)-C(9)	-112.3(4)
C(3)-C(2)-C(4)-C(9)	121.4(4)
C(9)-C(4)-C(5)-C(6)	-1.4(6)
C(2)-C(4)-C(5)-C(6)	177.6(4)
C(4)-C(5)-C(6)-C(7)	-0.5(6)
C(5)-C(6)-C(7)-C(8)	1.4(6)
C(6)-C(7)-C(8)-C(9)	-0.5(6)
C(6)-C(7)-C(8)-C(10)	-177.1(3)
C(5)-C(4)-C(9)-C(8)	2.3(5)
C(2)-C(4)-C(9)-C(8)	-176.7(3)
C(5)-C(4)-C(9)-N(2)	-177.1(3)
C(2)-C(4)-C(9)-N(2)	4.0(5)
C(7)-C(8)-C(9)-C(4)	-1.4(5)
C(10)-C(8)-C(9)-C(4)	175.0(3)
C(7)-C(8)-C(9)-N(2)	178.0(3)
C(10)-C(8)-C(9)-N(2)	-5.6(5)
C(7)-C(8)-C(10)-C(11)	-51.1(5)
C(9)-C(8)-C(10)-C(11)	132.5(4)
C(7)-C(8)-C(10)-C(12)	73.8(5)
C(9)-C(8)-C(10)-C(12)	-102.7(4)
C(15)-C(14)-C(16)-C(21)	-126.5(4)
C(13)-C(14)-C(16)-C(21)	108.8(4)
C(15)-C(14)-C(16)-C(17)	53.0(5)
C(13)-C(14)-C(16)-C(17)	-71.7(5)
C(21)-C(16)-C(17)-C(18)	1.1(6)
C(14)-C(16)-C(17)-C(18)	-178.4(4)
C(16)-C(17)-C(18)-C(19)	0.0(7)
C(17)-C(18)-C(19)-C(20)	-1.2(6)
C(18)-C(19)-C(20)-C(21)	1.2(6)
C(18)-C(19)-C(20)-C(22)	179.3(4)
C(19)-C(20)-C(21)-C(16)	0.0(5)
C(22)-C(20)-C(21)-C(16)	-178.1(3)
C(19)-C(20)-C(21)-N(1)	-177.5(3)
C(22)-C(20)-C(21)-N(1)	4.5(5)
C(17)-C(16)-C(21)-C(20)	-1.1(5)
C(14)-C(16)-C(21)-C(20)	178.4(4)
C(17)-C(16)-C(21)-N(1)	176.4(3)
C(14)-C(16)-C(21)-N(1)	-4.1(5)

C(19)-C(20)-C(22)-C(24)	-74.5(5)
C(21)-C(20)-C(22)-C(24)	103.6(5)
C(19)-C(20)-C(22)-C(23)	50.0(6)
C(21)-C(20)-C(22)-C(23)	-131.9(5)
C(30)-C(25)-C(26)-C(27)	0.3(6)
Si(1)-C(25)-C(26)-C(27)	-178.6(3)
C(25)-C(26)-C(27)-C(28)	0.4(7)
C(26)-C(27)-C(28)-C(29)	-0.6(9)
C(27)-C(28)-C(29)-C(30)	0.1(10)
C(26)-C(25)-C(30)-C(29)	-0.8(7)
Si(1)-C(25)-C(30)-C(29)	178.1(4)
C(28)-C(29)-C(30)-C(25)	0.6(9)
C(36)-C(31)-C(32)-C(33)	-1.6(6)
Si(1)-C(31)-C(32)-C(33)	170.8(3)
C(31)-C(32)-C(33)-C(34)	1.7(7)
C(32)-C(33)-C(34)-C(35)	-1.1(7)
C(33)-C(34)-C(35)-C(36)	0.5(7)
C(32)-C(31)-C(36)-C(35)	1.0(6)
Si(1)-C(31)-C(36)-C(35)	-171.3(3)
C(34)-C(35)-C(36)-C(31)	-0.5(6)
O(1)-C(37)-C(38)-C(39)	-41.2(14)
C(37)-C(38)-C(39)-C(40)	58.5(13)
C(38)-C(39)-C(40)-O(1)	-61.3(13)
C(20)-C(21)-N(1)-Si(1)	-89.5(4)
C(16)-C(21)-N(1)-Si(1)	93.0(4)
C(20)-C(21)-N(1)-Ge(1)	113.2(3)
C(16)-C(21)-N(1)-Ge(1)	-64.2(4)
N(2)-Ge(1)-N(1)-C(21)	165.1(3)
Si(1)-Ge(1)-N(1)-C(21)	164.9(3)
N(2)-Ge(1)-N(1)-Si(1)	0.22(12)
C(4)-C(9)-N(2)-Si(1)	88.2(4)
C(8)-C(9)-N(2)-Si(1)	-91.1(4)
C(4)-C(9)-N(2)-Ge(1)	-119.1(3)
C(8)-C(9)-N(2)-Ge(1)	61.6(4)
N(1)-Ge(1)-N(2)-C(9)	-160.5(3)
Si(1)-Ge(1)-N(2)-C(9)	-160.3(4)
N(1)-Ge(1)-N(2)-Si(1)	-0.22(12)
C(39)-C(40)-O(1)-C(37)	36.9(13)
C(38)-C(37)-O(1)-C(40)	2.7(14)
C(21)-N(1)-Si(1)-N(2)	-161.7(3)
Ge(1)-N(1)-Si(1)-N(2)	-0.24(13)
C(21)-N(1)-Si(1)-C(31)	-43.0(4)
Ge(1)-N(1)-Si(1)-C(31)	118.46(14)
C(21)-N(1)-Si(1)-C(25)	80.7(4)

Ge(1)-N(1)-Si(1)-C(25)	-117.88(15)
C(21)-N(1)-Si(1)-Ge(1)	-161.4(4)
C(9)-N(2)-Si(1)-N(1)	159.2(3)
Ge(1)-N(2)-Si(1)-N(1)	0.24(13)
C(9)-N(2)-Si(1)-C(31)	39.4(4)
Ge(1)-N(2)-Si(1)-C(31)	-119.56(14)
C(9)-N(2)-Si(1)-C(25)	-83.9(3)
Ge(1)-N(2)-Si(1)-C(25)	117.13(15)
C(9)-N(2)-Si(1)-Ge(1)	159.0(4)
C(36)-C(31)-Si(1)-N(1)	-142.3(3)
C(32)-C(31)-Si(1)-N(1)	45.6(3)
C(36)-C(31)-Si(1)-N(2)	-38.6(3)
C(32)-C(31)-Si(1)-N(2)	149.4(3)
C(36)-C(31)-Si(1)-C(25)	89.7(3)
C(32)-C(31)-Si(1)-C(25)	-82.4(3)
C(36)-C(31)-Si(1)-Ge(1)	-90.0(3)
C(32)-C(31)-Si(1)-Ge(1)	97.9(3)
C(26)-C(25)-Si(1)-N(1)	52.7(3)
C(30)-C(25)-Si(1)-N(1)	-126.2(3)
C(26)-C(25)-Si(1)-N(2)	-49.3(4)
C(30)-C(25)-Si(1)-N(2)	131.8(3)
C(26)-C(25)-Si(1)-C(31)	-177.8(3)
C(30)-C(25)-Si(1)-C(31)	3.3(4)
C(26)-C(25)-Si(1)-Ge(1)	1.9(4)
C(30)-C(25)-Si(1)-Ge(1)	-177.0(3)
N(2)-Ge(1)-Si(1)-N(1)	-179.66(19)
N(1)-Ge(1)-Si(1)-N(2)	179.66(19)
N(2)-Ge(1)-Si(1)-C(31)	89.15(19)
N(1)-Ge(1)-Si(1)-C(31)	-91.20(18)
N(2)-Ge(1)-Si(1)-C(25)	-90.50(19)
N(1)-Ge(1)-Si(1)-C(25)	89.16(18)

Symmetry transformations used to generate equivalent atoms:

S-2. Crystallographic data for **4**

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

Identification code	f91027b
Empirical formula	C26 H40 N2 Si Sn
Formula weight	527.38
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 17.83(4) A alpha = 90 deg. b = 8.55(2) A beta = 90 deg. c = 36.69(8) A gamma = 90 deg.
Volume	5595(22) A^3
Z, Calculated density	8, 1.252 Mg/m^3
Absorption coefficient	0.970 mm^-1
F(000)	2192
Crystal size	0.18 x 0.16 x 0.13 mm
Theta range for data collection	2.22 to 25.01 deg.
Limiting indices	-21<=h<=19, -7<=k<=10, -24<=l<=43
Reflections collected / unique	18142 / 7707 [R(int) = 0.0626]
Completeness to theta = 25.01	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8843 and 0.8448
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	7707 / 32 / 561
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0762, wR2 = 0.1880
R indices (all data)	R1 = 0.1125, wR2 = 0.2050
Absolute structure parameter	0.00(17)
Largest diff. peak and hole	1.142 and -0.862 e.A^-3

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

	x	y	z	U(eq)
Sn(1)	1910(1)	11308(1)	2681(1)	71(1)
Si(1)	3073(2)	9133(4)	2523(1)	54(1)
N(1)	3054(7)	11095(11)	2626(4)	63(3)
N(2)	2108(6)	9040(9)	2530(3)	41(3)
C(1)	3502(7)	8687(16)	2070(5)	70(5)
C(2)	3512(12)	7870(20)	2851(6)	106(8)
C(3)	3628(6)	12291(13)	2629(4)	40(3)
C(4)	3991(10)	12642(17)	2931(5)	62(5)
C(5)	4603(7)	13767(19)	2904(5)	61(4)
C(6)	4696(8)	14600(20)	2635(7)	81(6)
C(7)	4299(9)	14327(16)	2325(5)	64(5)
C(8)	3711(8)	13191(14)	2314(4)	49(4)
C(9)	3893(9)	11830(20)	3284(5)	68(4)
C(10)	3398(11)	12650(30)	3558(5)	95(7)
C(11)	4593(8)	11250(20)	3485(6)	95(6)
C(12)	3273(12)	12970(20)	1968(6)	87(6)
C(13)	3749(14)	12860(30)	1614(6)	119(9)
C(14)	2642(14)	14070(20)	1957(8)	139(10)
C(15)	1621(9)	7823(14)	2455(5)	56(4)
C(16)	1376(7)	6787(17)	2728(4)	51(4)
C(17)	856(8)	5607(17)	2657(6)	65(4)
C(18)	653(9)	5390(20)	2300(7)	82(6)
C(19)	843(7)	6329(16)	2055(4)	45(3)
C(20)	1309(7)	7533(14)	2095(4)	40(4)
C(21)	1616(10)	7053(17)	3129(5)	71(5)
C(22)	1902(13)	5600(30)	3298(6)	122(9)
C(23)	848(15)	7790(40)	3336(7)	144(11)
C(24)	1535(9)	8650(20)	1786(6)	85(6)
C(25)	1716(14)	7800(30)	1416(5)	107(8)
C(26)	975(13)	9910(30)	1739(6)	115(8)
Sn(2)	10549(1)	6182(1)	4903(1)	75(1)
Si(2)	9374(2)	3864(4)	5002(1)	46(1)
N(3)	10375(5)	3806(10)	5011(3)	42(3)

N(4)	9382(4)	5900(9)	4920(4)	40(2)
C(27)	8922(8)	3245(19)	5395(5)	69(4)
C(28)	8966(7)	2725(17)	4618(5)	64(5)
C(29)	10892(7)	2604(13)	5087(4)	32(3)
C(30)	11083(10)	2266(19)	5422(5)	62(5)
C(31)	11640(11)	1090(20)	5526(7)	97(7)
C(32)	11894(9)	197(19)	5202(6)	79(6)
C(33)	11680(6)	553(16)	4862(5)	67(5)
C(34)	11175(9)	1731(16)	4779(5)	65(5)
C(35)	10869(8)	3299(19)	5749(4)	61(4)
C(36)	10679(14)	2410(30)	6074(6)	107(8)
C(37)	11476(12)	4510(30)	5855(6)	116(8)
C(38)	10998(9)	2080(20)	4391(5)	74(5)
C(39)	11510(13)	2910(40)	4194(6)	130(10)
C(40)	10815(13)	620(30)	4176(7)	124(9)
C(41)	8846(6)	7021(11)	4936(4)	40(3)
C(42)	8422(7)	7489(16)	4618(5)	49(4)
C(43)	7936(7)	8689(19)	4646(7)	83(6)
C(44)	7800(8)	9307(18)	4981(6)	69(5)
C(45)	8213(8)	8868(16)	5288(5)	59(4)
C(46)	8664(8)	7706(15)	5265(4)	47(4)
C(47)	8623(8)	6820(20)	4248(5)	67(4)
C(48)	7981(13)	6480(30)	4024(5)	126(9)
C(49)	9120(20)	8030(40)	4056(8)	210(20)
C(50)	9094(10)	7377(17)	5619(5)	63(5)
C(51)	9623(12)	8600(20)	5735(6)	103(7)
C(52)	8485(14)	6900(30)	5938(7)	121(8)

Table 3. Bond lengths [A] and angles [deg] for **4**.

Sn(1)-N(2)	2.048(9)
Sn(1)-N(1)	2.059(14)
Sn(1)-Si(1)	2.845(6)
Si(1)-N(1)	1.721(11)
Si(1)-N(2)	1.723(12)
Si(1)-C(2)	1.796(18)
Si(1)-C(1)	1.870(19)
N(1)-C(3)	1.447(15)
N(2)-C(15)	1.383(18)
C(3)-C(4)	1.32(2)
C(3)-C(8)	1.40(2)
C(4)-C(5)	1.46(2)
C(4)-C(9)	1.48(3)
C(5)-C(6)	1.23(2)
C(6)-C(7)	1.36(3)
C(7)-C(8)	1.43(2)
C(8)-C(12)	1.50(3)
C(9)-C(10)	1.51(2)
C(9)-C(11)	1.53(2)
C(12)-C(14)	1.47(3)
C(12)-C(13)	1.56(3)
C(15)-C(16)	1.41(2)
C(15)-C(20)	1.45(2)
C(16)-C(17)	1.395(19)
C(16)-C(21)	1.55(2)
C(17)-C(18)	1.37(3)
C(18)-C(19)	1.25(2)
C(19)-C(20)	1.331(18)
C(20)-C(24)	1.54(2)
C(21)-C(22)	1.48(3)
C(21)-C(23)	1.69(3)
C(24)-C(26)	1.48(2)
C(24)-C(25)	1.57(3)
Sn(2)-N(3)	2.094(9)
Sn(2)-N(4)	2.096(9)
Sn(2)-Si(2)	2.907(6)
Si(2)-C(27)	1.735(18)
Si(2)-N(4)	1.766(9)
Si(2)-N(3)	1.786(10)
Si(2)-C(28)	1.861(16)

N(3)-C(29)	1.408(15)
N(4)-C(41)	1.355(14)
C(29)-C(30)	1.31(2)
C(29)-C(34)	1.45(2)
C(30)-C(31)	1.46(3)
C(30)-C(35)	1.54(2)
C(31)-C(32)	1.48(3)
C(32)-C(33)	1.34(2)
C(33)-C(34)	1.385(19)
C(34)-C(38)	1.49(2)
C(35)-C(36)	1.45(3)
C(35)-C(37)	1.55(2)
C(38)-C(39)	1.36(3)
C(38)-C(40)	1.51(3)
C(41)-C(46)	1.38(2)
C(41)-C(42)	1.45(2)
C(42)-C(43)	1.347(19)
C(42)-C(47)	1.52(2)
C(43)-C(44)	1.36(3)
C(44)-C(45)	1.40(2)
C(45)-C(46)	1.280(19)
C(46)-C(50)	1.54(2)
C(47)-C(48)	1.44(3)
C(47)-C(49)	1.53(3)
C(50)-C(51)	1.47(2)
C(50)-C(52)	1.64(3)

N(2)-Sn(1)-N(1)	73.7(4)
N(2)-Sn(1)-Si(1)	36.9(3)
N(1)-Sn(1)-Si(1)	36.9(3)
N(1)-Si(1)-N(2)	91.3(5)
N(1)-Si(1)-C(2)	116.4(9)
N(2)-Si(1)-C(2)	113.5(9)
N(1)-Si(1)-C(1)	113.7(7)
N(2)-Si(1)-C(1)	114.3(6)
C(2)-Si(1)-C(1)	107.2(9)
N(1)-Si(1)-Sn(1)	45.9(5)
N(2)-Si(1)-Sn(1)	45.5(3)
C(2)-Si(1)-Sn(1)	125.0(7)
C(1)-Si(1)-Sn(1)	127.8(5)
C(3)-N(1)-Si(1)	132.7(10)
C(3)-N(1)-Sn(1)	129.6(8)
Si(1)-N(1)-Sn(1)	97.3(6)
C(15)-N(2)-Si(1)	131.2(9)

C(15)-N(2)-Sn(1)	131.2(9)
Si(1)-N(2)-Sn(1)	97.6(4)
C(4)-C(3)-C(8)	121.2(12)
C(4)-C(3)-N(1)	121.0(14)
C(8)-C(3)-N(1)	117.2(13)
C(3)-C(4)-C(5)	117.4(17)
C(3)-C(4)-C(9)	124.7(15)
C(5)-C(4)-C(9)	117.3(15)
C(6)-C(5)-C(4)	122.7(16)
C(5)-C(6)-C(7)	120.0(16)
C(6)-C(7)-C(8)	121.5(16)
C(3)-C(8)-C(7)	115.3(13)
C(3)-C(8)-C(12)	125.1(14)
C(7)-C(8)-C(12)	119.4(15)
C(4)-C(9)-C(10)	115.6(15)
C(4)-C(9)-C(11)	118.5(15)
C(10)-C(9)-C(11)	107.8(15)
C(14)-C(12)-C(8)	110.0(18)
C(14)-C(12)-C(13)	116(2)
C(8)-C(12)-C(13)	115.4(17)
N(2)-C(15)-C(16)	121.7(15)
N(2)-C(15)-C(20)	123.3(14)
C(16)-C(15)-C(20)	115.0(13)
C(17)-C(16)-C(15)	121.8(15)
C(17)-C(16)-C(21)	117.8(15)
C(15)-C(16)-C(21)	120.0(13)
C(18)-C(17)-C(16)	116.8(16)
C(19)-C(18)-C(17)	122.0(17)
C(18)-C(19)-C(20)	125.8(16)
C(19)-C(20)-C(15)	118.1(14)
C(19)-C(20)-C(24)	124.2(14)
C(15)-C(20)-C(24)	117.7(12)
C(22)-C(21)-C(16)	111.7(15)
C(22)-C(21)-C(23)	113.8(19)
C(16)-C(21)-C(23)	105.0(15)
C(26)-C(24)-C(20)	111.2(16)
C(26)-C(24)-C(25)	112.1(17)
C(20)-C(24)-C(25)	113.8(16)
N(3)-Sn(2)-N(4)	74.6(3)
N(3)-Sn(2)-Si(2)	37.6(3)
N(4)-Sn(2)-Si(2)	37.1(2)
C(27)-Si(2)-N(4)	116.4(7)
C(27)-Si(2)-N(3)	116.0(6)
N(4)-Si(2)-N(3)	91.3(4)

C(27)-Si(2)-C(28)	106.7(8)
N(4)-Si(2)-C(28)	113.1(6)
N(3)-Si(2)-C(28)	113.0(6)
C(27)-Si(2)-Sn(2)	130.2(6)
N(4)-Si(2)-Sn(2)	45.6(3)
N(3)-Si(2)-Sn(2)	45.7(3)
C(28)-Si(2)-Sn(2)	123.0(5)
C(29)-N(3)-Si(2)	132.8(7)
C(29)-N(3)-Sn(2)	130.4(7)
Si(2)-N(3)-Sn(2)	96.7(4)
C(41)-N(4)-Si(2)	133.2(7)
C(41)-N(4)-Sn(2)	128.3(6)
Si(2)-N(4)-Sn(2)	97.3(4)
C(30)-C(29)-N(3)	121.1(14)
C(30)-C(29)-C(34)	122.0(14)
N(3)-C(29)-C(34)	116.9(13)
C(29)-C(30)-C(31)	124.9(18)
C(29)-C(30)-C(35)	122.8(16)
C(31)-C(30)-C(35)	111.1(17)
C(30)-C(31)-C(32)	110.6(18)
C(33)-C(32)-C(31)	122.9(14)
C(32)-C(33)-C(34)	123.7(16)
C(33)-C(34)-C(29)	115.6(15)
C(33)-C(34)-C(38)	119.6(15)
C(29)-C(34)-C(38)	124.7(13)
C(36)-C(35)-C(30)	113.5(16)
C(36)-C(35)-C(37)	107.8(16)
C(30)-C(35)-C(37)	114.0(14)
C(39)-C(38)-C(34)	118.0(17)
C(39)-C(38)-C(40)	107(2)
C(34)-C(38)-C(40)	112.2(18)
N(4)-C(41)-C(46)	120.2(14)
N(4)-C(41)-C(42)	122.1(13)
C(46)-C(41)-C(42)	117.6(12)
C(43)-C(42)-C(41)	119.1(17)
C(43)-C(42)-C(47)	120.4(17)
C(41)-C(42)-C(47)	119.6(12)
C(42)-C(43)-C(44)	119(2)
C(43)-C(44)-C(45)	122.0(15)
C(46)-C(45)-C(44)	119.1(16)
C(45)-C(46)-C(41)	122.3(15)
C(45)-C(46)-C(50)	113.6(14)
C(41)-C(46)-C(50)	123.0(13)
C(48)-C(47)-C(42)	113.7(15)

C(48)-C(47)-C(49)	110(2)
C(42)-C(47)-C(49)	107.2(17)
C(51)-C(50)-C(46)	115.8(15)
C(51)-C(50)-C(52)	113.2(18)
C(46)-C(50)-C(52)	108.4(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **4**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sn(1)	51(1)	56(1)	107(1)	-10(1)	1(1)	4(1)
Si(1)	48(2)	44(2)	70(3)	-2(2)	-15(2)	2(2)
N(1)	77(7)	52(6)	62(9)	-11(7)	-2(7)	-7(6)
N(2)	55(5)	11(4)	58(7)	-9(4)	5(4)	-4(4)
C(1)	44(7)	45(8)	121(15)	-3(9)	-2(8)	14(7)
C(2)	123(16)	94(13)	100(16)	-5(12)	-46(13)	68(13)
C(3)	29(5)	28(5)	64(8)	3(6)	5(5)	-12(4)
C(4)	72(11)	47(9)	66(13)	-9(8)	-35(10)	6(7)
C(5)	30(7)	69(10)	84(13)	1(10)	-19(7)	7(7)
C(6)	48(8)	64(11)	133(19)	-34(13)	-2(12)	-2(8)
C(7)	67(10)	37(7)	90(14)	9(7)	9(9)	-20(7)
C(8)	53(8)	25(6)	68(11)	3(7)	-3(7)	-1(6)
C(9)	75(10)	76(11)	53(11)	-27(10)	-15(9)	11(9)
C(10)	81(12)	128(18)	75(15)	22(12)	22(10)	47(12)
C(11)	46(9)	132(16)	105(16)	10(13)	-5(8)	18(10)
C(12)	109(15)	59(10)	94(17)	12(11)	-12(13)	15(11)
C(13)	150(20)	134(19)	71(16)	13(14)	-11(15)	-49(17)
C(14)	150(20)	107(17)	160(30)	-2(16)	-79(19)	35(16)
C(15)	88(11)	13(5)	68(12)	0(7)	5(10)	11(6)
C(16)	51(7)	61(9)	40(10)	-20(8)	-10(7)	12(6)
C(17)	75(10)	57(8)	63(12)	10(10)	14(10)	-34(7)
C(18)	55(10)	78(12)	113(19)	-19(13)	27(11)	-4(9)
C(19)	38(6)	63(8)	34(8)	-1(7)	-27(6)	1(7)
C(20)	25(6)	48(8)	48(11)	5(7)	-18(6)	-9(5)
C(21)	100(13)	33(7)	79(14)	10(9)	18(10)	12(8)
C(22)	180(20)	106(16)	83(17)	34(13)	-65(15)	-27(15)
C(23)	140(20)	210(30)	81(19)	-70(18)	6(16)	40(20)
C(24)	52(9)	87(12)	115(17)	22(12)	-19(9)	-7(9)
C(25)	117(17)	170(20)	33(12)	8(12)	-1(12)	6(16)
C(26)	126(18)	127(19)	94(16)	48(14)	-6(13)	7(15)
Sn(2)	49(1)	54(1)	123(1)	10(1)	-1(1)	-1(1)
Si(2)	36(2)	43(2)	58(3)	0(2)	-17(2)	5(2)
N(3)	30(4)	21(4)	75(9)	11(5)	-9(5)	-9(4)
N(4)	19(4)	30(4)	73(8)	2(6)	-6(5)	-14(4)

C(27)	56(7)	70(8)	82(9)	−14(7)	−17(6)	19(6)
C(28)	32(7)	62(9)	98(14)	18(9)	−18(7)	12(6)
C(29)	18(5)	34(7)	45(10)	0(6)	9(6)	−15(5)
C(30)	85(12)	56(10)	44(12)	1(8)	−2(9)	−45(9)
C(31)	80(12)	101(15)	108(17)	32(14)	13(12)	34(12)
C(32)	73(11)	51(9)	113(16)	5(9)	−44(11)	38(8)
C(33)	30(6)	63(8)	107(15)	−30(10)	−31(8)	16(6)
C(34)	66(9)	41(8)	88(15)	4(8)	4(9)	8(7)
C(35)	52(8)	89(11)	43(10)	−1(9)	−12(7)	0(8)
C(36)	125(19)	136(19)	61(17)	−15(13)	5(14)	3(15)
C(37)	122(17)	123(17)	104(17)	−39(14)	16(13)	−74(15)
C(38)	56(9)	106(13)	60(13)	−20(10)	−6(8)	42(9)
C(39)	89(15)	250(30)	54(15)	6(16)	7(11)	14(16)
C(40)	141(19)	105(16)	130(20)	−68(15)	−39(16)	10(15)
C(41)	52(6)	9(4)	57(7)	7(6)	8(6)	−7(4)
C(42)	19(6)	70(10)	58(12)	17(7)	15(7)	4(6)
C(43)	22(7)	68(10)	160(20)	7(12)	−3(9)	10(7)
C(44)	38(7)	62(9)	108(16)	−29(11)	−7(9)	−2(6)
C(45)	50(8)	52(9)	74(12)	−23(8)	13(8)	−30(7)
C(46)	48(6)	28(6)	65(8)	−13(6)	−3(6)	−8(5)
C(47)	59(9)	79(11)	63(12)	15(10)	−5(9)	13(8)
C(48)	113(17)	210(30)	55(14)	−9(15)	3(12)	−32(18)
C(49)	330(50)	160(30)	150(30)	−40(20)	60(30)	−150(30)
C(50)	71(10)	47(9)	70(13)	−14(8)	4(9)	18(8)
C(51)	113(16)	99(15)	98(17)	−11(12)	−29(13)	6(13)
C(52)	114(17)	130(20)	110(20)	−36(17)	−4(15)	9(16)

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

	x	y	z	U(eq)
H(1A)	3321	9419	1892	105
H(1B)	3368	7645	1997	105
H(1C)	4038	8769	2087	105
H(2A)	4030	8156	2877	158
H(2B)	3476	6808	2771	158
H(2C)	3264	7982	3082	158
H(5)	4937	13855	3097	73
H(6)	5039	15420	2644	98
H(7)	4413	14892	2115	77
H(9)	3618	10871	3222	82
H(10A)	3226	11906	3736	142
H(10B)	2975	13097	3435	142
H(10C)	3679	13457	3677	142
H(11A)	4917	12118	3537	142
H(11B)	4855	10506	3336	142
H(11C)	4447	10756	3710	142
H(12)	3039	11939	1993	105
H(13A)	3465	12335	1429	178
H(13B)	4200	12283	1663	178
H(13C)	3876	13893	1533	178
H(14A)	2441	14198	2198	208
H(14B)	2260	13671	1798	208
H(14C)	2813	15064	1868	208
H(17)	657	4995	2843	78
H(18)	364	4527	2238	98
H(19)	641	6170	1824	54
H(21)	2014	7841	3134	85
H(22A)	1642	4713	3198	183
H(22B)	1820	5634	3557	183
H(22C)	2429	5496	3250	183
H(23A)	959	7989	3588	215
H(23B)	444	7054	3319	215
H(23C)	706	8751	3220	215
H(24)	2001	9154	1863	102
H(25A)	1325	7060	1362	160

H(25B)	2186	7254	1437	160
H(25C)	1748	8554	1224	160
H(26A)	509	9473	1657	173
H(26B)	1154	10649	1561	173
H(26C)	900	10436	1968	173
H(27A)	9159	3707	5604	104
H(27B)	8952	2126	5412	104
H(27C)	8405	3558	5386	104
H(28A)	9239	2948	4398	96
H(28B)	8449	3012	4586	96
H(28C)	8999	1629	4671	96
H(31)	11810	924	5763	116
H(32)	12216	−646	5236	95
H(33)	11883	−23	4671	80
H(35)	10421	3889	5679	74
H(36A)	10357	1558	6009	161
H(36B)	10424	3081	6244	161
H(36C)	11129	2016	6184	161
H(37A)	11242	5397	5967	174
H(37B)	11742	4831	5641	174
H(37C)	11821	4040	6024	174
H(38)	10539	2708	4394	89
H(39A)	11388	4001	4204	195
H(39B)	11500	2564	3945	195
H(39C)	12001	2746	4293	195
H(40A)	10585	903	3949	186
H(40B)	10476	−24	4314	186
H(40C)	11268	45	4129	186
H(43)	7699	9086	4440	100
H(44)	7421	10045	5006	83
H(45)	8161	9412	5506	70
H(47)	8912	5859	4284	81
H(48A)	7694	5656	4134	190
H(48B)	8147	6150	3787	190
H(48C)	7676	7397	4001	190
H(49A)	8850	8991	4030	321
H(49B)	9258	7641	3820	321
H(49C)	9564	8203	4198	321
H(50)	9394	6437	5574	75
H(51A)	9895	8971	5527	155
H(51B)	9968	8167	5909	155
H(51C)	9352	9444	5844	155
H(52A)	8733	6868	6170	181
H(52B)	8274	5897	5884	181

H(52C)	8092	7671	5945	181

S-3. Crystallographic data for **5a**

Table 1. Crystal data and structure refinement for **5a**.

Identification code	a00527a
Empirical formula	C13 H20 N Pb0.50 Si0.50
Formula weight	307.94
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.444(4) A alpha = 90 deg. b = 18.724(6) A beta = 116.420(4) deg. c = 12.638(4) A gamma = 90 deg.
Volume	2637.3(16) A^3
Z, Calculated density	8, 1.551 Mg/m^3
Absorption coefficient	6.457 mm^-1
F(000)	1224
Crystal size	0.20 x 0.18 x 0.15 mm
Theta range for data collection	1.91 to 26.01 deg.
Limiting indices	-15<=h<=15, -14<=k<=23, -14<=l<=15
Reflections collected / unique	11715 / 5195 [R(int) = 0.0350]
Completeness to theta = 26.01	100.0 %
Absorption correction	Semi-empirical from equivalents

Max. and min. transmission	0.4442 and 0.3583
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5195 / 0 / 271
Goodness-of-fit on F^2	0.944
Final R indices [I>2sigma(I)]	R1 = 0.0259, wR2 = 0.0563
R indices (all data)	R1 = 0.0403, wR2 = 0.0593
Largest diff. peak and hole	1.168 and -0.775 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pb(1)	10078(1)	740(1)	10837(1)	32(1)
Si(1)	7604(1)	476(1)	8807(1)	30(1)
N(1)	8158(3)	512(2)	10311(3)	30(1)
N(2)	8989(3)	525(2)	8738(3)	27(1)
C(1)	7560(3)	651(2)	11036(3)	29(1)
C(2)	7129(4)	86(2)	11479(3)	33(1)
C(3)	6583(4)	239(3)	12201(4)	42(1)
C(4)	6481(4)	923(3)	12529(4)	51(1)
C(5)	6908(4)	1474(3)	12119(4)	47(1)
C(6)	7436(4)	1362(2)	11360(4)	36(1)
C(7)	7851(4)	2008(2)	10909(4)	45(1)
C(8)	6825(5)	2541(3)	10285(5)	64(2)
C(9)	8922(5)	2377(3)	11906(6)	74(2)
C(10)	7243(4)	-697(2)	11201(4)	38(1)
C(11)	6022(5)	-1066(3)	10546(5)	65(2)
C(12)	8005(5)	-1107(3)	12328(4)	57(1)
C(13)	6573(4)	1217(3)	7952(4)	52(1)
C(14)	6718(4)	-358(3)	8165(4)	45(1)
C(15)	9010(4)	941(2)	7763(3)	32(1)
C(16)	8666(4)	609(2)	6632(4)	40(1)
C(17)	8675(4)	1015(3)	5712(4)	51(1)
C(18)	8976(4)	1730(3)	5839(4)	55(1)
C(19)	9275(4)	2045(3)	6892(5)	50(1)
C(20)	9293(4)	1678(2)	7869(4)	38(1)
C(21)	9644(4)	2116(2)	9003(4)	43(1)
C(22)	10989(5)	2211(3)	9686(5)	72(2)
C(23)	9001(6)	2849(3)	8779(6)	84(2)
C(24)	8305(5)	-167(3)	6369(4)	50(1)
C(25)	9257(7)	-581(3)	6172(6)	79(2)
C(26)	7062(5)	-245(3)	5328(4)	74(2)

Table 3. Bond lengths [A] and angles [deg] for **5a**.

Pb(1)-N(1)	2.218(3)
Pb(1)-N(2)	2.417(3)
Pb(1)-N(2)#1	2.587(3)
Pb(1)-Si(1)	3.0457(14)
Pb(1)-Pb(1)#1	3.4404(9)
Si(1)-N(1)	1.711(3)
Si(1)-N(2)	1.766(3)
Si(1)-C(13)	1.873(5)
Si(1)-C(14)	1.875(5)
N(1)-C(1)	1.438(5)
N(2)-C(15)	1.468(5)
N(2)-Pb(1)#1	2.587(3)
C(1)-C(2)	1.409(5)
C(1)-C(6)	1.423(5)
C(2)-C(3)	1.389(6)
C(2)-C(10)	1.529(6)
C(3)-C(4)	1.368(7)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.364(7)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.399(6)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.522(6)
C(7)-C(9)	1.532(7)
C(7)-C(8)	1.534(7)
C(7)-H(7A)	0.9800
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-C(12)	1.523(6)
C(10)-C(11)	1.534(7)
C(10)-H(10A)	0.9800
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600

C(12)-H(12C)	0.9600
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-C(20)	1.415(5)
C(15)-C(16)	1.437(6)
C(16)-C(17)	1.394(6)
C(16)-C(24)	1.515(6)
C(17)-C(18)	1.381(7)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.348(7)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.404(6)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.536(6)
C(21)-C(22)	1.514(7)
C(21)-C(23)	1.550(6)
C(21)-H(21A)	0.9800
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-C(25)	1.525(8)
C(24)-C(26)	1.527(7)
C(24)-H(24A)	0.9800
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600

N(1)-Pb(1)-N(2)	68.62(11)
N(1)-Pb(1)-N(2)#1	102.11(11)
N(2)-Pb(1)-N(2)#1	93.21(10)
N(1)-Pb(1)-Si(1)	33.48(8)
N(2)-Pb(1)-Si(1)	35.41(8)
N(2)#1-Pb(1)-Si(1)	102.59(7)
N(1)-Pb(1)-Pb(1)#1	84.36(8)

N(2)-Pb(1)-Pb(1)#1	48.67(7)
N(2)#1-Pb(1)-Pb(1)#1	44.54(7)
Si(1)-Pb(1)-Pb(1)#1	65.88(3)
N(1)-Si(1)-N(2)	97.68(16)
N(1)-Si(1)-C(13)	116.5(2)
N(2)-Si(1)-C(13)	111.45(19)
N(1)-Si(1)-C(14)	112.48(19)
N(2)-Si(1)-C(14)	114.91(19)
C(13)-Si(1)-C(14)	104.3(2)
N(1)-Si(1)-Pb(1)	45.66(11)
N(2)-Si(1)-Pb(1)	52.46(11)
C(13)-Si(1)-Pb(1)	122.82(17)
C(14)-Si(1)-Pb(1)	132.81(16)
C(1)-N(1)-Si(1)	130.4(3)
C(1)-N(1)-Pb(1)	124.6(2)
Si(1)-N(1)-Pb(1)	100.86(15)
C(15)-N(2)-Si(1)	116.9(3)
C(15)-N(2)-Pb(1)	128.5(2)
Si(1)-N(2)-Pb(1)	92.13(13)
C(15)-N(2)-Pb(1)#1	119.1(2)
Si(1)-N(2)-Pb(1)#1	107.42(14)
Pb(1)-N(2)-Pb(1)#1	86.79(10)
C(2)-C(1)-C(6)	118.6(4)
C(2)-C(1)-N(1)	120.9(3)
C(6)-C(1)-N(1)	120.4(3)
C(3)-C(2)-C(1)	119.4(4)
C(3)-C(2)-C(10)	118.1(4)
C(1)-C(2)-C(10)	122.5(4)
C(4)-C(3)-C(2)	122.0(4)
C(4)-C(3)-H(3A)	119.0
C(2)-C(3)-H(3A)	119.0
C(5)-C(4)-C(3)	119.3(4)
C(5)-C(4)-H(4A)	120.4
C(3)-C(4)-H(4A)	120.4
C(4)-C(5)-C(6)	121.9(4)
C(4)-C(5)-H(5A)	119.0
C(6)-C(5)-H(5A)	119.0
C(5)-C(6)-C(1)	118.8(4)
C(5)-C(6)-C(7)	118.7(4)
C(1)-C(6)-C(7)	122.6(4)
C(6)-C(7)-C(9)	111.5(4)
C(6)-C(7)-C(8)	111.4(4)
C(9)-C(7)-C(8)	110.5(4)
C(6)-C(7)-H(7A)	107.7

C(9)-C(7)-H(7A)	107.7
C(8)-C(7)-H(7A)	107.7
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(12)-C(10)-C(2)	110.6(4)
C(12)-C(10)-C(11)	109.4(4)
C(2)-C(10)-C(11)	112.7(4)
C(12)-C(10)-H(10A)	108.0
C(2)-C(10)-H(10A)	108.0
C(11)-C(10)-H(10A)	108.0
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1)-C(13)-H(13A)	109.5
Si(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(1)-C(14)-H(14A)	109.5
Si(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5

C(20)-C(15)-C(16)	117.9(4)
C(20)-C(15)-N(2)	122.3(4)
C(16)-C(15)-N(2)	119.7(3)
C(17)-C(16)-C(15)	119.0(4)
C(17)-C(16)-C(24)	116.8(4)
C(15)-C(16)-C(24)	124.2(4)
C(18)-C(17)-C(16)	122.3(5)
C(18)-C(17)-H(17A)	118.9
C(16)-C(17)-H(17A)	118.8
C(19)-C(18)-C(17)	118.7(4)
C(19)-C(18)-H(18A)	120.6
C(17)-C(18)-H(18A)	120.6
C(18)-C(19)-C(20)	122.9(4)
C(18)-C(19)-H(19A)	118.5
C(20)-C(19)-H(19A)	118.5
C(19)-C(20)-C(15)	119.2(4)
C(19)-C(20)-C(21)	116.4(4)
C(15)-C(20)-C(21)	124.4(4)
C(22)-C(21)-C(20)	112.3(4)
C(22)-C(21)-C(23)	110.5(4)
C(20)-C(21)-C(23)	113.2(4)
C(22)-C(21)-H(21A)	106.8
C(20)-C(21)-H(21A)	106.8
C(23)-C(21)-H(21A)	106.8
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(16)-C(24)-C(25)	110.4(4)
C(16)-C(24)-C(26)	111.6(4)
C(25)-C(24)-C(26)	111.9(5)
C(16)-C(24)-H(24A)	107.6
C(25)-C(24)-H(24A)	107.6
C(26)-C(24)-H(24A)	107.6
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5

H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **5a**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pb(1)	31(1)	26(1)	37(1)	-3(1)	13(1)	-1(1)
Si(1)	28(1)	31(1)	31(1)	1(1)	12(1)	2(1)
N(1)	31(2)	32(2)	31(2)	-2(1)	17(2)	-1(1)
N(2)	29(2)	24(2)	30(2)	3(1)	15(2)	-3(1)
C(1)	25(2)	36(2)	26(2)	-3(2)	10(2)	0(2)
C(2)	28(2)	40(2)	30(2)	6(2)	12(2)	4(2)
C(3)	39(3)	56(3)	34(2)	8(2)	19(2)	2(2)
C(4)	44(3)	77(4)	37(2)	-4(2)	23(2)	11(3)
C(5)	50(3)	49(3)	43(3)	-12(2)	22(2)	3(2)
C(6)	30(2)	40(3)	36(2)	-4(2)	13(2)	2(2)
C(7)	45(3)	31(2)	61(3)	-9(2)	25(2)	2(2)
C(8)	76(4)	44(3)	84(4)	7(3)	46(3)	15(3)
C(9)	55(4)	58(4)	100(5)	-23(3)	27(3)	-16(3)
C(10)	45(3)	33(2)	42(2)	5(2)	24(2)	0(2)
C(11)	60(4)	55(3)	69(4)	0(3)	18(3)	-11(3)
C(12)	51(3)	57(3)	64(3)	20(3)	25(3)	9(3)
C(13)	41(3)	61(3)	54(3)	9(3)	20(2)	14(2)
C(14)	31(3)	58(3)	42(3)	-5(2)	13(2)	-11(2)
C(15)	30(2)	35(2)	34(2)	7(2)	15(2)	3(2)
C(16)	35(3)	50(3)	34(2)	7(2)	13(2)	-1(2)
C(17)	53(3)	67(3)	32(2)	10(2)	18(2)	-5(3)
C(18)	51(3)	67(4)	50(3)	27(3)	25(3)	3(3)
C(19)	51(3)	38(3)	65(3)	20(2)	30(3)	1(2)
C(20)	39(3)	31(2)	46(3)	9(2)	21(2)	4(2)
C(21)	57(3)	26(2)	52(3)	12(2)	31(3)	6(2)
C(22)	80(4)	70(4)	65(4)	-18(3)	31(3)	-29(3)
C(23)	132(6)	32(3)	111(5)	13(3)	77(5)	16(3)
C(24)	67(3)	51(3)	28(2)	-1(2)	19(2)	-11(3)
C(25)	119(6)	66(4)	69(4)	-12(3)	58(4)	0(4)
C(26)	77(4)	87(4)	39(3)	-2(3)	8(3)	-36(3)

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

	x	y	z	U(eq)
H(3A)	6277	-135	12471	50
H(4A)	6125	1010	13026	61
H(5A)	6845	1937	12351	56
H(7A)	8113	1838	10328	54
H(8A)	6166	2303	9657	96
H(8B)	7099	2926	9966	96
H(8C)	6566	2727	10842	96
H(9A)	9560	2039	12281	110
H(9B)	8682	2563	12477	110
H(9C)	9196	2762	11585	110
H(10A)	7650	-713	10692	46
H(11A)	5543	-811	9831	98
H(11B)	5618	-1072	11040	98
H(11C)	6140	-1548	10357	98
H(12A)	8771	-878	12736	86
H(12B)	8119	-1588	12131	86
H(12C)	7607	-1116	12827	86
H(13A)	5843	1019	7355	78
H(13B)	6953	1503	7585	78
H(13C)	6393	1509	8477	78
H(14A)	5960	-235	7520	67
H(14B)	6583	-604	8762	67
H(14C)	7156	-663	7883	67
H(17A)	8472	796	4987	61
H(18A)	8972	1990	5210	66
H(19A)	9478	2527	6976	60
H(21A)	9386	1842	9509	51
H(22A)	11374	1753	9825	108
H(22B)	11174	2438	10429	108
H(22C)	11272	2503	9238	108
H(23A)	9251	3097	9516	125
H(23B)	8149	2776	8426	125
H(23C)	9205	3128	8257	125
H(24A)	8267	-370	7066	59
H(25A)	10022	-523	6846	118

H(25B)	9301	-402	5480	118
H(25C)	9048	-1078	6066	118
H(26A)	6488	16	5489	111
H(26B)	6842	-741	5215	111
H(26C)	7077	-60	4626	111

S-4. Crystallographic data for **5b**

Table 1. Crystal data and structure refinement for **5b**.

Identification code	110721cm
Empirical formula	C36 H44 N2 Pb Si
Formula weight	740.01
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Tetragonal, P4(3)2(1)2
Unit cell dimensions	a = 12.4575(10) A alpha = 90 deg. b = 12.4575(10) A beta = 90 deg. c = 43.426(7) A gamma = 90 deg.
Volume	6739.2(13) A^3
Z, Calculated density	8, 1.459 Mg/m^3
Absorption coefficient	5.068 mm^-1
F(000)	2960
Crystal size	0.48 x 0.42 x 0.31 mm
Theta range for data collection	1.88 to 27.00 deg.
Limiting indices	-14<=h<=15, -15<=k<=15, -46<=l<=55
Reflections collected / unique	38768 / 7339 [R(int) = 0.1244]
Completeness to theta = 27.00	99.9 %

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.3026 and 0.1947
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7339 / 0 / 369
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0618, wR2 = 0.1129
R indices (all data)	R1 = 0.0946, wR2 = 0.1233
Absolute structure parameter	0.032(12)
Largest diff. peak and hole	1.432 and -1.313 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6739(14)	-2359(13)	533(4)	101(5)
C(2)	5970(11)	-1426(9)	529(2)	58(3)
C(3)	4832(11)	-1808(12)	468(3)	81(4)
C(4)	6320(9)	-546(9)	298(2)	49(3)
C(5)	6300(10)	-793(10)	-17(3)	64(4)
C(6)	6590(13)	-56(13)	-231(3)	86(5)
C(7)	6955(11)	926(13)	-136(2)	74(4)
C(8)	7037(9)	1214(9)	173(2)	46(2)
C(9)	6733(8)	452(9)	396(2)	40(3)
C(10)	7462(9)	2315(9)	250(2)	51(3)
C(11)	8553(11)	2549(11)	108(3)	76(4)
C(12)	6668(12)	3185(11)	189(3)	87(5)
C(13)	9354(15)	4235(16)	876(3)	130(8)
C(14)	8290(10)	3843(10)	1007(2)	61(3)
C(15)	7471(16)	4652(11)	982(4)	129(8)
C(16)	8417(9)	3368(9)	1328(2)	42(2)
C(17)	8808(9)	4026(10)	1557(3)	59(3)
C(18)	8952(10)	3725(10)	1856(3)	54(3)
C(19)	8674(9)	2693(12)	1931(2)	57(3)
C(20)	8263(8)	1984(9)	1722(2)	42(3)
C(21)	8089(7)	2306(8)	1410(2)	35(2)
C(22)	7968(11)	855(10)	1821(2)	62(4)
C(23)	8899(19)	176(13)	1879(4)	131(7)
C(24)	7246(15)	879(15)	2101(3)	117(6)
C(25)	7684(9)	-782(8)	1178(2)	41(3)
C(26)	6735(9)	-1086(10)	1312(2)	51(3)
C(27)	6591(12)	-2030(11)	1469(3)	68(4)
C(28)	7436(18)	-2743(13)	1484(3)	94(6)
C(29)	8379(16)	-2518(11)	1350(3)	86(5)
C(30)	8531(10)	-1525(9)	1202(3)	55(3)
C(31)	9188(8)	501(8)	780(2)	39(2)
C(32)	9991(9)	1236(12)	844(3)	72(4)
C(33)	10933(11)	1212(14)	699(3)	98(6)

C(34)	11142(12)	485(15)	473(3)	100(6)
C(35)	10358(12)	-211(13)	392(3)	85(5)
C(36)	9381(10)	-190(11)	538(3)	66(4)
N(1)	6795(7)	708(6)	715(2)	37(2)
N(2)	7595(6)	1644(7)	1192(2)	34(2)
Pb(1)	6076(1)	2123(1)	940(1)	43(1)
Si(1)	7830(2)	535(2)	969(1)	34(1)

Table 3. Bond lengths [A] and angles [deg] for **5b**.

C(1)-C(2)	1.506(19)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(3)	1.519(17)
C(2)-C(4)	1.551(15)
C(2)-H(2)	0.9800
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-C(5)	1.403(14)
C(4)-C(9)	1.412(14)
C(5)-C(6)	1.353(17)
C(5)-H(5)	0.9300
C(6)-C(7)	1.369(18)
C(6)-H(6)	0.9300
C(7)-C(8)	1.394(14)
C(7)-H(7)	0.9300
C(8)-C(9)	1.406(14)
C(8)-C(10)	1.508(15)
C(9)-N(1)	1.423(11)
C(10)-C(12)	1.490(16)
C(10)-C(11)	1.520(16)
C(10)-H(10)	0.9800
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.524(19)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(15)	1.44(2)
C(14)-C(16)	1.523(15)
C(14)-H(14)	0.9800
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600

C(16)-C(17)	1.377(14)
C(16)-C(21)	1.429(14)
C(17)-C(18)	1.363(15)
C(17)-H(17)	0.9300
C(18)-C(19)	1.371(17)
C(18)-H(18)	0.9300
C(19)-C(20)	1.365(14)
C(19)-H(19)	0.9300
C(20)-C(21)	1.428(12)
C(20)-C(22)	1.516(16)
C(21)-N(2)	1.398(11)
C(22)-C(23)	1.46(2)
C(22)-C(24)	1.512(18)
C(22)-H(22)	0.9800
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(26)	1.372(14)
C(25)-C(30)	1.407(15)
C(25)-Si(1)	1.883(10)
C(26)-C(27)	1.370(16)
C(26)-H(26)	0.9300
C(27)-C(28)	1.38(2)
C(27)-H(27)	0.9300
C(28)-C(29)	1.34(2)
C(28)-H(28)	0.9300
C(29)-C(30)	1.408(18)
C(29)-H(29)	0.9300
C(30)-H(30)	0.9300
C(31)-C(36)	1.382(14)
C(31)-C(32)	1.384(14)
C(31)-Si(1)	1.881(10)
C(32)-C(33)	1.332(16)
C(32)-H(32)	0.9300
C(33)-C(34)	1.362(18)
C(33)-H(33)	0.9300
C(34)-C(35)	1.353(19)
C(34)-H(34)	0.9300
C(35)-C(36)	1.371(17)
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300

N(1)-Si(1)	1.712(8)
N(1)-Pb(1)	2.206(8)
N(2)-Si(1)	1.711(8)
N(2)-Pb(1)	2.267(7)
Pb(1)-Si(1)	2.950(3)

C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(1)-C(2)-C(3)	110.7(11)
C(1)-C(2)-C(4)	111.9(11)
C(3)-C(2)-C(4)	111.7(10)
C(1)-C(2)-H(2)	107.5
C(3)-C(2)-H(2)	107.5
C(4)-C(2)-H(2)	107.5
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(5)-C(4)-C(9)	119.6(10)
C(5)-C(4)-C(2)	118.2(10)
C(9)-C(4)-C(2)	122.0(9)
C(6)-C(5)-C(4)	120.9(11)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(5)-C(6)-C(7)	119.3(11)
C(5)-C(6)-H(6)	120.3
C(7)-C(6)-H(6)	120.3
C(6)-C(7)-C(8)	122.9(12)
C(6)-C(7)-H(7)	118.5
C(8)-C(7)-H(7)	118.5
C(7)-C(8)-C(9)	117.9(11)
C(7)-C(8)-C(10)	118.3(10)
C(9)-C(8)-C(10)	123.8(8)
C(8)-C(9)-C(4)	119.1(9)
C(8)-C(9)-N(1)	120.2(9)
C(4)-C(9)-N(1)	120.7(9)
C(12)-C(10)-C(8)	112.9(10)
C(12)-C(10)-C(11)	112.4(11)

C(8)-C(10)-C(11)	113.5(10)
C(12)-C(10)-H(10)	105.7
C(8)-C(10)-H(10)	105.7
C(11)-C(10)-H(10)	105.7
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(16)	114.6(12)
C(15)-C(14)-C(13)	111.4(14)
C(16)-C(14)-C(13)	112.2(11)
C(15)-C(14)-H(14)	106.0
C(16)-C(14)-H(14)	106.0
C(13)-C(14)-H(14)	106.0
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(21)	118.3(9)
C(17)-C(16)-C(14)	117.7(10)
C(21)-C(16)-C(14)	123.9(9)
C(18)-C(17)-C(16)	124.7(12)
C(18)-C(17)-H(17)	117.7
C(16)-C(17)-H(17)	117.7
C(17)-C(18)-C(19)	116.8(10)
C(17)-C(18)-H(18)	121.6
C(19)-C(18)-H(18)	121.6
C(20)-C(19)-C(18)	123.0(10)

C(20)-C(19)-H(19)	118.5
C(18)-C(19)-H(19)	118.5
C(19)-C(20)-C(21)	120.3(11)
C(19)-C(20)-C(22)	120.2(10)
C(21)-C(20)-C(22)	119.5(9)
N(2)-C(21)-C(20)	122.9(9)
N(2)-C(21)-C(16)	120.2(8)
C(20)-C(21)-C(16)	116.8(8)
C(23)-C(22)-C(24)	110.2(12)
C(23)-C(22)-C(20)	113.3(13)
C(24)-C(22)-C(20)	110.7(11)
C(23)-C(22)-H(22)	107.5
C(24)-C(22)-H(22)	107.5
C(20)-C(22)-H(22)	107.5
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(30)	115.6(10)
C(26)-C(25)-Si(1)	121.9(9)
C(30)-C(25)-Si(1)	122.5(9)
C(27)-C(26)-C(25)	124.1(12)
C(27)-C(26)-H(26)	117.9
C(25)-C(26)-H(26)	117.9
C(26)-C(27)-C(28)	118.5(13)
C(26)-C(27)-H(27)	120.8
C(28)-C(27)-H(27)	120.8
C(29)-C(28)-C(27)	120.9(14)
C(29)-C(28)-H(28)	119.6
C(27)-C(28)-H(28)	119.6
C(28)-C(29)-C(30)	120.0(14)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(25)-C(30)-C(29)	120.7(12)
C(25)-C(30)-H(30)	119.6
C(29)-C(30)-H(30)	119.6

C(36)-C(31)-C(32)	116.0(10)
C(36)-C(31)-Si(1)	120.2(8)
C(32)-C(31)-Si(1)	123.2(8)
C(33)-C(32)-C(31)	121.8(12)
C(33)-C(32)-H(32)	119.1
C(31)-C(32)-H(32)	119.1
C(32)-C(33)-C(34)	121.7(14)
C(32)-C(33)-H(33)	119.2
C(34)-C(33)-H(33)	119.2
C(35)-C(34)-C(33)	118.3(13)
C(35)-C(34)-H(34)	120.8
C(33)-C(34)-H(34)	120.8
C(34)-C(35)-C(36)	120.6(13)
C(34)-C(35)-H(35)	119.7
C(36)-C(35)-H(35)	119.7
C(35)-C(36)-C(31)	121.2(12)
C(35)-C(36)-H(36)	119.4
C(31)-C(36)-H(36)	119.4
C(9)-N(1)-Si(1)	129.9(7)
C(9)-N(1)-Pb(1)	126.0(6)
Si(1)-N(1)-Pb(1)	96.9(3)
C(21)-N(2)-Si(1)	141.6(7)
C(21)-N(2)-Pb(1)	122.6(6)
Si(1)-N(2)-Pb(1)	94.7(3)
N(1)-Pb(1)-N(2)	70.4(3)
N(1)-Pb(1)-Si(1)	35.2(2)
N(2)-Pb(1)-Si(1)	35.3(2)
N(2)-Si(1)-N(1)	97.8(4)
N(2)-Si(1)-C(31)	114.7(4)
N(1)-Si(1)-C(31)	113.4(4)
N(2)-Si(1)-C(25)	114.5(4)
N(1)-Si(1)-C(25)	110.4(4)
C(31)-Si(1)-C(25)	106.1(5)
N(2)-Si(1)-Pb(1)	50.0(2)
N(1)-Si(1)-Pb(1)	48.0(3)
C(31)-Si(1)-Pb(1)	131.5(3)
C(25)-Si(1)-Pb(1)	122.3(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **5b**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	100(14)	81(13)	123(13)	15(10)	-15(10)	-4(10)
C(2)	73(9)	56(9)	44(6)	-17(5)	-5(6)	-16(7)
C(3)	69(10)	80(11)	94(10)	-11(8)	5(8)	-15(8)
C(4)	53(8)	51(7)	42(5)	-3(5)	-1(5)	-7(6)
C(5)	73(10)	58(9)	59(7)	-28(6)	1(6)	-17(7)
C(6)	137(15)	89(12)	33(6)	-21(7)	5(7)	-6(10)
C(7)	77(10)	100(12)	46(6)	2(7)	2(6)	-16(9)
C(8)	41(7)	54(8)	43(5)	-2(5)	-12(5)	2(6)
C(9)	21(6)	59(8)	39(5)	-13(5)	-4(4)	2(5)
C(10)	66(8)	57(8)	30(5)	0(5)	8(5)	-7(6)
C(11)	79(11)	61(10)	88(9)	-1(7)	6(8)	-18(7)
C(12)	83(11)	50(9)	128(12)	17(8)	3(9)	12(8)
C(13)	154(18)	157(19)	80(10)	11(10)	-4(10)	-88(15)
C(14)	72(9)	51(8)	58(7)	-10(6)	-18(6)	-20(7)
C(15)	190(20)	38(9)	163(15)	20(10)	-100(15)	-16(10)
C(16)	41(7)	34(6)	51(6)	-2(5)	-10(5)	-5(5)
C(17)	48(7)	53(7)	75(7)	-12(7)	-13(7)	-5(6)
C(18)	41(7)	58(9)	61(7)	-31(6)	-7(6)	6(6)
C(19)	36(7)	93(11)	43(6)	-11(6)	-2(5)	9(6)
C(20)	43(7)	41(7)	41(5)	-12(5)	-5(4)	1(5)
C(21)	23(6)	42(6)	42(5)	-16(4)	-7(4)	0(4)
C(22)	86(10)	63(9)	38(6)	2(5)	-19(6)	-19(8)
C(23)	180(20)	58(12)	159(17)	-7(11)	-13(16)	1(14)
C(24)	138(17)	131(16)	82(9)	42(10)	8(10)	-37(13)
C(25)	54(8)	35(7)	35(5)	-5(4)	-1(5)	0(5)
C(26)	50(7)	47(7)	56(6)	-2(6)	4(5)	4(6)
C(27)	80(10)	65(10)	59(7)	7(7)	-7(6)	-21(8)
C(28)	159(19)	57(10)	66(9)	14(7)	-7(10)	-2(11)
C(29)	119(15)	47(10)	92(10)	6(8)	-15(10)	29(9)
C(30)	56(9)	33(7)	76(8)	0(6)	11(6)	5(5)
C(31)	30(6)	49(7)	38(5)	-5(4)	-3(4)	3(5)
C(32)	23(6)	109(12)	83(8)	-44(8)	9(6)	-27(7)
C(33)	35(8)	140(16)	119(11)	-58(11)	9(8)	-27(9)
C(34)	47(9)	161(17)	91(9)	-57(10)	30(8)	-23(10)

C(35)	72(11)	117(14)	65(8)	-40(8)	7(7)	-23(9)
C(36)	36(7)	71(10)	92(9)	-35(7)	22(6)	-5(6)
N(1)	41(5)	27(5)	42(4)	-8(3)	-1(4)	2(3)
N(2)	13(4)	48(5)	41(4)	-8(4)	-5(3)	4(3)
Pb(1)	31(1)	45(1)	53(1)	-12(1)	-6(1)	6(1)
Si(1)	28(1)	34(2)	40(1)	-7(1)	-1(1)	3(1)

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

	x	y	z	U(eq)
H(1A)	6571	-2823	702	152
H(1B)	7460	-2097	554	152
H(1C)	6675	-2752	343	152
H(2)	5980	-1104	735	69
H(3A)	4817	-2215	280	121
H(3B)	4365	-1199	449	121
H(3C)	4596	-2251	635	121
H(5)	6085	-1473	-81	76
H(6)	6541	-215	-439	104
H(7)	7158	1424	-285	89
H(10)	7576	2316	473	61
H(11A)	9060	2018	175	114
H(11B)	8791	3248	172	114
H(11C)	8495	2530	-112	114
H(12A)	6532	3229	-28	130
H(12B)	6951	3857	261	130
H(12C)	6011	3029	296	130
H(13A)	9273	4379	660	195
H(13B)	9892	3692	905	195
H(13C)	9569	4880	980	195
H(14)	8060	3250	875	73
H(15A)	6837	4418	1088	194
H(15B)	7305	4768	768	194
H(15C)	7724	5309	1071	194
H(17)	8988	4727	1503	70
H(18)	9225	4197	2002	64
H(19)	8770	2466	2133	69
H(22)	7561	527	1652	75
H(23A)	9397	239	1712	197
H(23B)	8672	-558	1898	197
H(23C)	9241	398	2067	197
H(24A)	7092	158	2165	176
H(24B)	6587	1239	2050	176
H(24C)	7599	1256	2265	176
H(26)	6153	-623	1296	61

H(27)	5939	−2187	1563	82
H(28)	7351	−3389	1588	113
H(29)	8933	−3018	1356	103
H(30)	9198	−1359	1118	66
H(32)	9870	1762	992	86
H(33)	11461	1703	754	118
H(34)	11808	468	376	120
H(35)	10482	−709	236	102
H(36)	8839	−649	472	79

Table 6. Torsion angles [deg] for **5b**.

C(1)-C(2)-C(4)-C(5)	66.5(15)
C(3)-C(2)-C(4)-C(5)	-58.2(15)
C(1)-C(2)-C(4)-C(9)	-108.4(13)
C(3)-C(2)-C(4)-C(9)	126.9(11)
C(9)-C(4)-C(5)-C(6)	-5.4(19)
C(2)-C(4)-C(5)-C(6)	179.6(13)
C(4)-C(5)-C(6)-C(7)	3(2)
C(5)-C(6)-C(7)-C(8)	-1(2)
C(6)-C(7)-C(8)-C(9)	0(2)
C(6)-C(7)-C(8)-C(10)	179.3(13)
C(7)-C(8)-C(9)-C(4)	-2.6(16)
C(10)-C(8)-C(9)-C(4)	178.5(10)
C(7)-C(8)-C(9)-N(1)	-179.7(11)
C(10)-C(8)-C(9)-N(1)	1.4(16)
C(5)-C(4)-C(9)-C(8)	5.1(16)
C(2)-C(4)-C(9)-C(8)	179.9(10)
C(5)-C(4)-C(9)-N(1)	-177.9(10)
C(2)-C(4)-C(9)-N(1)	-3.1(16)
C(7)-C(8)-C(10)-C(12)	74.6(15)
C(9)-C(8)-C(10)-C(12)	-106.5(12)
C(7)-C(8)-C(10)-C(11)	-54.9(14)
C(9)-C(8)-C(10)-C(11)	124.1(11)
C(15)-C(14)-C(16)-C(17)	-67.9(15)
C(13)-C(14)-C(16)-C(17)	60.4(16)
C(15)-C(14)-C(16)-C(21)	108.0(13)
C(13)-C(14)-C(16)-C(21)	-123.7(13)
C(21)-C(16)-C(17)-C(18)	2.9(17)
C(14)-C(16)-C(17)-C(18)	179.0(11)
C(16)-C(17)-C(18)-C(19)	-0.6(18)
C(17)-C(18)-C(19)-C(20)	-0.5(17)
C(18)-C(19)-C(20)-C(21)	-0.8(17)
C(18)-C(19)-C(20)-C(22)	-179.7(11)
C(19)-C(20)-C(21)-N(2)	-175.0(9)
C(22)-C(20)-C(21)-N(2)	3.9(15)
C(19)-C(20)-C(21)-C(16)	3.1(14)
C(22)-C(20)-C(21)-C(16)	-178.0(10)
C(17)-C(16)-C(21)-N(2)	174.1(9)
C(14)-C(16)-C(21)-N(2)	-1.7(15)
C(17)-C(16)-C(21)-C(20)	-4.1(14)
C(14)-C(16)-C(21)-C(20)	-179.9(10)

C(19)-C(20)-C(22)-C(23)	-72.6(15)
C(21)-C(20)-C(22)-C(23)	108.5(13)
C(19)-C(20)-C(22)-C(24)	51.7(16)
C(21)-C(20)-C(22)-C(24)	-127.2(11)
C(30)-C(25)-C(26)-C(27)	1.7(15)
Si(1)-C(25)-C(26)-C(27)	-179.4(9)
C(25)-C(26)-C(27)-C(28)	-2.5(18)
C(26)-C(27)-C(28)-C(29)	0(2)
C(27)-C(28)-C(29)-C(30)	2(2)
C(26)-C(25)-C(30)-C(29)	1.1(16)
Si(1)-C(25)-C(30)-C(29)	-177.8(9)
C(28)-C(29)-C(30)-C(25)	-3(2)
C(36)-C(31)-C(32)-C(33)	-6(2)
Si(1)-C(31)-C(32)-C(33)	-177.8(12)
C(31)-C(32)-C(33)-C(34)	2(3)
C(32)-C(33)-C(34)-C(35)	1(3)
C(33)-C(34)-C(35)-C(36)	-1(3)
C(34)-C(35)-C(36)-C(31)	-3(2)
C(32)-C(31)-C(36)-C(35)	6.5(19)
Si(1)-C(31)-C(36)-C(35)	178.6(11)
C(8)-C(9)-N(1)-Si(1)	-90.3(11)
C(4)-C(9)-N(1)-Si(1)	92.7(11)
C(8)-C(9)-N(1)-Pb(1)	53.0(12)
C(4)-C(9)-N(1)-Pb(1)	-124.0(9)
C(20)-C(21)-N(2)-Si(1)	-74.2(14)
C(16)-C(21)-N(2)-Si(1)	107.8(12)
C(20)-C(21)-N(2)-Pb(1)	121.1(9)
C(16)-C(21)-N(2)-Pb(1)	-56.9(11)
C(9)-N(1)-Pb(1)-N(2)	-149.1(8)
Si(1)-N(1)-Pb(1)-N(2)	3.4(3)
C(9)-N(1)-Pb(1)-Si(1)	-152.5(9)
C(21)-N(2)-Pb(1)-N(1)	167.2(8)
Si(1)-N(2)-Pb(1)-N(1)	-3.4(3)
C(21)-N(2)-Pb(1)-Si(1)	170.5(9)
C(21)-N(2)-Si(1)-N(1)	-163.0(11)
Pb(1)-N(2)-Si(1)-N(1)	4.1(4)
C(21)-N(2)-Si(1)-C(31)	-42.7(12)
Pb(1)-N(2)-Si(1)-C(31)	124.4(4)
C(21)-N(2)-Si(1)-C(25)	80.4(12)
Pb(1)-N(2)-Si(1)-C(25)	-112.5(4)
C(21)-N(2)-Si(1)-Pb(1)	-167.1(12)
C(9)-N(1)-Si(1)-N(2)	146.6(9)
Pb(1)-N(1)-Si(1)-N(2)	-4.2(4)
C(9)-N(1)-Si(1)-C(31)	25.3(10)

Pb(1)-N(1)-Si(1)-C(31)	-125.5(4)
C(9)-N(1)-Si(1)-C(25)	-93.6(9)
Pb(1)-N(1)-Si(1)-C(25)	115.6(4)
C(9)-N(1)-Si(1)-Pb(1)	150.8(10)
C(36)-C(31)-Si(1)-N(2)	-163.7(9)
C(32)-C(31)-Si(1)-N(2)	7.8(12)
C(36)-C(31)-Si(1)-N(1)	-52.4(11)
C(32)-C(31)-Si(1)-N(1)	119.0(10)
C(36)-C(31)-Si(1)-C(25)	68.9(10)
C(32)-C(31)-Si(1)-C(25)	-119.7(10)
C(36)-C(31)-Si(1)-Pb(1)	-106.2(10)
C(32)-C(31)-Si(1)-Pb(1)	65.3(11)
C(26)-C(25)-Si(1)-N(2)	60.2(9)
C(30)-C(25)-Si(1)-N(2)	-121.0(8)
C(26)-C(25)-Si(1)-N(1)	-49.0(9)
C(30)-C(25)-Si(1)-N(1)	129.9(8)
C(26)-C(25)-Si(1)-C(31)	-172.2(8)
C(30)-C(25)-Si(1)-C(31)	6.6(9)
C(26)-C(25)-Si(1)-Pb(1)	3.4(9)
C(30)-C(25)-Si(1)-Pb(1)	-177.8(7)
N(1)-Pb(1)-Si(1)-N(2)	174.5(5)
N(2)-Pb(1)-Si(1)-N(1)	-174.5(5)
N(1)-Pb(1)-Si(1)-C(31)	85.3(5)
N(2)-Pb(1)-Si(1)-C(31)	-89.3(5)
N(1)-Pb(1)-Si(1)-C(25)	-89.1(5)
N(2)-Pb(1)-Si(1)-C(25)	96.4(5)

Symmetry transformations used to generate equivalent atoms:

S-5. Crystallographic data for **6**

Table 1. Crystal data and structure refinement for **6**.

Identification code	a00413c
Empirical formula	C56 H86 Ge2 N4 O3 Si2
Formula weight	1064.65
Temperature	293(2) K
Wavelength	0.71073 A

Crystal system, space group	Monoclinic, P2/n
Unit cell dimensions	a = 13.449(4) A alpha = 90 deg. b = 10.478(4) A beta = 90.705(5) deg. c = 21.692(7) A gamma = 90 deg.
Volume	3056.5(18) A^3
Z, Calculated density	2, 1.157 Mg/m^3
Absorption coefficient	1.064 mm^-1
F(000)	1132
Crystal size	0.25 x 0.15 x 0.14 mm
Theta range for data collection	1.77 to 25.01 deg.
Limiting indices	-15<=h<=14, -12<=k<=12, -23<=l<=25
Reflections collected / unique	12377 / 5382 [R(int) = 0.0605]
Completeness to theta = 25.01	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8654 and 0.7769
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5382 / 0 / 317
Goodness-of-fit on F^2	0.871
Final R indices [I>2sigma(I)]	R1 = 0.0739, wR2 = 0.1946
R indices (all data)	R1 = 0.1385, wR2 = 0.2312
Largest diff. peak and hole	1.207 and -0.508 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ge(1)	2335(1)	764(1)	1909(1)	87(1)
Si(1)	2059(1)	561(2)	733(1)	100(1)
N(1)	3048(3)	985(5)	1212(2)	72(1)
N(2)	1340(3)	299(6)	1384(2)	86(2)
O(1)	2500	1952(11)	2500	192(4)
O(2)	2500	-528(8)	2500	146(3)
C(1)	1559(6)	1863(11)	222(4)	169(4)
C(2)	2324(7)	-870(10)	248(4)	170(5)
C(3)	353(4)	-108(7)	1482(2)	66(2)
C(4)	-390(4)	802(7)	1590(3)	72(2)
C(5)	-1350(4)	375(8)	1683(3)	92(2)
C(6)	-1590(5)	-869(9)	1683(4)	101(2)
C(7)	-868(5)	-1754(7)	1581(3)	90(2)
C(8)	117(4)	-1387(8)	1481(3)	79(2)
C(9)	882(6)	-2446(8)	1389(4)	110(2)
C(10)	1039(7)	-3198(10)	1987(5)	176(5)
C(11)	625(7)	-3291(9)	850(5)	154(4)
C(12)	-178(5)	2207(8)	1619(3)	103(2)
C(13)	-833(8)	2982(9)	1156(5)	158(4)
C(14)	-329(7)	2742(8)	2270(4)	134(3)
C(15)	4025(4)	1445(7)	1115(2)	70(2)
C(16)	4831(4)	567(7)	1114(2)	70(2)
C(17)	5767(4)	1073(8)	1035(3)	85(2)
C(18)	5940(5)	2339(9)	945(3)	102(2)
C(19)	5158(5)	3176(7)	944(3)	99(2)
C(20)	4197(4)	2751(8)	1035(3)	84(2)
C(21)	3371(6)	3761(8)	1049(4)	120(3)
C(22)	3313(9)	4493(10)	452(6)	176(5)
C(23)	3502(7)	4605(10)	1625(5)	175(5)
C(24)	4709(5)	-825(8)	1205(3)	90(2)
C(25)	5116(8)	-1223(10)	1832(4)	148(4)
C(26)	5215(7)	-1584(8)	711(4)	126(3)
C(27)	7140(20)	5250(30)	1985(19)	310(20)

C (28)	6630 (40)	5740 (50)	1850 (20)	193 (18)
C (29)	7150 (20)	5720 (30)	1278 (19)	195 (16)
O (3)	7771 (17)	5634 (16)	2207 (9)	158 (7)

Table 3. Bond lengths [A] and angles [deg] for **6**.

Ge(1)-O(1)	1.799(8)
Ge(1)-N(2)	1.812(4)
Ge(1)-N(1)	1.816(4)
Ge(1)-O(2)	1.875(6)
Ge(1)-Si(1)	2.5816(19)
Ge(1)-Ge(1)#1	2.5972(14)
Si(1)-N(1)	1.735(4)
Si(1)-N(2)	1.744(5)
Si(1)-C(2)	1.869(8)
Si(1)-C(1)	1.876(9)
N(1)-C(15)	1.418(6)
N(2)-C(3)	1.412(6)
O(1)-Ge(1)#1	1.799(8)
O(2)-Ge(1)#1	1.875(6)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-C(8)	1.377(8)
C(3)-C(4)	1.404(8)
C(4)-C(5)	1.384(8)
C(4)-C(12)	1.501(9)
C(5)-C(6)	1.343(9)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.363(9)
C(6)-H(6A)	0.9300
C(7)-C(8)	1.398(8)
C(7)-H(7A)	0.9300
C(8)-C(9)	1.528(9)
C(9)-C(11)	1.503(10)
C(9)-C(10)	1.530(11)
C(9)-H(9A)	0.9800
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600

C(12)-C(14)	1.534(10)
C(12)-C(13)	1.556(10)
C(12)-H(12A)	0.9800
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-C(20)	1.399(8)
C(15)-C(16)	1.420(8)
C(16)-C(17)	1.378(8)
C(16)-C(24)	1.481(8)
C(17)-C(18)	1.361(9)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.370(9)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.384(8)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.535(9)
C(21)-C(22)	1.506(12)
C(21)-C(23)	1.540(12)
C(21)-H(21A)	0.9800
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-C(26)	1.503(9)
C(24)-C(25)	1.520(10)
C(24)-H(24A)	0.9800
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-C(28)	0.89(5)
C(27)-O(3)	1.05(3)
C(27)-C(29)	1.61(5)
C(27)-O(3)#2	1.80(4)
C(28)-C(29)	1.44(6)
C(28)-O(3)	1.71(6)

O(3)-O(3)#2	1.47(4)
O(3)-C(27)#2	1.80(4)
O(1)-Ge(1)-N(2)	135.8(2)
O(1)-Ge(1)-N(1)	116.3(2)
N(2)-Ge(1)-N(1)	84.54(19)
O(1)-Ge(1)-O(2)	90.0(3)
N(2)-Ge(1)-O(2)	108.4(2)
N(1)-Ge(1)-O(2)	127.02(18)
O(1)-Ge(1)-Si(1)	140.9(3)
N(2)-Ge(1)-Si(1)	42.41(14)
N(1)-Ge(1)-Si(1)	42.15(13)
O(2)-Ge(1)-Si(1)	129.1(2)
O(1)-Ge(1)-Ge(1)#1	43.8(3)
N(2)-Ge(1)-Ge(1)#1	137.41(15)
N(1)-Ge(1)-Ge(1)#1	137.42(13)
O(2)-Ge(1)-Ge(1)#1	46.17(19)
Si(1)-Ge(1)-Ge(1)#1	175.03(6)
N(1)-Si(1)-N(2)	89.1(2)
N(1)-Si(1)-C(2)	113.1(4)
N(2)-Si(1)-C(2)	116.2(3)
N(1)-Si(1)-C(1)	115.7(4)
N(2)-Si(1)-C(1)	113.2(3)
C(2)-Si(1)-C(1)	108.7(5)
N(1)-Si(1)-Ge(1)	44.61(14)
N(2)-Si(1)-Ge(1)	44.50(15)
C(2)-Si(1)-Ge(1)	126.6(3)
C(1)-Si(1)-Ge(1)	124.7(3)
C(15)-N(1)-Si(1)	134.7(3)
C(15)-N(1)-Ge(1)	131.8(3)
Si(1)-N(1)-Ge(1)	93.24(19)
C(3)-N(2)-Si(1)	134.5(4)
C(3)-N(2)-Ge(1)	132.4(3)
Si(1)-N(2)-Ge(1)	93.1(2)
Ge(1)-O(1)-Ge(1)#1	92.4(6)
Ge(1)#1-O(2)-Ge(1)	87.7(4)
Si(1)-C(1)-H(1A)	109.5
Si(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Si(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
Si(1)-C(2)-H(2A)	109.5
Si(1)-C(2)-H(2B)	109.5

H(2A)-C(2)-H(2B)	109.5
Si(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(8)-C(3)-C(4)	119.8(5)
C(8)-C(3)-N(2)	120.7(6)
C(4)-C(3)-N(2)	119.4(6)
C(5)-C(4)-C(3)	118.2(6)
C(5)-C(4)-C(12)	119.2(6)
C(3)-C(4)-C(12)	122.6(5)
C(6)-C(5)-C(4)	122.6(6)
C(6)-C(5)-H(5A)	118.7
C(4)-C(5)-H(5A)	118.7
C(5)-C(6)-C(7)	119.2(6)
C(5)-C(6)-H(6A)	120.4
C(7)-C(6)-H(6A)	120.4
C(6)-C(7)-C(8)	121.1(7)
C(6)-C(7)-H(7A)	119.4
C(8)-C(7)-H(7A)	119.4
C(3)-C(8)-C(7)	119.0(6)
C(3)-C(8)-C(9)	123.5(6)
C(7)-C(8)-C(9)	117.5(7)
C(11)-C(9)-C(8)	112.4(7)
C(11)-C(9)-C(10)	112.6(8)
C(8)-C(9)-C(10)	110.4(6)
C(11)-C(9)-H(9A)	107.0
C(8)-C(9)-H(9A)	107.0
C(10)-C(9)-H(9A)	107.0
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(4)-C(12)-C(14)	111.7(7)
C(4)-C(12)-C(13)	112.2(6)
C(14)-C(12)-C(13)	108.8(7)
C(4)-C(12)-H(12A)	108.0

C(14)-C(12)-H(12A)	108.0
C(13)-C(12)-H(12A)	108.0
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(20)-C(15)-N(1)	120.3(6)
C(20)-C(15)-C(16)	120.4(5)
N(1)-C(15)-C(16)	119.3(6)
C(17)-C(16)-C(15)	116.7(7)
C(17)-C(16)-C(24)	119.8(6)
C(15)-C(16)-C(24)	123.5(5)
C(18)-C(17)-C(16)	123.4(6)
C(18)-C(17)-H(17A)	118.3
C(16)-C(17)-H(17A)	118.3
C(17)-C(18)-C(19)	119.4(6)
C(17)-C(18)-H(18A)	120.3
C(19)-C(18)-H(18A)	120.3
C(18)-C(19)-C(20)	120.8(7)
C(18)-C(19)-H(19A)	119.6
C(20)-C(19)-H(19A)	119.6
C(19)-C(20)-C(15)	119.2(6)
C(19)-C(20)-C(21)	117.3(7)
C(15)-C(20)-C(21)	123.5(6)
C(22)-C(21)-C(20)	111.4(7)
C(22)-C(21)-C(23)	114.2(9)
C(20)-C(21)-C(23)	109.6(7)
C(22)-C(21)-H(21A)	107.1
C(20)-C(21)-H(21A)	107.1
C(23)-C(21)-H(21A)	107.1
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(16)-C(24)-C(26)	112.0(6)
C(16)-C(24)-C(25)	110.5(7)
C(26)-C(24)-C(25)	109.4(7)
C(16)-C(24)-H(24A)	108.3
C(26)-C(24)-H(24A)	108.3
C(25)-C(24)-H(24A)	108.3
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(28)-C(27)-O(3)	122(7)
C(28)-C(27)-C(29)	63(5)
O(3)-C(27)-C(29)	108(3)
C(28)-C(27)-O(3)#2	103(6)
O(3)-C(27)-O(3)#2	55(3)
C(29)-C(27)-O(3)#2	149(3)
C(27)-C(28)-C(29)	84(6)
C(27)-C(28)-O(3)	31(4)
C(29)-C(28)-O(3)	87(3)
C(28)-C(29)-C(27)	33(2)
C(27)-O(3)-O(3)#2	89(3)
C(27)-O(3)-C(28)	26(3)
O(3)#2-O(3)-C(28)	86(3)
C(27)-O(3)-C(27)#2	114(3)
O(3)#2-O(3)-C(27)#2	35.7(11)
C(28)-O(3)-C(27)#2	120(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,y,-z+1/2 #2 -x+3/2,y,-z+1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **6**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ge(1)	41(1)	173(1)	47(1)	5(1)	2(1)	-7(1)
Si(1)	50(1)	206(2)	43(1)	-4(1)	2(1)	-30(1)
N(1)	41(2)	130(4)	46(2)	4(2)	4(2)	-9(2)
N(2)	50(3)	159(5)	50(3)	-8(3)	2(2)	-15(3)
O(1)	133(7)	287(12)	157(8)	0	97(6)	0
O(2)	84(5)	182(8)	172(9)	0	2(5)	0
C(1)	102(6)	324(14)	80(6)	75(7)	-24(4)	-29(7)
C(2)	122(7)	291(13)	98(6)	-92(7)	49(5)	-84(7)
C(3)	38(3)	108(5)	52(3)	2(3)	0(2)	-10(3)
C(4)	54(3)	93(5)	68(4)	4(3)	2(3)	-5(3)
C(5)	50(4)	121(6)	105(5)	-1(4)	3(3)	14(4)
C(6)	46(3)	133(7)	124(6)	11(5)	1(4)	-21(4)
C(7)	82(5)	92(5)	97(5)	6(4)	2(4)	-17(4)
C(8)	58(4)	115(6)	63(4)	2(4)	-1(3)	17(4)
C(9)	102(5)	132(7)	97(6)	1(5)	11(4)	25(5)
C(10)	163(9)	214(11)	151(9)	58(8)	21(7)	105(8)
C(11)	157(9)	144(8)	160(9)	-43(7)	11(7)	38(6)
C(12)	78(4)	133(7)	98(5)	-8(5)	-6(4)	-4(4)
C(13)	189(10)	129(8)	155(9)	34(6)	-61(8)	-21(7)
C(14)	138(7)	155(8)	108(7)	-37(6)	-3(5)	10(6)
C(15)	51(3)	114(5)	44(3)	-4(3)	11(2)	-8(3)
C(16)	47(3)	116(6)	48(3)	-9(3)	9(2)	-5(3)
C(17)	50(3)	137(7)	69(4)	-19(4)	0(3)	6(4)
C(18)	54(4)	142(7)	112(6)	-41(5)	18(3)	-25(4)
C(19)	83(5)	103(6)	111(6)	-16(4)	20(4)	-19(4)
C(20)	64(4)	123(6)	67(4)	-14(4)	8(3)	7(4)
C(21)	98(6)	119(7)	144(8)	-4(6)	22(5)	19(5)
C(22)	168(10)	165(10)	195(12)	67(8)	15(9)	48(7)
C(23)	137(8)	197(11)	193(11)	-85(9)	4(7)	62(7)
C(24)	70(4)	125(7)	76(5)	5(4)	3(3)	0(4)
C(25)	174(9)	191(9)	79(6)	25(6)	13(6)	37(7)
C(26)	159(8)	124(6)	95(6)	-5(5)	19(5)	5(6)
C(27)	240(40)	190(30)	510(70)	-30(20)	140(40)	-70(20)
C(28)	200(40)	210(40)	170(30)	30(30)	-50(30)	30(20)

C(29)	160(20)	106(17)	320(50)	70(20)	−90(30)	−52(15)
0(3)	173(19)	108(11)	191(18)	46(9)	−28(13)	−50(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **6**.

	x	y	z	U(eq)
H(1A)	1523	1563	-195	253
H(1B)	1992	2590	246	253
H(1C)	907	2101	356	253
H(2A)	2155	-688	-174	255
H(2B)	1936	-1579	388	255
H(2C)	3018	-1078	280	255
H(5A)	-1849	973	1747	111
H(6A)	-2241	-1124	1753	121
H(7A)	-1032	-2616	1578	108
H(9A)	1516	-2031	1295	132
H(10A)	1235	-2625	2311	264
H(10B)	1549	-3826	1929	264
H(10C)	430	-3616	2095	264
H(11A)	566	-2783	483	231
H(11B)	5	-3714	925	231
H(11C)	1139	-3916	799	231
H(12A)	520	2338	1511	124
H(13A)	-742	2656	747	237
H(13B)	-643	3864	1170	237
H(13C)	-1520	2902	1266	237
H(14A)	85	2284	2558	201
H(14B)	-1013	2647	2382	201
H(14C)	-153	3630	2277	201
H(17A)	6308	521	1044	102
H(18A)	6584	2633	884	123
H(19A)	5274	4041	881	119
H(21A)	2739	3305	1091	144
H(22A)	3208	3910	116	264
H(22B)	3924	4949	393	264
H(22C)	2771	5088	467	264
H(23A)	2976	5224	1637	263
H(23B)	4131	5035	1609	263
H(23C)	3481	4081	1988	263
H(24A)	3997	-1023	1189	109
H(25A)	4787	-747	2148	222

H(25B)	5817	−1054	1853	222
H(25C)	5001	−2118	1893	222
H(26A)	4956	−1337	314	189
H(26B)	5094	−2477	776	189
H(26C)	5917	−1424	728	189