

Table 1. Crystal data and structure refinement for 1.

Identification code	1	
Empirical formula	C ₃₂ H ₃₇ As	
Formula weight	496.54	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.0510(6) Å	α = 90°.
	b = 20.3953(12) Å	β = 107.3800(10)°.
	c = 13.4192(7) Å	γ = 90°.
Volume	2625.3(3) Å ³	
Z	4	
Density (calculated)	1.256 Mg/m ³	
Absorption coefficient	1.312 mm ⁻¹	
F(000)	1048	
Crystal size	0.1 x 0.3 x 0.4 mm ³	
Theta range for data collection	1.88 to 26.37°.	
Index ranges	-11 ≤ h ≤ 12, -25 ≤ k ≤ 25, -16 ≤ l ≤ 14	
Reflections collected	19834	
Independent reflections	5372 [R(int) = 0.0503]	
Completeness to theta = 26.37°	100.0 %	
Absorption correction	Semi-empirical	
Max. and min. transmission	1.000000 and 0.833509	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5372 / 0 / 307	
Goodness-of-fit on F ²	0.932	
Final R indices [I > 2σ(I)]	R1 = 0.0354, wR2 = 0.0709	
R indices (all data)	R1 = 0.0646, wR2 = 0.0787	
Largest diff. peak and hole	0.428 and -0.344 e.Å ⁻³	

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

	x	y	z	U(eq)
As(1)	1163(1)	1159(1)	1650(1)	28(1)
C(1)	780(2)	318(1)	1576(2)	29(1)
C(2)	345(2)	-287(1)	1353(2)	27(1)
C(3)	-904(2)	-605(1)	1521(2)	31(1)
C(4)	-2045(3)	-337(1)	1758(2)	41(1)
C(5)	-3102(3)	-754(2)	1820(2)	49(1)
C(6)	-3055(3)	-1414(2)	1640(2)	50(1)
C(7)	-1939(3)	-1686(1)	1385(2)	42(1)
C(8)	-863(3)	-1277(1)	1321(2)	32(1)
C(9)	383(3)	-1414(1)	1002(2)	29(1)
C(10)	875(3)	-1995(1)	698(2)	38(1)
C(11)	2045(3)	-1967(1)	359(2)	44(1)
C(12)	2718(3)	-1381(1)	330(2)	43(1)
C(13)	2247(3)	-805(1)	637(2)	34(1)
C(14)	1078(2)	-821(1)	977(2)	26(1)
C(15)	2632(2)	1225(1)	3027(2)	22(1)
C(16)	4040(2)	1284(1)	3016(2)	23(1)
C(17)	5088(2)	1255(1)	3966(2)	23(1)
C(18)	4831(2)	1191(1)	4921(2)	22(1)
C(19)	3440(2)	1185(1)	4904(2)	24(1)
C(20)	2329(2)	1216(1)	3996(2)	22(1)
C(21)	4502(3)	1407(1)	2023(2)	29(1)
C(22)	4180(3)	828(1)	1257(2)	37(1)
C(23)	6094(3)	1502(2)	2299(2)	42(1)
C(24)	3857(3)	2045(1)	1485(2)	42(1)
C(25)	5981(2)	1141(1)	5957(2)	26(1)
C(26)	7442(2)	1196(1)	5836(2)	38(1)
C(27)	5824(3)	1701(1)	6689(2)	35(1)
C(28)	5866(3)	477(1)	6464(2)	35(1)
C(29)	845(2)	1244(1)	4115(2)	29(1)
C(30)	884(3)	1431(2)	5241(2)	40(1)
C(31)	-52(3)	1771(1)	3409(2)	41(1)
C(32)	143(3)	571(1)	3901(2)	39(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for 1.

As(1)-C(1)	1.754(2)
As(1)-C(15)	1.996(2)
C(1)-C(2)	1.314(3)
C(2)-C(14)	1.485(3)
C(2)-C(3)	1.489(3)
C(3)-C(4)	1.390(3)
C(3)-C(8)	1.400(3)
C(4)-C(5)	1.383(4)
C(5)-C(6)	1.371(4)
C(6)-C(7)	1.383(4)
C(7)-C(8)	1.389(3)
C(8)-C(9)	1.465(3)
C(9)-C(10)	1.392(3)
C(9)-C(14)	1.401(3)
C(10)-C(11)	1.382(4)
C(11)-C(12)	1.380(4)
C(12)-C(13)	1.375(4)
C(13)-C(14)	1.383(3)
C(15)-C(20)	1.421(3)
C(15)-C(16)	1.425(3)
C(16)-C(17)	1.390(3)
C(16)-C(21)	1.558(3)
C(17)-C(18)	1.388(3)
C(18)-C(19)	1.392(3)
C(18)-C(25)	1.523(3)
C(19)-C(20)	1.387(3)
C(20)-C(29)	1.548(3)
C(21)-C(22)	1.534(3)
C(21)-C(24)	1.535(3)
C(21)-C(23)	1.543(3)
C(25)-C(26)	1.529(3)
C(25)-C(28)	1.534(3)
C(25)-C(27)	1.545(3)
C(29)-C(32)	1.529(3)
C(29)-C(31)	1.535(3)
C(29)-C(30)	1.548(3)

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C(1)-As(1)-C(15)	101.94(9)
C(2)-C(1)-As(1)	169.72(19)
C(1)-C(2)-C(14)	127.0(2)
C(1)-C(2)-C(3)	127.8(2)
C(14)-C(2)-C(3)	104.9(2)
C(4)-C(3)-C(8)	120.2(2)
C(4)-C(3)-C(2)	130.8(2)
C(8)-C(3)-C(2)	108.8(2)
C(5)-C(4)-C(3)	118.2(3)
C(6)-C(5)-C(4)	121.7(3)
C(5)-C(6)-C(7)	120.7(3)
C(6)-C(7)-C(8)	118.6(3)
C(7)-C(8)-C(3)	120.5(2)
C(7)-C(8)-C(9)	130.8(2)
C(3)-C(8)-C(9)	108.6(2)
C(10)-C(9)-C(14)	120.3(2)
C(10)-C(9)-C(8)	131.1(2)
C(14)-C(9)-C(8)	108.6(2)
C(11)-C(10)-C(9)	118.3(2)
C(12)-C(11)-C(10)	121.1(2)
C(13)-C(12)-C(11)	121.1(3)
C(12)-C(13)-C(14)	118.8(3)
C(13)-C(14)-C(9)	120.5(2)
C(13)-C(14)-C(2)	130.7(2)
C(9)-C(14)-C(2)	108.9(2)
C(20)-C(15)-C(16)	119.71(19)
C(20)-C(15)-As(1)	123.00(16)
C(16)-C(15)-As(1)	117.29(15)
C(17)-C(16)-C(15)	118.04(19)
C(17)-C(16)-C(21)	116.95(19)
C(15)-C(16)-C(21)	125.0(2)
C(18)-C(17)-C(16)	123.4(2)
C(17)-C(18)-C(19)	116.7(2)
C(17)-C(18)-C(25)	123.37(19)
C(19)-C(18)-C(25)	119.97(18)
C(20)-C(19)-C(18)	123.8(2)
C(19)-C(20)-C(15)	117.87(19)
C(19)-C(20)-C(29)	117.32(19)
C(15)-C(20)-C(29)	124.81(19)

C(22)-C(21)-C(24)	111.3(2)
C(22)-C(21)-C(23)	104.7(2)
C(24)-C(21)-C(23)	105.5(2)
C(22)-C(21)-C(16)	113.10(19)
C(24)-C(21)-C(16)	110.31(19)
C(23)-C(21)-C(16)	111.54(19)
C(18)-C(25)-C(26)	112.89(18)
C(18)-C(25)-C(28)	109.09(19)
C(26)-C(25)-C(28)	108.3(2)
C(18)-C(25)-C(27)	109.69(19)
C(26)-C(25)-C(27)	107.3(2)
C(28)-C(25)-C(27)	109.55(19)
C(32)-C(29)-C(31)	111.1(2)
C(32)-C(29)-C(20)	110.62(19)
C(31)-C(29)-C(20)	111.60(19)
C(32)-C(29)-C(30)	106.3(2)
C(31)-C(29)-C(30)	105.6(2)
C(20)-C(29)-C(30)	111.46(19)

Symmetry transformations used to generate equivalent atoms:

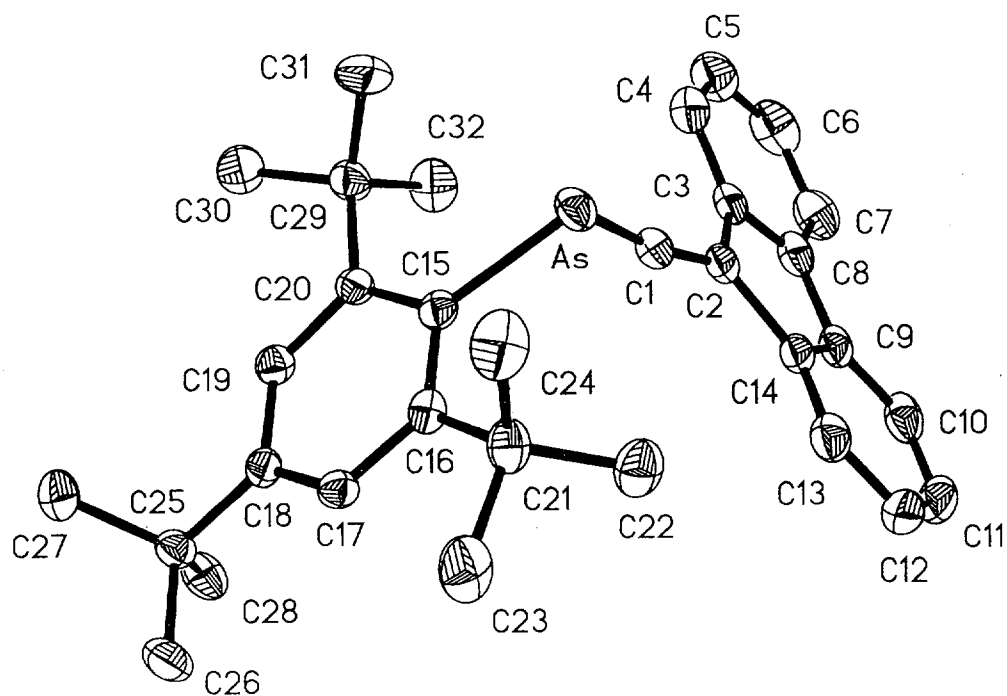
Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
As(1)	31(1)	26(1)	22(1)	3(1)	0(1)	1(1)
C(1)	28(1)	34(1)	21(1)	-1(1)	2(1)	4(1)
C(2)	29(1)	29(1)	19(1)	-2(1)	0(1)	4(1)
C(3)	30(1)	39(2)	19(1)	-3(1)	0(1)	-1(1)
C(4)	40(2)	50(2)	30(1)	-7(1)	7(1)	4(1)
C(5)	31(2)	77(2)	39(2)	-4(2)	13(1)	-4(2)
C(6)	45(2)	64(2)	40(2)	5(2)	10(1)	-17(2)
C(7)	44(2)	42(2)	35(2)	5(1)	5(1)	-9(1)
C(8)	36(1)	34(2)	20(1)	2(1)	2(1)	-3(1)
C(9)	37(1)	29(1)	17(1)	1(1)	1(1)	4(1)
C(10)	51(2)	28(1)	25(1)	1(1)	-1(1)	4(1)
C(11)	56(2)	39(2)	33(2)	-7(1)	5(1)	20(1)
C(12)	41(2)	57(2)	29(1)	-5(1)	10(1)	13(1)
C(13)	38(2)	39(2)	23(1)	-1(1)	7(1)	0(1)
C(14)	29(1)	28(1)	19(1)	-2(1)	2(1)	3(1)
C(15)	27(1)	16(1)	23(1)	1(1)	6(1)	3(1)
C(16)	28(1)	20(1)	21(1)	-2(1)	8(1)	-1(1)
C(17)	20(1)	24(1)	25(1)	-1(1)	8(1)	0(1)
C(18)	23(1)	20(1)	21(1)	-2(1)	6(1)	1(1)
C(19)	26(1)	27(1)	20(1)	1(1)	9(1)	1(1)
C(20)	22(1)	19(1)	24(1)	0(1)	6(1)	0(1)
C(21)	37(1)	30(1)	21(1)	0(1)	11(1)	-5(1)
C(22)	41(2)	41(2)	32(1)	-2(1)	17(1)	-2(1)
C(23)	46(2)	60(2)	29(1)	-6(1)	22(1)	-14(1)
C(24)	61(2)	35(2)	34(2)	5(1)	20(1)	-5(1)
C(25)	23(1)	31(1)	22(1)	2(1)	4(1)	1(1)
C(26)	23(1)	56(2)	31(1)	-2(1)	2(1)	1(1)
C(27)	38(2)	39(2)	26(1)	-6(1)	6(1)	-1(1)
C(28)	35(2)	38(1)	25(1)	7(1)	-1(1)	1(1)
C(29)	21(1)	37(1)	30(1)	-4(1)	8(1)	-3(1)
C(30)	27(1)	60(2)	42(2)	-12(1)	20(1)	-5(1)
C(31)	23(1)	48(2)	49(2)	1(1)	9(1)	7(1)
C(32)	37(2)	44(2)	40(2)	-3(1)	19(1)	-13(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(4)	-2097	121	1874	49
H(5)	-3881	-579	1992	58
H(6)	-3797	-1688	1692	60
H(7)	-1909	-2143	1256	50
H(10)	418	-2400	722	45
H(11)	2391	-2359	144	53
H(12)	3520	-1376	94	51
H(13)	2717	-404	616	40
H(17)	6030	1281	3960	27
H(19)	3240	1158	5551	29
H(22A)	3180	820	884	55
H(22B)	4447	417	1644	55
H(22C)	4708	877	755	55
H(23A)	6567	1097	2601	64
H(23B)	6384	1860	2806	64
H(23C)	6341	1611	1665	64
H(24A)	4190	2127	880	63
H(24B)	4131	2410	1978	63
H(24C)	2839	2005	1253	63
H(26A)	7584	842	5384	57
H(26B)	8139	1161	6523	57
H(26C)	7540	1620	5522	57
H(27A)	5860	2124	6352	53
H(27B)	6584	1676	7345	53
H(27C)	4928	1657	6833	53
H(28A)	4946	439	6570	53
H(28B)	6590	447	7139	53
H(28C)	5990	123	6007	53
H(30A)	-66	1517	5264	61
H(30B)	1454	1826	5457	61
H(30C)	1289	1069	5716	61
H(31A)	-320	1622	2682	61
H(31B)	483	2179	3475	61

H(31C)	-892	1849	3619	61
H(32A)	-787	596	3994	58
H(32B)	707	249	4390	58
H(32C)	59	438	3184	58



1

Table 7. Crystal data and structure refinement for 4.

Identification code	4	
Empirical formula	C ₂₂ H ₃₈ As Br Si	
Formula weight	485.44	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.6357(19) Å	$\alpha = 90^\circ$.
	b = 12.498(3) Å	$\beta = 94.640(3)^\circ$.
	c = 20.452(4) Å	$\gamma = 90^\circ$.
Volume	2455.0(8) Å ³	
Z	4	
Density (calculated)	1.313 Mg/m ³	
Absorption coefficient	3.064 mm ⁻¹	
F(000)	1008	
Crystal size	0.05 x 0.1 x 0.3 mm ³	
Theta range for data collection	1.91 to 24.71°	
Index ranges	-11 ≤ h ≤ 8, -14 ≤ k ≤ 13, -24 ≤ l ≤ 24	
Reflections collected	14860	
Independent reflections	4186 [R(int) = 0.0931]	
Completeness to theta = 24.71°	99.9 %	
Absorption correction	Semi-empirical	
Max. and min. transmission	1.000000 and 0.571648	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4186 / 0 / 238	
Goodness-of-fit on F ²	1.059	
Final R indices [I > 2σ(I)]	R1 = 0.0417, wR2 = 0.0970	
R indices (all data)	R1 = 0.0508, wR2 = 0.1038	
Largest diff. peak and hole	0.431 and -0.576 e.Å ⁻³	

Table 8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1625(4)	6602(2)	3519(2)	23(1)
Br(1)	845(1)	7777(1)	3022(1)	32(1)
As(1)	1250(1)	5218(1)	3365(1)	23(1)
C(2)	-64(4)	5317(2)	2577(2)	21(1)
C(3)	-1511(4)	5459(3)	2645(2)	22(1)
C(4)	-2332(4)	5878(3)	2119(2)	26(1)
C(5)	-1806(4)	6152(3)	1525(2)	23(1)
C(6)	-432(4)	5892(3)	1455(2)	24(1)
C(7)	453(3)	5447(3)	1957(2)	22(1)
C(8)	-2236(4)	5178(3)	3277(2)	28(1)
C(9)	-2154(4)	6127(3)	3752(2)	38(1)
C(10)	-1613(5)	4182(3)	3631(2)	43(1)
C(11)	-3777(5)	4917(5)	3103(2)	53(1)
C(12)	-2756(4)	6657(3)	972(2)	27(1)
C(13)	-3657(4)	7545(3)	1239(2)	37(1)
C(14)	-3722(4)	5784(3)	656(2)	38(1)
C(15)	-1925(5)	7154(4)	437(2)	44(1)
C(16)	1942(4)	5137(3)	1776(2)	27(1)
C(17)	2650(4)	4262(3)	2214(2)	34(1)
C(18)	1868(4)	4678(3)	1074(2)	37(1)
C(19)	2871(4)	6137(3)	1806(2)	43(1)
Si(1)	2899(1)	7053(1)	4204(1)	28(1)
C(20)	3642(5)	5850(4)	4639(2)	46(1)
C(21)	1984(5)	7903(4)	4782(2)	44(1)
C(22)	4293(5)	7832(4)	3839(2)	47(1)

Table 9. Bond lengths [Å] and angles [°] for 4.

C(1)-As(1)	1.789(3)
C(1)-Si(1)	1.873(4)
C(1)-Br(1)	1.906(3)
As(1)-C(2)	1.971(3)
C(2)-C(7)	1.409(5)
C(2)-C(3)	1.424(5)
C(3)-C(4)	1.386(5)
C(3)-C(8)	1.557(4)
C(4)-C(5)	1.396(5)
C(5)-C(6)	1.382(5)
C(5)-C(12)	1.532(5)
C(6)-C(7)	1.396(5)
C(7)-C(16)	1.559(5)
C(8)-C(9)	1.530(5)
C(8)-C(11)	1.534(6)
C(8)-C(10)	1.538(5)
C(12)-C(13)	1.536(5)
C(12)-C(15)	1.538(5)
C(12)-C(14)	1.542(5)
C(16)-C(19)	1.536(5)
C(16)-C(17)	1.538(5)
C(16)-C(18)	1.544(5)
Si(1)-C(20)	1.860(4)
Si(1)-C(22)	1.863(4)
Si(1)-C(21)	1.864(4)
As(1)-C(1)-Si(1)	122.22(18)
As(1)-C(1)-Br(1)	125.83(19)
Si(1)-C(1)-Br(1)	111.94(17)
C(1)-As(1)-C(2)	100.97(14)
C(7)-C(2)-C(3)	119.6(3)
C(7)-C(2)-As(1)	119.5(2)
C(3)-C(2)-As(1)	119.8(2)
C(4)-C(3)-C(2)	118.2(3)
C(4)-C(3)-C(8)	117.7(3)
C(2)-C(3)-C(8)	124.2(3)
C(3)-C(4)-C(5)	123.0(3)

C(6)-C(5)-C(4)	116.8(3)
C(6)-C(5)-C(12)	122.7(3)
C(4)-C(5)-C(12)	120.4(3)
C(5)-C(6)-C(7)	123.4(3)
C(6)-C(7)-C(2)	117.9(3)
C(6)-C(7)-C(16)	116.3(3)
C(2)-C(7)-C(16)	125.7(3)
C(9)-C(8)-C(11)	108.2(3)
C(9)-C(8)-C(10)	109.3(3)
C(11)-C(8)-C(10)	105.7(3)
C(9)-C(8)-C(3)	110.4(3)
C(11)-C(8)-C(3)	110.2(3)
C(10)-C(8)-C(3)	112.9(3)
C(5)-C(12)-C(13)	110.9(3)
C(5)-C(12)-C(15)	112.1(3)
C(13)-C(12)-C(15)	107.6(3)
C(5)-C(12)-C(14)	108.7(3)
C(13)-C(12)-C(14)	108.7(3)
C(15)-C(12)-C(14)	108.6(3)
C(19)-C(16)-C(17)	109.0(3)
C(19)-C(16)-C(18)	108.8(3)
C(17)-C(16)-C(18)	105.2(3)
C(19)-C(16)-C(7)	109.4(3)
C(17)-C(16)-C(7)	114.4(3)
C(18)-C(16)-C(7)	109.8(3)
C(20)-Si(1)-C(22)	110.6(2)
C(20)-Si(1)-C(21)	110.0(2)
C(22)-Si(1)-C(21)	110.5(2)
C(20)-Si(1)-C(1)	108.55(18)
C(22)-Si(1)-C(1)	107.90(19)
C(21)-Si(1)-C(1)	109.30(19)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(2)	21(2)	22(2)	2(1)	-1(1)	7(1)
Br(1)	37(1)	23(1)	34(1)	5(1)	-3(1)	7(1)
As(1)	28(1)	20(1)	22(1)	2(1)	-3(1)	2(1)
C(2)	24(2)	19(2)	21(2)	0(1)	1(1)	-2(1)
C(3)	24(2)	22(2)	20(2)	-3(1)	2(1)	-4(1)
C(4)	19(2)	32(2)	26(2)	-1(1)	4(1)	0(1)
C(5)	25(2)	23(2)	20(2)	0(1)	0(1)	-4(1)
C(6)	22(2)	28(2)	22(2)	1(1)	1(1)	-3(1)
C(7)	19(2)	23(2)	24(2)	-3(1)	-1(1)	-4(1)
C(8)	27(2)	35(2)	21(2)	1(1)	7(2)	-7(2)
C(9)	38(2)	43(2)	35(2)	-4(2)	13(2)	1(2)
C(10)	54(3)	37(2)	39(2)	9(2)	19(2)	-4(2)
C(11)	36(2)	86(4)	39(2)	7(2)	11(2)	-18(2)
C(12)	27(2)	30(2)	25(2)	2(1)	-3(1)	-1(2)
C(13)	35(2)	30(2)	45(2)	2(2)	-4(2)	4(2)
C(14)	34(2)	39(2)	39(2)	-4(2)	-13(2)	1(2)
C(15)	38(2)	58(3)	34(2)	19(2)	-5(2)	-1(2)
C(16)	20(2)	30(2)	32(2)	-3(2)	7(2)	-1(1)
C(17)	23(2)	39(2)	40(2)	-1(2)	3(2)	6(2)
C(18)	34(2)	46(2)	32(2)	-4(2)	10(2)	8(2)
C(19)	28(2)	40(2)	63(3)	-5(2)	19(2)	-7(2)
Si(1)	25(1)	32(1)	26(1)	-7(1)	-3(1)	3(1)
C(20)	44(3)	51(2)	40(2)	-2(2)	-16(2)	16(2)
C(21)	45(3)	49(2)	40(2)	-15(2)	7(2)	1(2)
C(22)	33(2)	49(3)	59(3)	-15(2)	7(2)	-12(2)

Table 11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4.

	x	y	z	U(eq)
H(4)	-3296	5983	2164	31
H(6)	-71	6023	1043	29
H(9A)	-2650	5951	4137	57
H(9B)	-2582	6756	3532	57
H(9C)	-1176	6281	3889	57
H(10A)	-698	4360	3848	64
H(10B)	-1511	3610	3311	64
H(10C)	-2232	3943	3959	64
H(11A)	-4202	4684	3498	80
H(11B)	-3854	4344	2775	80
H(11C)	-4259	5556	2924	80
H(13A)	-4194	7253	1584	56
H(13B)	-4296	7825	882	56
H(13C)	-3056	8124	1419	56
H(14A)	-4264	5464	992	57
H(14B)	-3160	5229	465	57
H(14C)	-4356	6103	311	57
H(15A)	-2569	7488	102	66
H(15B)	-1392	6593	235	66
H(15C)	-1286	7696	633	66
H(17A)	3450	3974	2004	51
H(17B)	1984	3685	2276	51
H(17C)	2969	4568	2641	51
H(18A)	1557	5237	760	55
H(18B)	1209	4080	1038	55
H(18C)	2792	4424	977	55
H(19A)	2962	6415	2255	65
H(19B)	2449	5685	1510	65
H(19C)	3793	5950	1671	65
H(20A)	4060	5380	4325	69
H(20B)	2901	5464	4841	69
H(20C)	4357	6071	4980	69
H(21A)	2656	8165	5130	66

