

Table 1. Crystal data and structure refinement for $11 \cdot 2\text{CH}_2\text{Cl}_2$.

Identification code	11·2CH ₂ Cl ₂		
Empirical formula	C ₂₅ H ₃₇ Cl ₄ N O ₄ Si		
Formula weight	585.45		
Temperature	173(2) K		
Wavelength	0.71073 Å		
Crystal system	Monoclinic		
Space group	P2(1)/c		
Unit cell dimensions	a = 11.440(2) Å alpha = 90 deg. b = 15.188(3) Å beta = 100.20(3) deg. c = 17.037(3) Å gamma = 90 deg.		
Volume, Z	2913.1(10) Å ³ , 4		
Density (calculated)	1.335 Mg/m ³		
Absorption coefficient	0.478 mm ⁻¹		
F(000)	1232		
Crystal size	0.5 x 0.4 x 0.3 mm		
Theta range for data collection	2.25 to 26.37 deg.		
Limiting indices	-14<=h<=14, -18<=k<=18, -21<=l<=21		
Reflections collected	42961		
Independent reflections	5952 [R(int) = 0.0533]		
Absorption correction	None		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	5952 / 26 / 384		
Goodness-of-fit on F ²	1.049		
Final R indices [I>2sigma(I)]	R1 = 0.0342, wR2 = 0.0898		
R indices (all data)	R1 = 0.0424, wR2 = 0.0940		
Largest diff. peak and hole	0.285 and -0.161 e.Å ⁻³		

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $11 \cdot 2\text{CH}_2\text{Cl}_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Si	1217(1)	1501(1)	2223(1)	30(1)
O(1)	1417(1)	358(1)	1850(1)	34(1)
O(2)	2631(1)	1703(1)	2072(1)	32(1)
O(3)	1052(1)	2612(1)	2465(1)	33(1)
O(4)	-262(1)	3935(1)	2791(1)	41(1)
C(1)	891(2)	1017(1)	3172(1)	45(1)
C(2)	-29(1)	1617(1)	1320(1)	33(1)
N	-650(1)	2504(1)	1182(1)	30(1)
C(3)	2486(1)	260(1)	1634(1)	29(1)
C(4)	3172(1)	1026(1)	1743(1)	29(1)
C(5)	4276(1)	1067(1)	1532(1)	36(1)
C(6)	4712(1)	315(1)	1207(1)	42(1)
C(7)	4043(1)	-451(1)	1111(1)	41(1)
C(8)	2924(1)	-488(1)	1329(1)	36(1)
C(9)	1434(1)	3054(1)	3155(1)	30(1)
C(10)	742(1)	3766(1)	3329(1)	31(1)
C(11)	1100(2)	4249(1)	4018(1)	39(1)
C(12)	2150(2)	4043(1)	4532(1)	45(1)
C(13)	2834(2)	3344(1)	4362(1)	48(1)
C(14)	2471(1)	2851(1)	3676(1)	40(1)
C(15)	-361(1)	2990(1)	440(1)	37(1)
C(16)	-905(2)	3909(1)	428(1)	51(1)
C(17)	-2211(2)	3906(1)	460(1)	59(1)
C(18)	-2424(2)	3440(1)	1203(1)	56(1)
C(19)	-1967(1)	2485(1)	1286(1)	43(1)
C(20)	-813(2)	2493(1)	-333(1)	45(1)
C(21)	989(2)	3083(1)	558(1)	50(1)
C(22)	-2726(2)	1879(1)	678(1)	55(1)
C(23)	-1982(2)	2163(2)	2129(1)	59(1)
C(24)	-4961(9)	3835(5)	-1361(5)	63(2)
Cl(1)	-4358(2)	2812(2)	-1521(2)	53(1)
Cl(2)	-5473(2)	3893(2)	-462(1)	71(1)
C(25)	-6477(13)	3923(9)	2141(8)	73(4)
Cl(3)	-7437(5)	4828(4)	1983(5)	100(2)
Cl(4)	-5803(6)	3751(2)	1320(5)	74(1)
C(26)	-4750(20)	3970(11)	-1317(12)	56(4)
Cl(5)	-4300(7)	2892(6)	-1432(6)	92(3)
Cl(6)	-5661(13)	4031(10)	-599(11)	127(3)
C(27)	-6492(9)	3853(6)	2249(7)	38(2)
Cl(7)	-7419(4)	4788(3)	2084(3)	58(1)
Cl(8)	-5428(10)	3832(3)	1643(8)	83(2)

Table 3. Selected bond lengths [Å] and angles [deg] for $11 \cdot 2\text{CH}_2\text{Cl}_2$.

Si-O(2)	1.7095(10)
Si-O(3)	1.7549(10)
Si-C(1)	1.8720(17)
Si-O(1)	1.8771(11)
Si-C(2)	1.9114(16)
O(2)-Si-O(3)	90.40(5)
O(2)-Si-C(1)	122.62(7)
O(3)-Si-C(1)	97.41(6)
O(2)-Si-O(1)	86.52(5)
O(3)-Si-O(1)	173.44(5)
C(1)-Si-O(1)	89.12(6)
O(2)-Si-C(2)	116.92(6)
O(3)-Si-C(2)	90.24(5)
C(1)-Si-C(2)	119.78(8)
O(1)-Si-C(2)	86.01(5)
C(3)-O(1)-Si	111.49(8)
C(4)-O(2)-Si	115.78(8)
C(9)-O(3)-Si	130.31(9)
Si-C(1)-H(1A)	109.5
Si-C(1)-H(1B)	109.5
Si-C(1)-H(1C)	109.5
N-C(2)-Si	117.86(9)
Si-C(2)-H(2A)	107.8
Si-C(2)-H(2B)	107.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [deg] for $11 \cdot 2\text{CH}_2\text{Cl}_2$.

Si-O(2)	1.7095(10)
Si-O(3)	1.7549(10)
Si-C(1)	1.8720(17)
Si-O(1)	1.8771(11)
Si-C(2)	1.9114(16)
O(1)-C(3)	1.3459(17)
O(2)-C(4)	1.3700(16)
O(3)-C(9)	1.3568(17)
O(4)-H(4O)	0.83(2)
O(4)-C(10)	1.3617(18)
O(4)-H(4O)	0.83(2)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-N	1.5212(17)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N-H	0.884(18)
N-C(19)	1.5482(18)
N-C(15)	1.5492(19)
N-H	0.884(18)
C(3)-C(8)	1.3804(19)
C(3)-C(4)	1.3971(19)
C(4)-C(5)	1.375(2)
C(5)-C(6)	1.399(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.385(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.395(2)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(14)	1.384(2)
C(9)-C(10)	1.4023(19)
C(10)-C(11)	1.384(2)
C(11)-C(12)	1.390(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.380(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.389(2)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(16)	1.527(2)
C(15)-C(20)	1.528(2)
C(15)-C(21)	1.528(2)
C(16)-C(17)	1.505(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.508(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.540(2)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(23)	1.520(3)
C(19)-C(22)	1.534(2)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800

C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-Cl(2)	1.736(6)
C(24)-Cl(1)	1.741(5)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-Cl(4)	1.732(9)
C(25)-Cl(3)	1.750(9)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
Cl(4)-Cl(8)	0.647(7)
C(26)-Cl(5)	1.739(11)
C(26)-Cl(6)	1.744(11)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-Cl(8)	1.730(8)
C(27)-Cl(7)	1.765(7)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
O(2)-Si-O(3)	90.40(5)
O(2)-Si-C(1)	122.62(7)
O(3)-Si-C(1)	97.41(6)
O(2)-Si-O(1)	86.52(5)
O(3)-Si-O(1)	173.44(5)
C(1)-Si-O(1)	89.12(6)
O(2)-Si-C(2)	116.92(6)
O(3)-Si-C(2)	90.24(5)
C(1)-Si-C(2)	119.78(8)
O(1)-Si-C(2)	86.01(5)
C(3)-O(1)-Si	111.49(8)
C(4)-O(2)-Si	115.78(8)
C(9)-O(3)-Si	130.31(9)
H(40)-O(4)-C(10)	109.4(16)
H(40)-O(4)-H(40)	0(5)
C(10)-O(4)-H(40)	109.4(16)
Si-C(1)-H(1A)	109.5
Si-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Si-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N-C(2)-Si	117.86(9)
N-C(2)-H(2A)	107.8
Si-C(2)-H(2A)	107.8
N-C(2)-H(2B)	107.8
Si-C(2)-H(2B)	107.8
H(2A)-C(2)-H(2B)	107.2
H-N-C(2)	103.3(11)
H-N-C(19)	103.3(11)
C(2)-N-C(19)	113.75(11)
H-N-C(15)	104.6(11)
C(2)-N-C(15)	112.81(11)
C(19)-N-C(15)	117.02(12)
H-N-H	0(4)
C(2)-N-H	103.3(11)

C(19)-N-H	103.3(11)
C(15)-N-H	104.6(11)
O(1)-C(3)-C(8)	127.02(12)
O(1)-C(3)-C(4)	112.77(12)
C(8)-C(3)-C(4)	120.21(13)
O(2)-C(4)-C(5)	125.16(12)
O(2)-C(4)-C(3)	113.32(12)
C(5)-C(4)-C(3)	121.51(13)
C(4)-C(5)-C(6)	118.37(13)
C(4)-C(5)-H(5)	120.8
C(6)-C(5)-H(5)	120.8
C(7)-C(6)-C(5)	120.24(14)
C(7)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(6)-C(7)-C(8)	121.09(13)
C(6)-C(7)-H(7)	119.5
C(8)-C(7)-H(7)	119.5
C(3)-C(8)-C(7)	118.55(13)
C(3)-C(8)-H(8)	120.7
C(7)-C(8)-H(8)	120.7
O(3)-C(9)-C(14)	123.58(12)
O(3)-C(9)-C(10)	117.21(12)
C(14)-C(9)-C(10)	119.19(13)
O(4)-C(10)-C(11)	123.99(13)
O(4)-C(10)-C(9)	116.34(12)
C(11)-C(10)-C(9)	119.67(13)
C(10)-C(11)-C(12)	120.53(14)
C(10)-C(11)-H(11)	119.7
C(12)-C(11)-H(11)	119.7
C(13)-C(12)-C(11)	119.93(14)
C(13)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(12)-C(13)-C(14)	119.72(15)
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1
C(9)-C(14)-C(13)	120.94(14)
C(9)-C(14)-H(14)	119.5
C(13)-C(14)-H(14)	119.5
C(16)-C(15)-C(20)	111.39(13)
C(16)-C(15)-C(21)	108.51(14)
C(20)-C(15)-C(21)	109.80(14)
C(16)-C(15)-N	107.60(13)
C(20)-C(15)-N	112.31(12)
C(21)-C(15)-N	107.06(12)
C(17)-C(16)-C(15)	113.68(14)
C(17)-C(16)-H(16A)	108.8
C(15)-C(16)-H(16A)	108.8
C(17)-C(16)-H(16B)	108.8
C(15)-C(16)-H(16B)	108.8
H(16A)-C(16)-H(16B)	107.7
C(16)-C(17)-C(18)	109.95(14)
C(16)-C(17)-H(17A)	109.7
C(18)-C(17)-H(17A)	109.7
C(16)-C(17)-H(17B)	109.7
C(18)-C(17)-H(17B)	109.7
H(17A)-C(17)-H(17B)	108.2
C(17)-C(18)-C(19)	114.60(15)
C(17)-C(18)-H(18A)	108.6
C(19)-C(18)-H(18A)	108.6
C(17)-C(18)-H(18B)	108.6
C(19)-C(18)-H(18B)	108.6
H(18A)-C(18)-H(18B)	107.6
C(23)-C(19)-C(22)	110.18(15)

C(23)-C(19)-C(18)	109.18(15)
C(22)-C(19)-C(18)	111.18(15)
C(23)-C(19)-N	106.72(13)
C(22)-C(19)-N	112.33(13)
C(18)-C(19)-N	107.08(13)
C(15)-C(20)-H(20A)	109.5
C(15)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(15)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(15)-C(21)-H(21A)	109.5
C(15)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(15)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(19)-C(23)-H(23A)	109.5
C(19)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(19)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
Cl(2)-C(24)-Cl(1)	112.9(4)
Cl(2)-C(24)-H(24A)	109.0
Cl(1)-C(24)-H(24A)	109.0
Cl(2)-C(24)-H(24B)	109.0
Cl(1)-C(24)-H(24B)	109.0
H(24A)-C(24)-H(24B)	107.8
Cl(4)-C(25)-Cl(3)	110.6(6)
Cl(4)-C(25)-H(25A)	109.5
Cl(3)-C(25)-H(25A)	109.5
Cl(4)-C(25)-H(25B)	109.5
Cl(3)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	108.1
Cl(8)-Cl(4)-C(25)	66.9(8)
Cl(5)-C(26)-Cl(6)	110.8(9)
Cl(5)-C(26)-H(26A)	109.5
Cl(6)-C(26)-H(26A)	109.5
Cl(5)-C(26)-H(26B)	109.5
Cl(6)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	108.1
Cl(8)-C(27)-Cl(7)	112.7(6)
Cl(8)-C(27)-H(27A)	109.1
Cl(7)-C(27)-H(27A)	109.1
Cl(8)-C(27)-H(27B)	109.1
Cl(7)-C(27)-H(27B)	109.1
H(27A)-C(27)-H(27B)	107.8
Cl(4)-Cl(8)-C(27)	94.6(9)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $11 \cdot 2\text{CH}_2\text{Cl}_2$.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Si	33(1)	26(1)	31(1)	-1(1)	8(1)	1(1)
O(1)	33(1)	26(1)	45(1)	-1(1)	11(1)	-2(1)
O(2)	33(1)	25(1)	37(1)	-5(1)	7(1)	-1(1)
O(3)	38(1)	30(1)	30(1)	-5(1)	4(1)	5(1)
O(4)	41(1)	34(1)	45(1)	-8(1)	0(1)	10(1)
C(1)	59(1)	39(1)	40(1)	4(1)	16(1)	0(1)
C(2)	36(1)	27(1)	37(1)	-3(1)	7(1)	0(1)
N	28(1)	28(1)	34(1)	-4(1)	5(1)	0(1)
C(3)	33(1)	27(1)	28(1)	2(1)	3(1)	1(1)
C(4)	34(1)	27(1)	26(1)	-1(1)	2(1)	2(1)
C(5)	33(1)	36(1)	40(1)	-2(1)	7(1)	-2(1)
C(6)	37(1)	44(1)	47(1)	-3(1)	12(1)	5(1)
C(7)	45(1)	35(1)	43(1)	-4(1)	10(1)	10(1)
C(8)	42(1)	27(1)	37(1)	-2(1)	4(1)	2(1)
C(9)	35(1)	27(1)	29(1)	-2(1)	8(1)	-1(1)
C(10)	36(1)	26(1)	32(1)	0(1)	8(1)	0(1)
C(11)	55(1)	28(1)	35(1)	-4(1)	11(1)	1(1)
C(12)	62(1)	40(1)	31(1)	-7(1)	2(1)	-3(1)
C(13)	50(1)	50(1)	38(1)	-3(1)	-5(1)	4(1)
C(14)	42(1)	40(1)	37(1)	-3(1)	3(1)	7(1)
C(15)	42(1)	35(1)	34(1)	1(1)	4(1)	-4(1)
C(16)	65(1)	35(1)	46(1)	1(1)	-7(1)	0(1)
C(17)	61(1)	46(1)	60(1)	-11(1)	-16(1)	19(1)
C(18)	34(1)	62(1)	71(1)	-23(1)	2(1)	12(1)
C(19)	28(1)	51(1)	52(1)	-11(1)	11(1)	-4(1)
C(20)	52(1)	48(1)	35(1)	-3(1)	5(1)	-3(1)
C(21)	44(1)	63(1)	46(1)	4(1)	11(1)	-14(1)
C(22)	34(1)	62(1)	67(1)	-16(1)	7(1)	-12(1)
C(23)	52(1)	73(1)	59(1)	-9(1)	27(1)	-16(1)
C(24)	68(3)	50(3)	65(3)	7(2)	-1(3)	-9(3)
Cl(1)	49(1)	58(1)	52(1)	0(1)	12(1)	2(1)
Cl(2)	63(1)	79(1)	68(2)	-29(1)	7(1)	-7(1)
C(25)	74(6)	72(6)	71(6)	6(4)	11(4)	-23(4)
Cl(3)	86(2)	72(2)	152(4)	-26(2)	46(2)	-12(2)
Cl(4)	65(2)	73(1)	92(2)	2(1)	41(2)	2(1)
C(26)	73(9)	42(6)	45(6)	5(4)	-12(5)	-11(5)
Cl(5)	95(4)	104(4)	67(3)	-19(2)	-16(2)	6(2)
Cl(6)	95(4)	82(3)	215(8)	-77(5)	59(4)	-19(3)
C(27)	39(3)	36(3)	42(3)	1(2)	16(2)	-5(2)
Cl(7)	62(2)	40(1)	81(2)	0(1)	36(1)	5(1)
Cl(8)	83(3)	68(1)	112(4)	15(2)	61(3)	12(1)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $11 \cdot 2\text{CH}_2\text{Cl}_2$.

	x	y	z	U(eq)
H(4O)	-620(20)	4359(15)	2949(14)	62
H(1A)	1610	739	3466	68
H(1B)	262	575	3047	68
H(1C)	631	1484	3499	68
H(2A)	303	1471	838	40
H(2B)	-640	1168	1369	40
H	-302(15)	2822(11)	1592(11)	36
H(5)	4732	1593	1606	43
H(6)	5469	329	1051	50
H(7)	4352	-958	894	49
H(8)	2474	-1017	1268	43
H(11)	625	4725	4142	47
H(12)	2396	4384	5000	54
H(13)	3551	3201	4712	57
H(14)	2940	2367	3562	48
H(16A)	-481	4248	888	61
H(16B)	-783	4215	-65	61
H(17A)	-2653	3604	-17	71
H(17B)	-2505	4520	460	71
H(18A)	-3288	3437	1209	68
H(18B)	-2034	3779	1674	68
H(20A)	-405	2710	-755	68
H(20B)	-1670	2588	-491	68
H(20C)	-655	1863	-251	68
H(21A)	1287	3319	1091	76
H(21B)	1199	3485	155	76
H(21C)	1346	2505	503	76
H(22A)	-2339	1303	678	82
H(22B)	-2811	2141	145	82
H(22C)	-3512	1806	822	82
H(23A)	-1762	1538	2170	89
H(23B)	-2780	2238	2253	89
H(23C)	-1412	2504	2507	89
H(24A)	-4349	4294	-1368	75
H(24B)	-5628	3960	-1802	75
H(25A)	-5861	4029	2618	87
H(25B)	-6929	3391	2239	87
H(26A)	-5188	4192	-1833	67
H(26B)	-4044	4348	-1155	67
H(27A)	-6091	3846	2814	46
H(27B)	-6986	3316	2152	46