

Figure 1: Ortep plot of [(3,5-*t*Bu₂-*N*-CH=C(SiMe₃)-pz)AlCl₂] (2).

Table 1: Crystal data and structure refinement for 2.

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

Table 3: Bond lengths and angles for 2.

Table 4: Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2.

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

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

Figure 2: Ortep plot of [(3,5-*t*Bu₂-*N*-CH=C(SiMe₃)-pz)AlCl(η^2 -3,5-*t*Bu₂pz)] (3)

Table 6: Crystal data and structure refinement for 3.

Table 7: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 8: Bond lengths and angles for 3.

Table 9: Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3.

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

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

Figure 3: Ortep plot of [(3,5-*t*Bu₂-*N*-CH=C(SiMe₃)-*pz*)Al(η^2 -3,5-*t*Bu₂*pz*)₂] (**4**).

Table 11: Crystal data and structure refinement for **4**.

Table 12: 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.

Table 13: Bond lengths and angles for **4**.

Table 14: Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4**.

The anisotropic displacement factor exponent takes the form: -2

$$\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

Table 15: Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4**.

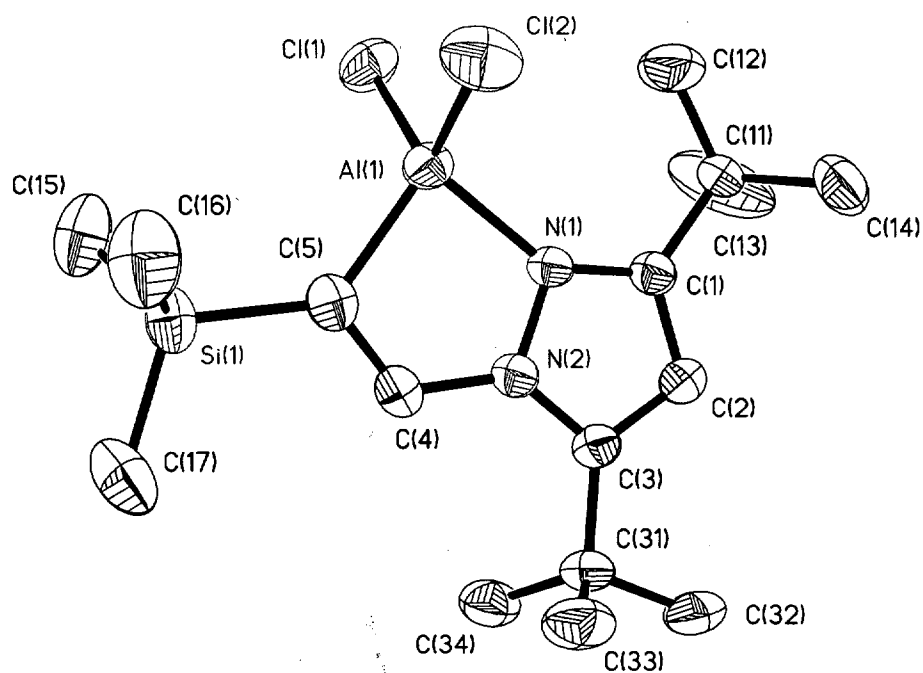


Figure 1: Ortep plot of $[(3,5\text{-}t\text{Bu}_2\text{-}N\text{-CH=C(SiMe}_3\text{)-pz)AlCl}_2]$ (**2**).

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

Identification code	roe883x	
Empirical formula	C ₁₆ H ₂₉ Al Cl ₂ N ₂ Si	
Formula weight	375.38	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.678(7) Å	α = 90°.
	b = 9.381(3) Å	β = 121.564(8)°.
	c = 18.093(5) Å	γ = 90°.
Volume	4292(2) Å ³	
Z	8	
Density (calculated)	1.162 Mg/m ³	
Absorption coefficient	0.398 mm ⁻¹	
F(000)	1600	
Crystal size	1.00 x 0.90 x 0.60 mm ³	
Theta range for data collection	3.75 to 25.06°.	
Index ranges	-35 ≤ h ≤ 35, -11 ≤ k ≤ 11, -21 ≤ l ≤ 21	
Reflections collected	8080	
Independent reflections	3785 [R(int) = 0.0807]	
Completeness to theta = 25.06°	99.3 %	
Max. and min. transmission	0.7961 and 0.6915	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3785 / 0 / 208	
Goodness-of-fit on F ²	1.033	
Final R indices [I > 2σ(I)]	R1 = 0.0524, wR2 = 0.1359	
R indices (all data)	R1 = 0.0574, wR2 = 0.1427	
Largest diff. peak and hole	0.403 and -0.542 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)
 For **2** (roe883x). U(eq) is defined as one third of the trace of the orthogonalized U^a tensor.

	x	y	z	U(eq)
Cl(1)	2041(1)	458(1)	650(1)	47(1)
Al(1)	1410(1)	360(1)	892(1)	34(1)
N(1)	1639(1)	-363(2)	2053(1)	32(1)
Si(1)	491(1)	-1884(1)	-723(1)	45(1)
C(1)	1952(1)	-155(2)	2910(1)	34(1)
Cl(2)	1034(1)	2379(1)	647(1)	60(1)
N(2)	1341(1)	-1564(2)	1953(1)	33(1)
C(2)	1854(1)	-1204(2)	3352(1)	39(1)
C(3)	1466(1)	-2086(2)	2739(1)	35(1)
C(4)	985(1)	-2024(2)	1075(1)	35(1)
C(5)	943(1)	-1293(2)	416(2)	37(1)
C(11)	2357(1)	1041(2)	3322(2)	39(1)
C(12)	2342(2)	2076(4)	2677(2)	84(1)
C(13)	2900(1)	354(4)	3805(4)	115(2)
C(14)	2264(2)	1806(5)	3956(3)	117(2)
C(15)	886(1)	-2057(4)	-1249(2)	68(1)
C(16)	-29(1)	-492(4)	-1287(2)	74(1)
C(17)	188(1)	-3647(4)	-762(2)	73(1)
C(31)	1211(1)	-3386(2)	2876(2)	41(1)
C(32)	1469(1)	-3595(3)	3860(2)	60(1)
C(33)	616(1)	-3124(3)	2473(2)	56(1)
C(34)	1313(1)	-4729(3)	2507(2)	50(1)

Table 3. Bond lengths [Å] and angles [°] for **2** (roe883x).

Cl(1)-Al(1)	2.1347(10)
Al(1)-C(5)	1.954(2)
Al(1)-N(1)	1.960(2)
Al(1)-Cl(2)	2.1243(10)
N(1)-C(1)	1.341(3)
N(1)-N(2)	1.385(2)
Si(1)-C(5)	1.861(2)
Si(1)-C(16)	1.863(3)
Si(1)-C(15)	1.864(3)
Si(1)-C(17)	1.866(3)
C(1)-C(2)	1.390(3)
C(1)-C(11)	1.524(3)
N(2)-C(3)	1.359(3)
N(2)-C(4)	1.439(3)
C(2)-C(3)	1.381(3)
C(3)-C(31)	1.522(3)
C(4)-C(5)	1.323(3)
C(11)-C(14)	1.497(4)
C(11)-C(12)	1.499(4)
C(11)-C(13)	1.516(5)
C(31)-C(34)	1.528(3)
C(31)-C(33)	1.537(4)
C(31)-C(32)	1.538(4)
C(5)-Al(1)-N(1)	88.03(9)
C(5)-Al(1)-Cl(2)	116.23(8)
N(1)-Al(1)-Cl(2)	112.43(6)
C(5)-Al(1)-Cl(1)	116.07(7)
N(1)-Al(1)-Cl(1)	112.67(6)
Cl(2)-Al(1)-Cl(1)	109.87(4)
C(1)-N(1)-N(2)	106.08(17)
C(1)-N(1)-Al(1)	146.25(15)
N(2)-N(1)-Al(1)	107.60(13)

C(5)-Si(1)-C(16)	108.00(13)
C(5)-Si(1)-C(15)	108.01(13)
C(16)-Si(1)-C(15)	110.01(17)
C(5)-Si(1)-C(17)	111.05(13)
C(16)-Si(1)-C(17)	110.93(17)
C(15)-Si(1)-C(17)	108.79(17)
N(1)-C(1)-C(2)	109.63(19)
N(1)-C(1)-C(11)	124.3(2)
C(2)-C(1)-C(11)	126.1(2)
C(3)-N(2)-N(1)	110.59(17)
C(3)-N(2)-C(4)	133.41(18)
N(1)-N(2)-C(4)	115.97(17)
C(3)-C(2)-C(1)	107.45(19)
N(2)-C(3)-C(2)	106.25(19)
N(2)-C(3)-C(31)	125.0(2)
C(2)-C(3)-C(31)	128.8(2)
C(5)-C(4)-N(2)	120.5(2)
C(4)-C(5)-Si(1)	121.09(18)
C(4)-C(5)-Al(1)	107.72(16)
Si(1)-C(5)-Al(1)	131.18(13)
C(14)-C(11)-C(12)	110.1(3)
C(14)-C(11)-C(13)	109.2(4)
C(12)-C(11)-C(13)	108.4(3)
C(14)-C(11)-C(1)	108.2(2)
C(12)-C(11)-C(1)	113.7(2)
C(13)-C(11)-C(1)	107.3(2)
C(3)-C(31)-C(34)	111.12(19)
C(3)-C(31)-C(33)	109.9(2)
C(34)-C(31)-C(33)	111.4(2)
C(3)-C(31)-C(32)	107.57(19)
C(34)-C(31)-C(32)	107.9(2)
C(33)-C(31)-C(32)	108.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2** (roe883x). 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}
Cl(1)	52(1)	53(1)	52(1)	6(1)	37(1)	5(1)
Al(1)	37(1)	31(1)	36(1)	2(1)	21(1)	4(1)
N(1)	35(1)	29(1)	35(1)	-2(1)	21(1)	-5(1)
Si(1)	40(1)	49(1)	35(1)	-6(1)	13(1)	7(1)
C(1)	35(1)	33(1)	37(1)	-4(1)	21(1)	-5(1)
Cl(2)	60(1)	39(1)	85(1)	9(1)	39(1)	15(1)
N(2)	35(1)	31(1)	36(1)	-3(1)	20(1)	-5(1)
C(2)	44(1)	42(1)	33(1)	-2(1)	22(1)	-9(1)
C(3)	38(1)	35(1)	38(1)	-1(1)	24(1)	-4(1)
C(4)	33(1)	34(1)	35(1)	-6(1)	16(1)	-2(1)
C(5)	34(1)	38(1)	38(1)	-4(1)	17(1)	4(1)
C(11)	47(1)	35(1)	39(1)	-8(1)	24(1)	-14(1)
C(12)	112(3)	77(2)	54(2)	-8(2)	38(2)	-58(2)
C(13)	52(2)	72(3)	161(5)	6(3)	14(3)	-24(2)
C(14)	195(5)	92(3)	145(4)	-82(3)	144(4)	-98(3)
C(15)	73(2)	88(2)	46(2)	-5(2)	32(2)	16(2)
C(16)	61(2)	83(2)	56(2)	0(2)	15(2)	27(2)
C(17)	63(2)	65(2)	67(2)	-20(2)	17(2)	-15(2)
C(31)	44(1)	37(1)	47(1)	-1(1)	29(1)	-10(1)
C(32)	76(2)	58(2)	52(2)	5(1)	38(2)	-22(1)
C(33)	48(2)	56(2)	78(2)	0(1)	43(2)	-8(1)
C(34)	58(2)	36(1)	64(2)	1(1)	36(1)	-5(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)
 For **2** (roe883x).

	x	y	z	U(eq)
H(2A)	2024	-1296	3964	47
H(4A)	777	-2858	967	42
H(12A)	2597	2843	2985	125
H(12B)	1986	2482	2331	125
H(12C)	2431	1581	2294	125
H(13A)	3172	1097	4068	173
H(13B)	2952	-207	3398	173
H(13C)	2927	-272	4259	173
H(14A)	2517	2593	4221	175
H(14B)	2312	1141	4410	175
H(14C)	1903	2184	3655	175
H(15A)	1027	-1122	-1267	102
H(15B)	659	-2417	-1842	102
H(15C)	1178	-2723	-916	102
H(16A)	138	411	-1286	111
H(16B)	-220	-367	-986	111
H(16C)	-276	-789	-1887	111
H(17A)	-17	-3571	-481	109
H(17B)	468	-4359	-457	109
H(17C)	-45	-3939	-1367	109
H(32A)	1850	-3744	4125	90
H(32B)	1313	-4429	3969	90
H(32C)	1408	-2746	4112	90
H(33A)	444	-3044	1842	84
H(33B)	563	-2240	2706	84
H(33C)	461	-3923	2614	84
H(34A)	1142	-4634	1877	75
H(34B)	1167	-5558	2641	75
H(34C)	1694	-4856	2768	75

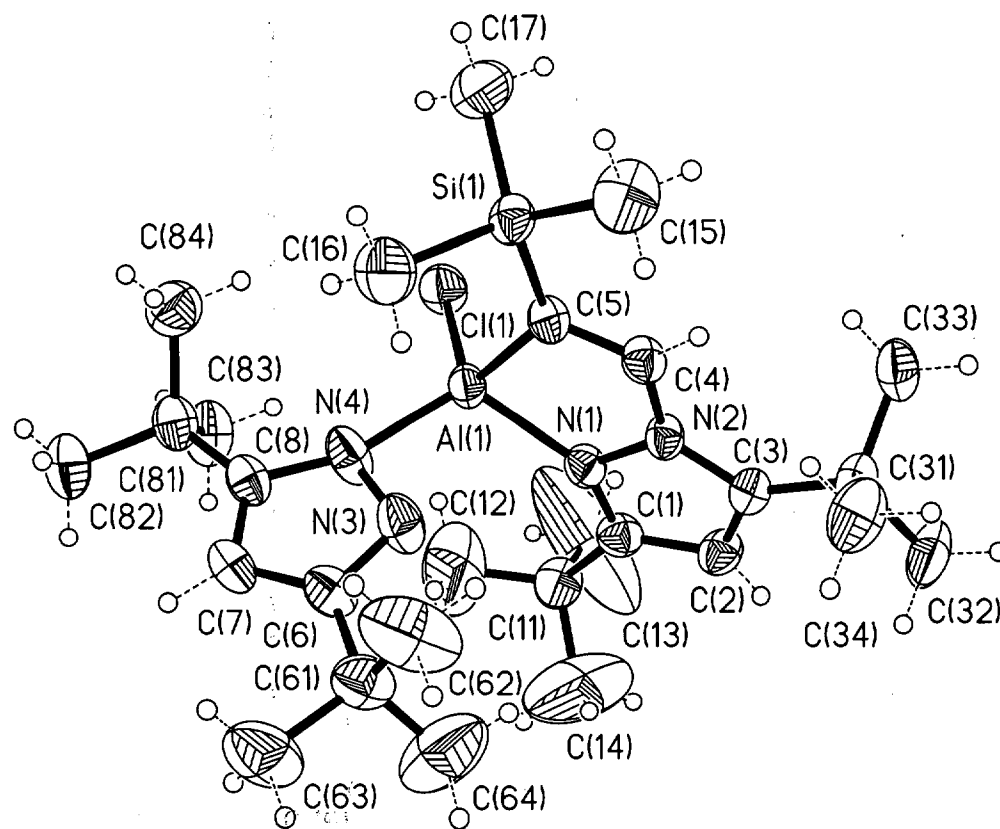


Figure 2: Ortep plot of [(3,5-*t*Bu₂-*N*-CH=C(SiMe₃)-pz)AlCl(η^2 -3,5-*t*Bu₂pz)] (3)

Table 6. Crystal data and structure refinement for **3** (roe892).

Identification code	roe892	
Empirical formula	C ₂₇ H ₄₈ Al Cl N ₄ Si	
Formula weight	519.21	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.2032(12) Å	$\alpha = 90^\circ$.
	b = 21.065(6) Å	$\beta = 105.961(12)^\circ$.
	c = 15.849(3) Å	$\gamma = 90^\circ$.
Volume	3275.2(11) Å ³	
Z	4	
Density (calculated)	1.053 Mg/m ³	
Absorption coefficient	0.200 mm ⁻¹	
F(000)	1128	
Crystal size	0.70 x 0.50 x 0.30 mm ³	
Theta range for data collection	3.57 to 25.03°	
Index ranges	-12 ≤ h ≤ 12, -6 ≤ k ≤ 25, -18 ≤ l ≤ 18	
Reflections collected	7790	
Independent reflections	5764 [R(int) = 0.0643]	
Completeness to theta = 25.03°	99.7 %	
Max. and min. transmission	0.9425 and 0.8728	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5764 / 0 / 322	
Goodness-of-fit on F ²	1.035	
Final R indices [I > 2σ(I)]	R1 = 0.0593, wR2 = 0.1458	
R indices (all data)	R1 = 0.0728, wR2 = 0.1573	
Largest diff. peak and hole	0.772 and -0.324 e.Å ⁻³	

Table 7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)
 For **3** (roe892). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^a tensor.

	x	y	z	$U(\text{eq})$
Al(1)	5164(1)	494(1)	6920(1)	34(1)
Cl(1)	3203(1)	176(1)	6132(1)	46(1)
Si(1)	6605(1)	1383(1)	5559(1)	37(1)
N(1)	6217(2)	-276(1)	7332(1)	34(1)
N(2)	7244(2)	-305(1)	6924(1)	31(1)
N(3)	6327(2)	1033(1)	8173(2)	49(1)
N(4)	4950(2)	1067(1)	7747(2)	47(1)
C(1)	6355(3)	-783(1)	7854(2)	39(1)
C(2)	7469(3)	-1140(1)	7774(2)	40(1)
C(3)	8021(3)	-833(1)	7192(2)	35(1)
C(4)	7334(3)	213(1)	6355(2)	35(1)
C(5)	6444(3)	682(1)	6230(2)	35(1)
C(6)	6558(3)	1429(1)	8847(2)	42(1)
C(7)	5334(3)	1722(1)	8868(2)	41(1)
C(8)	4332(3)	1485(1)	8165(2)	37(1)
C(11)	5415(3)	-926(1)	8436(2)	48(1)
C(12)	4589(7)	-366(3)	8545(5)	132(3)
C(13)	4516(11)	-1447(4)	8022(7)	256(7)
C(14)	6296(7)	-1097(6)	9316(4)	220(6)
C(15)	8216(4)	1362(2)	5224(3)	65(1)
C(16)	6578(4)	2101(2)	6237(2)	66(1)
C(17)	5148(4)	1412(2)	4562(2)	63(1)
C(31)	9254(3)	-1008(1)	6880(2)	42(1)
C(32)	9837(4)	-1635(2)	7330(3)	65(1)
C(33)	8861(4)	-1116(2)	5889(2)	59(1)
C(34)	10368(3)	-503(2)	7159(3)	67(1)
C(61)	7978(3)	1509(2)	9440(2)	54(1)
C(62)	8903(5)	1758(3)	8912(3)	106(2)
C(63)	7989(4)	1997(2)	10162(3)	83(1)
C(64)	8491(5)	884(2)	9878(4)	116(2)

C(81)	2824(3)	1630(1)	7860(2)	43(1)
C(82)	2463(4)	2139(2)	8447(2)	56(1)
C(83)	2002(3)	1027(2)	7906(2)	56(1)
C(84)	2453(4)	1872(2)	6909(2)	58(1)

Table 8. Bond lengths [Å] and angles [°] for **3** (roe892).

Al(1)-N(4)	1.838(2)
Al(1)-N(1)	1.956(2)
Al(1)-C(5)	1.961(3)
Al(1)-Cl(1)	2.1531(11)
Al(1)-N(3)	2.312(3)
Si(1)-C(17)	1.849(3)
Si(1)-C(5)	1.852(3)
Si(1)-C(16)	1.861(3)
Si(1)-C(15)	1.862(3)
N(1)-C(1)	1.335(3)
N(1)-N(2)	1.376(3)
N(2)-C(3)	1.364(3)
N(2)-C(4)	1.434(3)
N(3)-C(6)	1.326(4)
N(3)-N(4)	1.383(4)
N(4)-C(8)	1.358(3)
C(1)-C(2)	1.398(4)
C(1)-C(11)	1.532(4)
C(2)-C(3)	1.368(4)
C(3)-C(31)	1.518(4)
C(4)-C(5)	1.320(4)
C(6)-C(7)	1.402(4)
C(6)-C(61)	1.504(4)
C(7)-C(8)	1.382(4)
C(8)-C(81)	1.511(4)
C(11)-C(13)	1.465(7)
C(11)-C(14)	1.480(7)
C(11)-C(12)	1.488(6)
C(31)-C(33)	1.528(4)
C(31)-C(34)	1.529(4)
C(31)-C(32)	1.542(4)
C(61)-C(64)	1.515(6)
C(61)-C(62)	1.516(5)

C(61)-C(63)	1.536(5)
C(81)-C(82)	1.530(4)
C(81)-C(83)	1.535(4)
C(81)-C(84)	1.537(4)
N(4)-Al(1)-N(1)	117.91(11)
N(4)-Al(1)-C(5)	119.52(11)
N(1)-Al(1)-C(5)	87.99(10)
N(4)-Al(1)-Cl(1)	110.11(9)
N(1)-Al(1)-Cl(1)	105.87(8)
C(5)-Al(1)-Cl(1)	113.27(9)
N(4)-Al(1)-N(3)	36.75(10)
N(1)-Al(1)-N(3)	90.86(10)
C(5)-Al(1)-N(3)	96.67(10)
Cl(1)-Al(1)-N(3)	145.73(7)
C(17)-Si(1)-C(5)	109.89(15)
C(17)-Si(1)-C(16)	109.30(17)
C(5)-Si(1)-C(16)	107.33(14)
C(17)-Si(1)-C(15)	108.85(19)
C(5)-Si(1)-C(15)	111.67(14)
C(16)-Si(1)-C(15)	109.77(19)
C(1)-N(1)-N(2)	107.0(2)
C(1)-N(1)-Al(1)	145.59(18)
N(2)-N(1)-Al(1)	107.43(15)
C(3)-N(2)-N(1)	110.0(2)
C(3)-N(2)-C(4)	133.1(2)
N(1)-N(2)-C(4)	116.76(19)
C(6)-N(3)-N(4)	107.0(2)
C(6)-N(3)-Al(1)	159.6(2)
N(4)-N(3)-Al(1)	52.66(13)
C(8)-N(4)-N(3)	110.0(2)
C(8)-N(4)-Al(1)	159.4(2)
N(3)-N(4)-Al(1)	90.59(16)
N(1)-C(1)-C(2)	108.9(2)
N(1)-C(1)-C(11)	123.7(2)

C(2)-C(1)-C(11)	127.5(2)
C(3)-C(2)-C(1)	107.7(2)
N(2)-C(3)-C(2)	106.5(2)
N(2)-C(3)-C(31)	124.0(2)
C(2)-C(3)-C(31)	129.5(2)
C(5)-C(4)-N(2)	120.3(2)
C(4)-C(5)-Si(1)	121.1(2)
C(4)-C(5)-Al(1)	107.51(19)
Si(1)-C(5)-Al(1)	131.24(14)
N(3)-C(6)-C(7)	109.5(3)
N(3)-C(6)-C(61)	120.1(3)
C(7)-C(6)-C(61)	130.4(3)
C(8)-C(7)-C(6)	106.8(2)
N(4)-C(8)-C(7)	106.7(2)
N(4)-C(8)-C(81)	122.9(2)
C(7)-C(8)-C(81)	130.3(2)
C(13)-C(11)-C(14)	112.6(7)
C(13)-C(11)-C(12)	110.0(6)
C(14)-C(11)-C(12)	107.4(5)
C(13)-C(11)-C(1)	107.2(3)
C(14)-C(11)-C(1)	107.3(3)
C(12)-C(11)-C(1)	112.4(3)
C(3)-C(31)-C(33)	111.3(2)
C(3)-C(31)-C(34)	110.7(2)
C(33)-C(31)-C(34)	111.5(3)
C(3)-C(31)-C(32)	107.8(2)
C(33)-C(31)-C(32)	107.8(3)
C(34)-C(31)-C(32)	107.5(3)
C(6)-C(61)-C(64)	109.9(3)
C(6)-C(61)-C(62)	109.4(3)
C(64)-C(61)-C(62)	111.5(4)
C(6)-C(61)-C(63)	110.4(3)
C(64)-C(61)-C(63)	108.0(4)
C(62)-C(61)-C(63)	107.6(3)
C(8)-C(81)-C(82)	109.9(2)

C(8)-C(81)-C(83)	109.8(2)
C(82)-C(81)-C(83)	109.0(2)
C(8)-C(81)-C(84)	109.5(2)
C(82)-C(81)-C(84)	109.2(3)
C(83)-C(81)-C(84)	109.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3** (roe892). 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}
Al(1)	32(1)	34(1)	36(1)	-4(1)	12(1)	4(1)
Cl(1)	40(1)	50(1)	46(1)	-11(1)	6(1)	-4(1)
Si(1)	42(1)	28(1)	43(1)	2(1)	14(1)	1(1)
N(1)	35(1)	37(1)	35(1)	2(1)	16(1)	1(1)
N(2)	30(1)	31(1)	36(1)	1(1)	14(1)	2(1)
N(3)	39(1)	55(2)	56(2)	-19(1)	20(1)	-6(1)
N(4)	39(1)	55(2)	51(1)	-24(1)	18(1)	-9(1)
C(1)	40(2)	43(2)	36(1)	3(1)	13(1)	-2(1)
C(2)	40(2)	35(1)	46(2)	9(1)	15(1)	4(1)
C(3)	33(1)	32(1)	40(1)	1(1)	10(1)	2(1)
C(4)	37(1)	34(1)	37(1)	2(1)	17(1)	-1(1)
C(5)	37(1)	31(1)	38(1)	-4(1)	13(1)	-1(1)
C(6)	44(2)	46(2)	39(2)	-5(1)	18(1)	-12(1)
C(7)	49(2)	39(2)	40(2)	-10(1)	22(1)	-9(1)
C(8)	42(2)	34(1)	41(1)	-5(1)	22(1)	-7(1)
C(11)	50(2)	47(2)	53(2)	15(1)	26(1)	3(1)
C(12)	149(6)	134(5)	166(6)	59(4)	131(5)	47(4)
C(13)	334(12)	225(8)	333(12)	-171(9)	298(12)	-217(9)
C(14)	123(5)	454(15)	110(5)	157(8)	79(4)	93(8)
C(15)	62(2)	56(2)	88(3)	19(2)	38(2)	-4(2)
C(16)	92(3)	37(2)	65(2)	-8(2)	16(2)	0(2)
C(17)	68(2)	53(2)	59(2)	1(2)	1(2)	5(2)
C(31)	34(2)	41(2)	56(2)	6(1)	18(1)	8(1)
C(32)	57(2)	57(2)	90(3)	22(2)	33(2)	28(2)
C(33)	56(2)	66(2)	64(2)	-1(2)	31(2)	19(2)
C(34)	36(2)	70(2)	96(3)	4(2)	19(2)	-1(2)
C(61)	43(2)	70(2)	47(2)	-4(2)	11(1)	-10(2)
C(62)	57(3)	189(6)	74(3)	-19(3)	24(2)	-50(3)
C(63)	68(3)	109(3)	65(2)	-29(2)	6(2)	-22(2)
C(64)	81(3)	95(4)	138(5)	10(3)	-27(3)	3(3)

C(81)	41(2)	41(2)	52(2)	-4(1)	21(1)	-3(1)
C(82)	56(2)	50(2)	72(2)	-8(2)	32(2)	3(2)
C(83)	43(2)	51(2)	83(2)	-6(2)	29(2)	-7(1)
C(84)	55(2)	61(2)	58(2)	3(2)	14(2)	4(2)

Table 10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3** (roe892).

	x	y	z	U(eq)
H(2A)	7783	-1522	8066	48
H(4A)	8029	218	6070	42
H(7A)	5217	2021	9281	49
H(12A)	3942	-265	7988	199
H(12B)	5186	-5	8743	199
H(12C)	4101	-462	8975	199
H(13A)	4467	-1464	7402	385
H(13B)	3612	-1377	8091	385
H(13C)	4875	-1845	8298	385
H(14A)	7134	-854	9438	330
H(14B)	6506	-1547	9331	330
H(14C)	5823	-1002	9755	330
H(15A)	8273	1737	4881	98
H(15B)	8228	985	4874	98
H(15C)	8988	1352	5743	98
H(16A)	6604	2479	5892	99
H(16B)	7365	2097	6747	99
H(16C)	5751	2102	6426	99
H(17A)	5237	1780	4214	94
H(17B)	4304	1442	4729	94
H(17C)	5137	1030	4219	94
H(32A)	10649	-1749	7159	98
H(32B)	9161	-1968	7153	98
H(32C)	10068	-1583	7962	98
H(33A)	9666	-1232	5711	89
H(33B)	8473	-730	5590	89
H(33C)	8195	-1456	5737	89
H(34A)	11168	-637	6989	100
H(34B)	10603	-449	7791	100

H(34C)	10038	-104	6876	100
H(62A)	9814	1820	9297	159
H(62B)	8553	2160	8644	159
H(62C)	8934	1455	8458	159
H(63A)	8909	2040	10542	125
H(63B)	7389	1854	10504	125
H(63C)	7676	2404	9896	125
H(64A)	9358	950	10313	174
H(64B)	8609	584	9441	174
H(64C)	7834	717	10162	174
H(82A)	1497	2234	8243	84
H(82B)	2985	2521	8425	84
H(82C)	2680	1986	9047	84
H(83A)	1036	1121	7707	85
H(83B)	2228	876	8507	85
H(83C)	2225	702	7535	85
H(84A)	1494	1983	6724	87
H(84B)	2635	1542	6530	87
H(84C)	2997	2244	6875	87

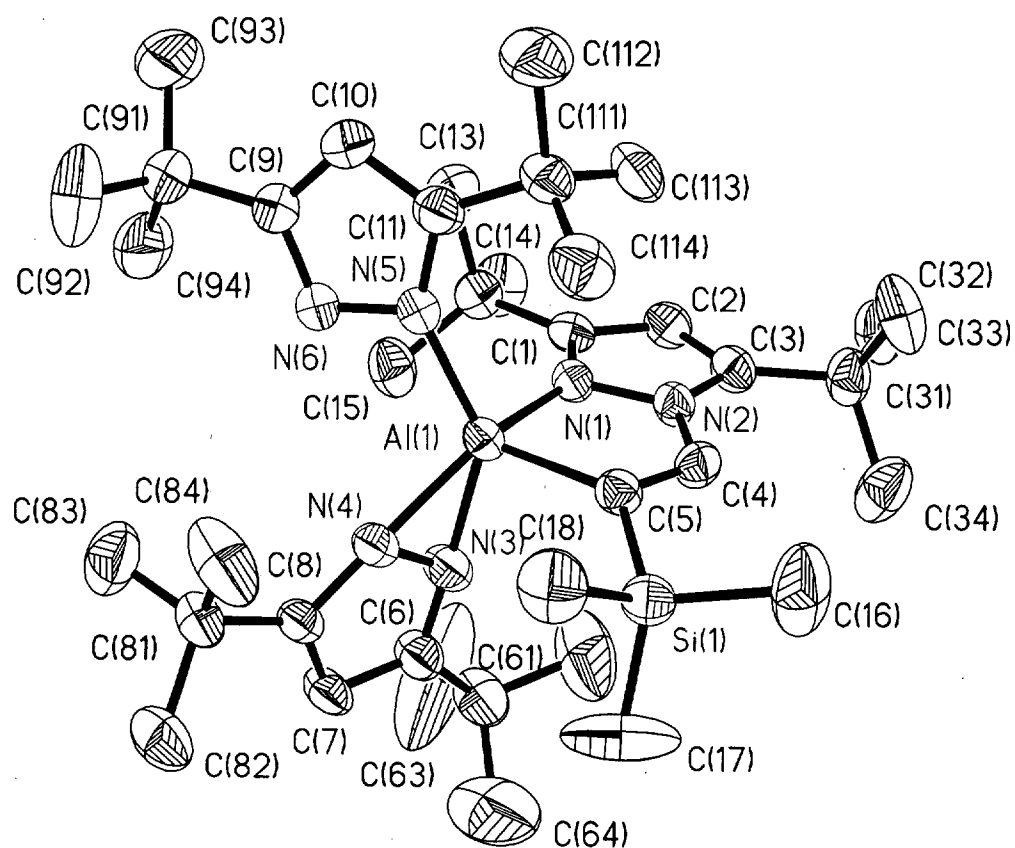


Figure 3: Ortep plot of $[(3,5\text{-}t\text{Bu}_2\text{-}N\text{-CH=C(SiMe}_3\text{)-pz)Al}(\eta^2\text{-}3,5\text{-}t\text{Bu}_2\text{pz})_2]$ (**4**).

Table 11. Crystal data and structure refinement for **4** (roe893x).

Identification code	roe893x	
Empirical formula	C ₃₈ H ₆₇ Al N ₆ Si	
Formula weight	663.05	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 19.888(5) Å	α = 90°.
	b = 11.5236(18) Å	β = 98.828(19)°.
	c = 18.789(3) Å	γ = 90°.
Volume	4255.1(14) Å ³	
Z	4	
Density (calculated)	1.035 Mg/m ³	
Absorption coefficient	0.107 mm ⁻¹	
F(000)	1456	
Crystal size	0.90 x 0.40 x 0.30 mm ³	
Theta range for data collection	3.52 to 25.03°	
Index ranges	-5 ≤ h ≤ 23, -13 ≤ k ≤ 2, -22 ≤ l ≤ 22	
Reflections collected	7510	
Independent reflections	7496 [R(int) = 0.1458]	
Completeness to theta = 25.03°	99.6 %	
Max. and min. transmission	0.9687 and 0.9101	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7496 / 0 / 437	
Goodness-of-fit on F ²	1.050	
Final R indices [I > 2σ(I)]	R1 = 0.0642, wR2 = 0.1440	
R indices (all data)	R1 = 0.0989, wR2 = 0.1708	
Extinction coefficient	0.0005(4)	
Largest diff. peak and hole	0.480 and -0.358 e.Å ⁻³	

Table 12. Atomic coordinates ($\times 10^3$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)
 For **4** (roe893x) $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{p} tensor.

	x	y	z	$U(\text{eq})$
Al(1)	2613(1)	5220(1)	1150(1)	32(1)
Si(1)	3996(1)	7003(1)	962(1)	43(1)
N(1)	2234(1)	4546(2)	192(1)	34(1)
N(2)	2571(1)	5039(2)	-316(1)	35(1)
N(3)	3240(1)	3887(2)	1435(1)	45(1)
N(4)	3081(1)	4542(2)	2006(1)	40(1)
N(5)	1836(1)	5943(2)	1415(1)	37(1)
N(6)	1587(1)	5206(2)	1902(1)	40(1)
C(1)	1794(1)	3776(2)	-152(2)	35(1)
C(2)	1850(2)	3793(3)	-884(2)	40(1)
C(3)	2339(2)	4593(3)	-982(1)	37(1)
C(4)	3096(1)	5857(3)	-61(2)	38(1)
C(5)	3216(1)	6148(2)	632(1)	35(1)
C(6)	3690(2)	3079(3)	1695(2)	45(1)
C(7)	3820(2)	3196(3)	2441(2)	45(1)
C(8)	3430(1)	4121(2)	2618(2)	36(1)
C(9)	991(2)	5638(3)	2013(2)	43(1)
C(10)	845(2)	6647(3)	1610(2)	49(1)
C(11)	1376(2)	6829(3)	1235(2)	40(1)
C(12)	1312(2)	3060(3)	224(2)	42(1)
C(13)	692(2)	3809(3)	301(2)	56(1)
C(14)	1089(2)	1995(3)	-244(2)	61(1)
C(15)	1656(2)	2639(3)	967(2)	54(1)
C(16)	4200(2)	8000(5)	245(2)	95(2)
C(17)	4696(2)	5957(4)	1236(3)	108(2)
C(18)	3896(2)	7900(3)	1757(2)	65(1)
C(31)	2579(2)	4981(3)	-1675(2)	48(1)
C(32)	2400(2)	6257(3)	-1815(2)	68(1)
C(33)	2201(2)	4252(3)	-2302(2)	58(1)
C(34)	3345(2)	4759(4)	-1652(2)	72(1)

C(61)	3982(2)	2251(3)	1202(2)	62(1)
C(62)	3875(3)	2734(4)	437(2)	107(2)
C(63)	3678(5)	1105(4)	1226(4)	206(5)
C(64)	4756(3)	2229(7)	1428(3)	152(3)
C(81)	3357(2)	4610(3)	3349(2)	43(1)
C(82)	4025(2)	4448(3)	3854(2)	62(1)
C(83)	2795(2)	3945(4)	3647(2)	76(1)
C(84)	3176(3)	5891(3)	3288(2)	83(2)
C(91)	571(2)	5055(3)	2519(2)	55(1)
C(92)	735(3)	5640(5)	3260(2)	102(2)
C(93)	-178(2)	5159(5)	2222(3)	111(2)
C(94)	756(2)	3780(4)	2612(2)	75(1)
C(111)	1454(2)	7780(3)	700(2)	46(1)
C(112)	882(2)	8678(3)	707(2)	76(1)
C(113)	1399(2)	7285(3)	-61(2)	59(1)
C(114)	2133(2)	8407(3)	894(2)	59(1)

Table 13. Bond lengths [Å] and angles [°] for 4 (roe893x).

Al(1)-N(5)	1.889(2)
Al(1)-N(4)	1.899(2)
Al(1)-C(5)	1.970(3)
Al(1)-N(3)	1.999(3)
Al(1)-N(1)	1.999(2)
Si(1)-C(17)	1.853(4)
Si(1)-C(18)	1.852(4)
Si(1)-C(5)	1.862(3)
Si(1)-C(16)	1.863(4)
N(1)-C(1)	1.340(3)
N(1)-N(2)	1.372(3)
N(2)-C(3)	1.366(3)
N(2)-C(4)	1.433(4)
N(3)-C(6)	1.332(4)
N(3)-N(4)	1.388(3)
N(4)-C(8)	1.338(3)
N(5)-C(11)	1.378(4)
N(5)-N(6)	1.393(3)
N(6)-C(9)	1.331(4)
C(1)-C(2)	1.398(4)
C(1)-C(12)	1.519(4)
C(2)-C(3)	1.372(4)
C(3)-C(31)	1.522(4)
C(4)-C(5)	1.331(4)
C(6)-C(7)	1.391(4)
C(6)-C(61)	1.508(4)
C(7)-C(8)	1.388(4)
C(8)-C(81)	1.513(4)
C(9)-C(10)	1.394(4)
C(9)-C(91)	1.515(4)
C(10)-C(11)	1.372(4)
C(11)-C(111)	1.512(4)
C(12)-C(13)	1.530(4)

C(12)-C(14)	1.535(4)
C(12)-C(15)	1.537(4)
C(31)-C(32)	1.527(5)
C(31)-C(34)	1.539(5)
C(31)-C(33)	1.544(4)
C(61)-C(63)	1.456(7)
C(61)-C(62)	1.525(5)
C(61)-C(64)	1.533(7)
C(81)-C(82)	1.520(5)
C(81)-C(84)	1.520(5)
C(81)-C(83)	1.530(5)
C(91)-C(93)	1.513(5)
C(91)-C(94)	1.518(5)
C(91)-C(92)	1.536(5)
C(111)-C(114)	1.527(5)
C(111)-C(113)	1.527(5)
C(111)-C(112)	1.538(5)
N(5)-Al(1)-N(4)	105.84(11)
N(5)-Al(1)-C(5)	118.38(12)
N(4)-Al(1)-C(5)	112.69(12)
N(5)-Al(1)-N(3)	140.38(11)
N(4)-Al(1)-N(3)	41.62(10)
C(5)-Al(1)-N(3)	98.50(12)
N(5)-Al(1)-N(1)	101.38(10)
N(4)-Al(1)-N(1)	132.13(11)
C(5)-Al(1)-N(1)	86.59(11)
N(3)-Al(1)-N(1)	94.34(10)
C(17)-Si(1)-C(18)	107.9(2)
C(17)-Si(1)-C(5)	107.50(17)
C(18)-Si(1)-C(5)	112.13(15)
C(17)-Si(1)-C(16)	111.4(3)
C(18)-Si(1)-C(16)	107.5(2)
C(5)-Si(1)-C(16)	110.39(16)
C(1)-N(1)-N(2)	106.9(2)

C(1)-N(1)-Al(1)	145.08(19)
N(2)-N(1)-Al(1)	107.95(16)
C(3)-N(2)-N(1)	110.4(2)
C(3)-N(2)-C(4)	132.9(2)
N(1)-N(2)-C(4)	116.7(2)
C(6)-N(3)-N(4)	108.4(2)
C(6)-N(3)-Al(1)	172.8(2)
N(4)-N(3)-Al(1)	65.33(14)
C(8)-N(4)-N(3)	108.5(2)
C(8)-N(4)-Al(1)	176.7(2)
N(3)-N(4)-Al(1)	73.06(15)
C(11)-N(5)-N(6)	108.9(2)
C(11)-N(5)-Al(1)	143.3(2)
N(6)-N(5)-Al(1)	107.00(17)
C(9)-N(6)-N(5)	106.8(2)
N(1)-C(1)-C(2)	108.7(2)
N(1)-C(1)-C(12)	123.2(2)
C(2)-C(1)-C(12)	128.0(3)
C(3)-C(2)-C(1)	107.8(3)
N(2)-C(3)-C(2)	106.1(2)
N(2)-C(3)-C(31)	124.5(3)
C(2)-C(3)-C(31)	129.3(3)
C(5)-C(4)-N(2)	120.3(3)
C(4)-C(5)-Si(1)	118.3(2)
C(4)-C(5)-Al(1)	108.4(2)
Si(1)-C(5)-Al(1)	131.41(15)
N(3)-C(6)-C(7)	108.2(3)
N(3)-C(6)-C(61)	121.1(3)
C(7)-C(6)-C(61)	130.7(3)
C(8)-C(7)-C(6)	107.0(3)
N(4)-C(8)-C(7)	107.9(2)
N(4)-C(8)-C(81)	122.4(3)
C(7)-C(8)-C(81)	129.6(3)
N(6)-C(9)-C(10)	110.0(3)
N(6)-C(9)-C(91)	121.5(3)

C(10)-C(9)-C(91)	128.5(3)
C(11)-C(10)-C(9)	107.1(3)
C(10)-C(11)-N(5)	107.2(3)
C(10)-C(11)-C(111)	128.1(3)
N(5)-C(11)-C(111)	124.7(3)
C(1)-C(12)-C(13)	108.2(3)
C(1)-C(12)-C(14)	108.5(3)
C(13)-C(12)-C(14)	109.8(3)
C(1)-C(12)-C(15)	111.7(3)
C(13)-C(12)-C(15)	110.2(3)
C(14)-C(12)-C(15)	108.5(3)
C(3)-C(31)-C(32)	109.5(3)
C(3)-C(31)-C(34)	111.5(3)
C(32)-C(31)-C(34)	111.6(3)
C(3)-C(31)-C(33)	108.2(3)
C(32)-C(31)-C(33)	108.6(3)
C(34)-C(31)-C(33)	107.2(3)
C(63)-C(61)-C(6)	110.7(3)
C(63)-C(61)-C(62)	111.2(5)
C(6)-C(61)-C(62)	109.8(3)
C(63)-C(61)-C(64)	112.3(5)
C(6)-C(61)-C(64)	107.7(3)
C(62)-C(61)-C(64)	104.8(4)
C(8)-C(81)-C(82)	109.0(3)
C(8)-C(81)-C(84)	110.3(3)
C(82)-C(81)-C(84)	109.9(3)
C(8)-C(81)-C(83)	108.8(3)
C(82)-C(81)-C(83)	109.1(3)
C(84)-C(81)-C(83)	109.7(3)
C(93)-C(91)-C(9)	109.8(3)
C(93)-C(91)-C(94)	109.1(4)
C(9)-C(91)-C(94)	110.7(3)
C(93)-C(91)-C(92)	111.1(4)
C(9)-C(91)-C(92)	108.3(3)
C(94)-C(91)-C(92)	107.8(4)

C(11)-C(111)-C(114)	111.1(3)
C(11)-C(111)-C(113)	110.6(3)
C(114)-C(111)-C(113)	109.5(3)
C(11)-C(111)-C(112)	109.3(3)
C(114)-C(111)-C(112)	107.9(3)
C(113)-C(111)-C(112)	108.2(3)

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4** (roe893x). 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}
Al(1)	32(1)	37(1)	26(1)	2(1)	0(1)	2(1)
Si(1)	35(1)	52(1)	39(1)	-2(1)	-2(1)	-9(1)
N(1)	33(1)	36(1)	31(1)	4(1)	3(1)	-1(1)
N(2)	34(1)	41(1)	28(1)	1(1)	2(1)	-5(1)
N(3)	45(2)	52(2)	36(1)	0(1)	-1(1)	10(1)
N(4)	38(1)	47(2)	34(1)	4(1)	2(1)	9(1)
N(5)	36(1)	42(1)	31(1)	5(1)	5(1)	3(1)
N(6)	38(1)	46(2)	35(1)	7(1)	7(1)	3(1)
C(1)	32(2)	33(2)	37(2)	-2(1)	-1(1)	1(1)
C(2)	41(2)	44(2)	34(2)	-5(1)	-2(1)	-3(1)
C(3)	42(2)	38(2)	31(2)	-2(1)	1(1)	1(1)
C(4)	32(2)	44(2)	38(2)	1(1)	5(1)	-8(1)
C(5)	34(2)	38(2)	32(2)	-1(1)	2(1)	0(1)
C(6)	50(2)	46(2)	37(2)	1(1)	4(1)	11(2)
C(7)	52(2)	48(2)	34(2)	6(1)	-2(1)	17(2)
C(8)	35(2)	38(2)	33(2)	4(1)	0(1)	3(1)
C(9)	38(2)	53(2)	37(2)	4(1)	7(1)	2(2)
C(10)	41(2)	56(2)	50(2)	7(2)	12(2)	12(2)
C(11)	39(2)	41(2)	38(2)	1(1)	2(1)	6(1)
C(12)	43(2)	39(2)	45(2)	-2(1)	4(1)	-7(1)
C(13)	43(2)	65(2)	62(2)	2(2)	10(2)	-6(2)
C(14)	69(2)	51(2)	64(2)	-11(2)	11(2)	-23(2)
C(15)	65(2)	50(2)	48(2)	9(2)	7(2)	-11(2)
C(16)	93(3)	133(4)	56(2)	6(3)	6(2)	-72(3)
C(17)	47(2)	82(3)	175(5)	-42(3)	-42(3)	15(2)
C(18)	69(3)	66(2)	57(2)	-13(2)	1(2)	-20(2)
C(31)	54(2)	61(2)	30(2)	-4(2)	8(1)	-11(2)
C(32)	108(3)	56(2)	37(2)	7(2)	5(2)	-15(2)
C(33)	75(3)	65(2)	32(2)	-6(2)	6(2)	-11(2)
C(34)	61(2)	106(3)	53(2)	-20(2)	23(2)	-18(2)

C(61)	80(3)	61(2)	46(2)	-4(2)	10(2)	32(2)
C(62)	179(6)	95(4)	53(3)	-10(2)	37(3)	39(4)
C(63)	378(12)	43(3)	260(9)	-46(4)	251(9)	-23(5)
C(64)	116(5)	244(8)	95(4)	-47(5)	9(3)	108(5)
C(81)	55(2)	41(2)	33(2)	2(1)	4(1)	5(2)
C(82)	72(3)	68(2)	41(2)	-7(2)	-8(2)	3(2)
C(83)	76(3)	103(3)	55(2)	-16(2)	27(2)	-13(3)
C(84)	144(4)	54(2)	47(2)	-5(2)	-2(2)	32(3)
C(91)	45(2)	74(2)	48(2)	10(2)	15(2)	4(2)
C(92)	146(5)	113(4)	60(3)	-7(3)	53(3)	-23(4)
C(93)	43(2)	173(5)	121(4)	72(4)	27(2)	3(3)
C(94)	70(3)	76(3)	84(3)	24(2)	28(2)	-6(2)
C(111)	44(2)	42(2)	50(2)	12(2)	4(1)	9(2)
C(112)	66(3)	63(2)	103(3)	34(2)	21(2)	25(2)
C(113)	62(2)	66(2)	45(2)	21(2)	-3(2)	4(2)
C(114)	64(2)	46(2)	65(2)	7(2)	5(2)	-2(2)

Table 15. Hydrogen coordinates ($\times 10^3$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)
 For **4** (roe893x).

	x	y	z	U(eq)
H(2A)	1595	3333	-1250	48
H(4A)	3360	6193	-388	46
H(7A)	4118	2732	2767	55
H(10A)	452	7121	1597	58
H(13A)	838	4491	597	84
H(13B)	369	3355	532	84
H(13C)	472	4062	-176	84
H(14A)	850	2249	-713	92
H(14B)	784	1515	-4	92
H(14C)	1490	1540	-312	92
H(15A)	1766	3308	1286	81
H(15B)	2075	2221	916	81
H(15C)	1347	2120	1174	81
H(16A)	3814	8519	97	142
H(16B)	4291	7545	-170	142
H(16C)	4603	8461	431	142
H(17A)	4576	5450	1616	161
H(17B)	5114	6382	1417	161
H(17C)	4768	5487	820	161
H(18A)	3735	7412	2123	98
H(18B)	3566	8519	1612	98
H(18C)	4336	8243	1956	98
H(32A)	1907	6362	-1842	102
H(32B)	2539	6498	-2270	102
H(32C)	2637	6730	-1421	102
H(33A)	1710	4386	-2339	86
H(33B)	2298	3428	-2210	86
H(33C)	2354	4481	-2753	86
H(34A)	3604	5266	-1290	108

H(34B)	3472	4925	-2125	108
H(34C)	3448	3947	-1525	108
H(62A)	3388	2745	248	161
H(62B)	4113	2242	130	161
H(62C)	4057	3525	442	161
H(63A)	3201	1134	995	309
H(63B)	3700	861	1729	309
H(63C)	3928	549	971	309
H(64A)	4866	1832	1893	229
H(64B)	4929	3026	1472	229
H(64C)	4966	1814	1064	229
H(82A)	4391	4844	3655	93
H(82B)	4129	3618	3906	93
H(82C)	3985	4777	4327	93
H(83A)	2372	3996	3305	114
H(83B)	2726	4284	4109	114
H(83C)	2928	3129	3718	114
H(84A)	3540	6316	3104	125
H(84B)	3123	6194	3764	125
H(84C)	2749	5990	2957	125
H(92A)	609	6462	3217	154
H(92B)	1223	5571	3437	154
H(92C)	478	5259	3599	154
H(93A)	-298	5980	2149	166
H(93B)	-447	4818	2564	166
H(93C)	-273	4747	1762	166
H(94A)	634	3378	2151	113
H(94B)	507	3434	2970	113
H(94C)	1246	3705	2775	113
H(11A)	922	9032	1186	115
H(11B)	440	8292	592	115
H(11C)	922	9281	348	115
H(11D)	1763	6717	-78	88
H(11E)	1442	7914	-402	88
H(11F)	956	6905	-191	88

H(11G)	2507	7853	890	88
H(11H)	2161	8749	1375	88
H(11I)	2169	9022	542	88
