

Organoaluminum(III) complexes of the bis-N,N'-(2,6-diisopropylphenyl)imidazolin-2-imine ligand

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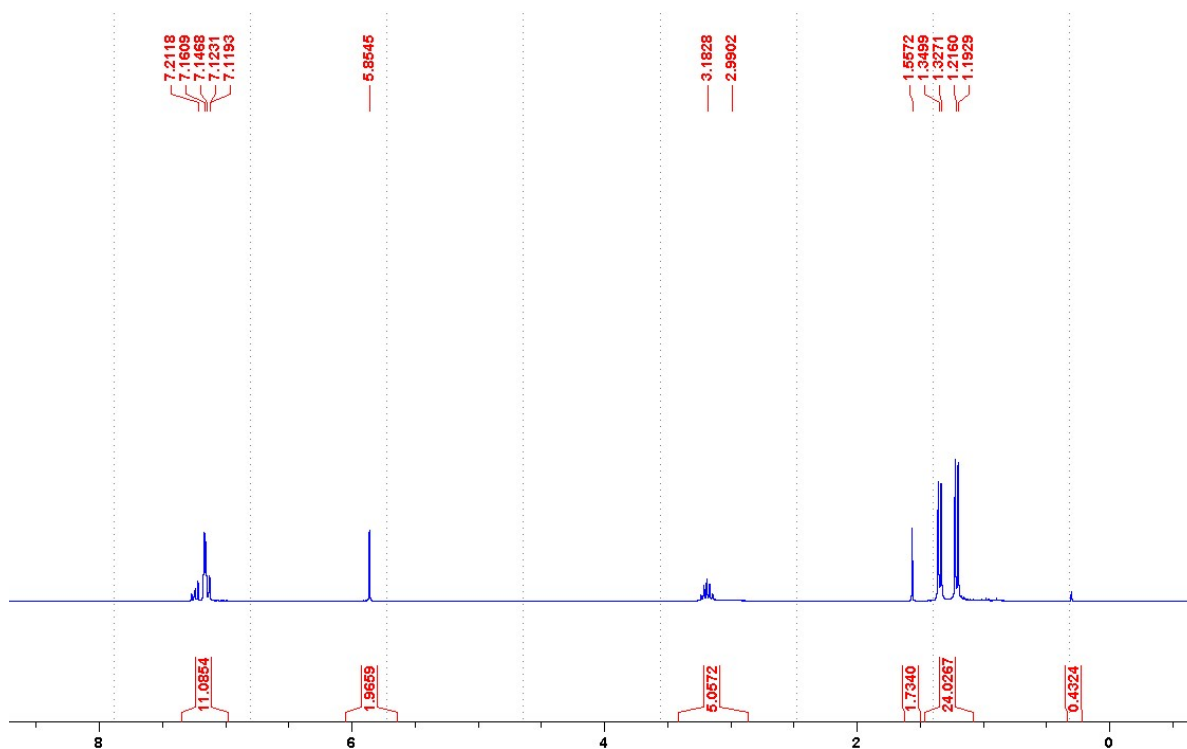
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Supporting Information

¹H NMR Spectra for compounds 1, 2, 3 and 5	S2
¹³C NMR Spectra for compounds 2, 3 and 5	S4
Crystallography tables for compound 2	S7
Crystallography tables for compound 3	S25
Crystallography tables for compound 4	S45
Crystallography tables for compound 5	S93
Crystallography tables for compound 6	S106
Crystallography tables for compound 7	S127

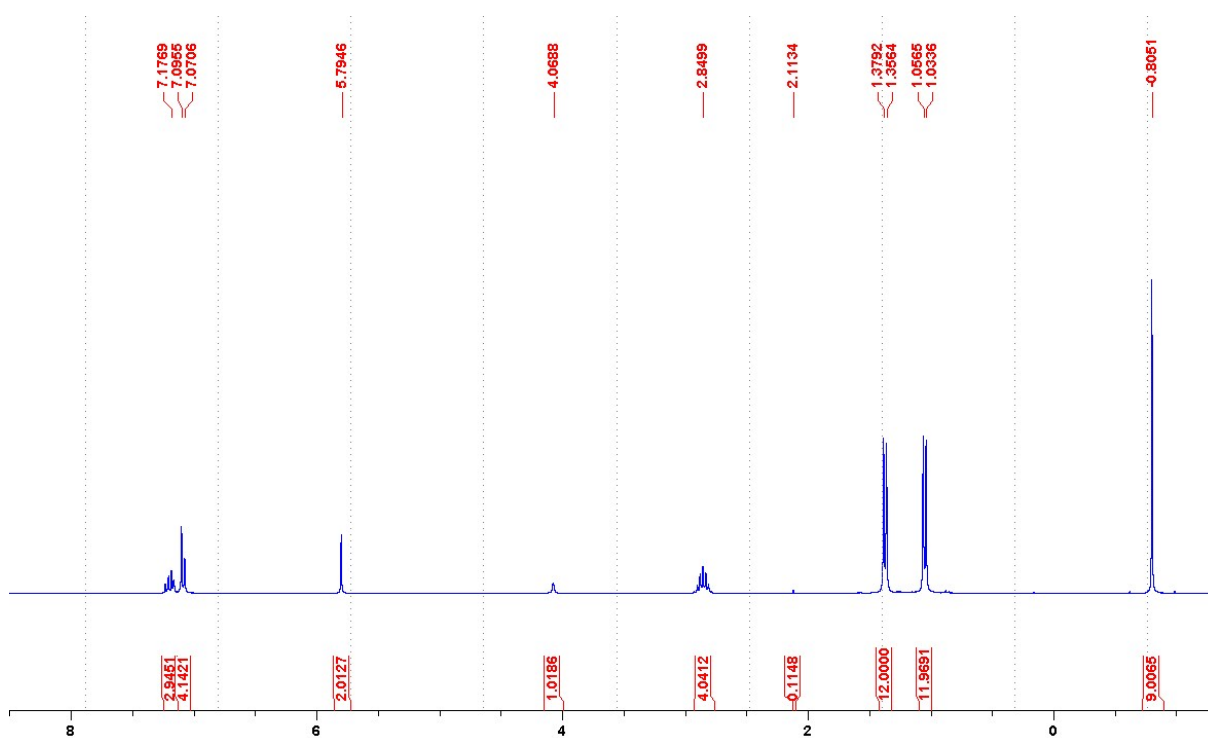
¹H NMR Spectra for compounds 1, 2, 3 and 5
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Ligand 1 (iPrNH)* in C₆D₆

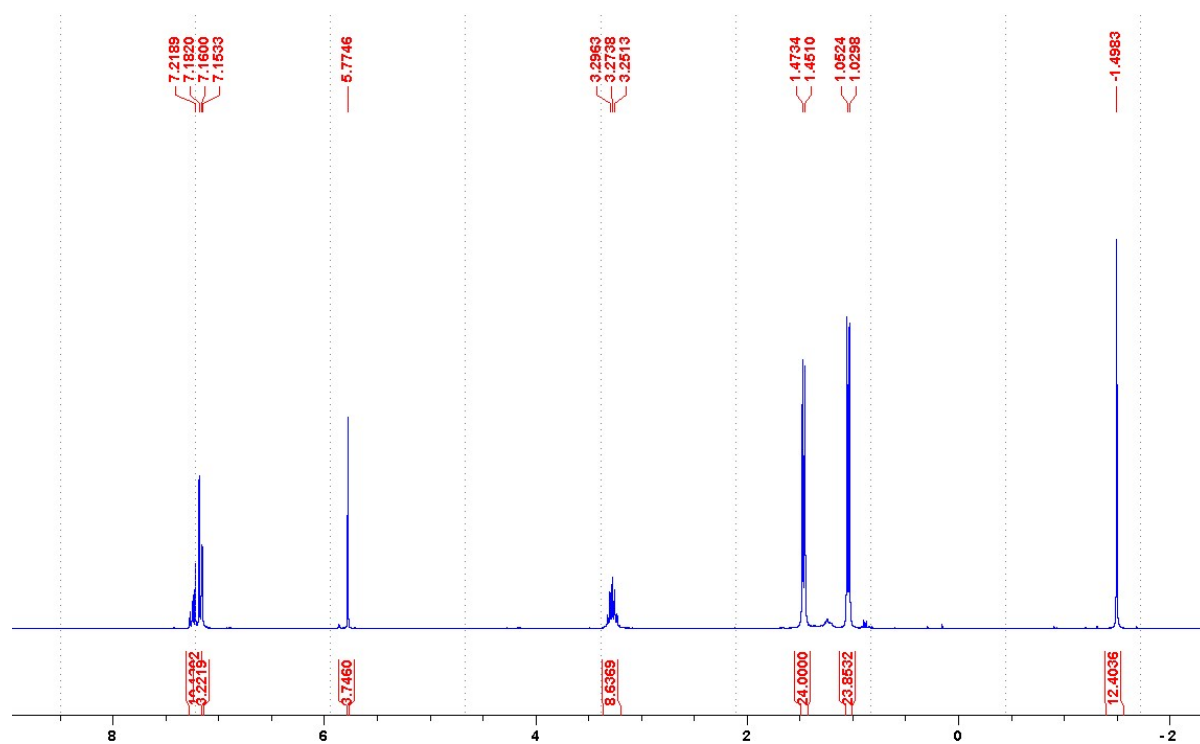


*NMR wet with solvent. Septet and broad imine proton overlap resulting in 5H

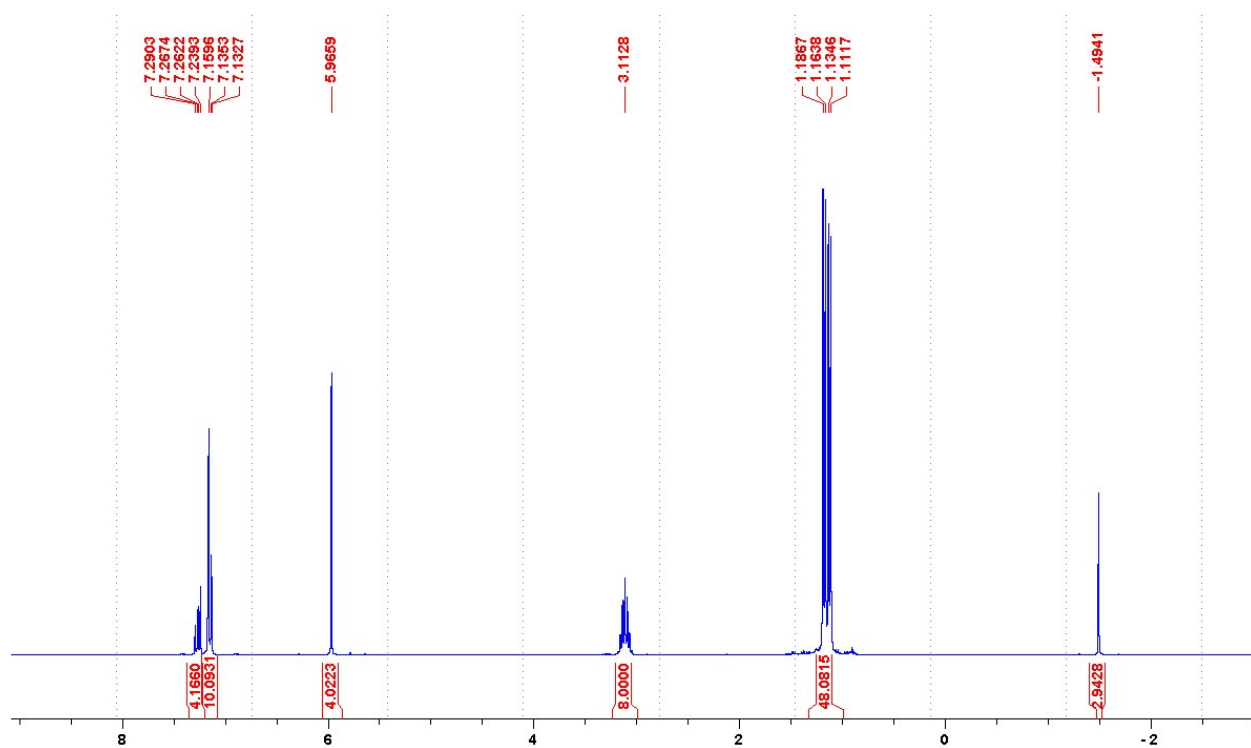
Product 2 (iPrNH-AlMe₃) in C₆D₆



Product 3 ((iPrN-AlMe₂)₂) in C₆D₆

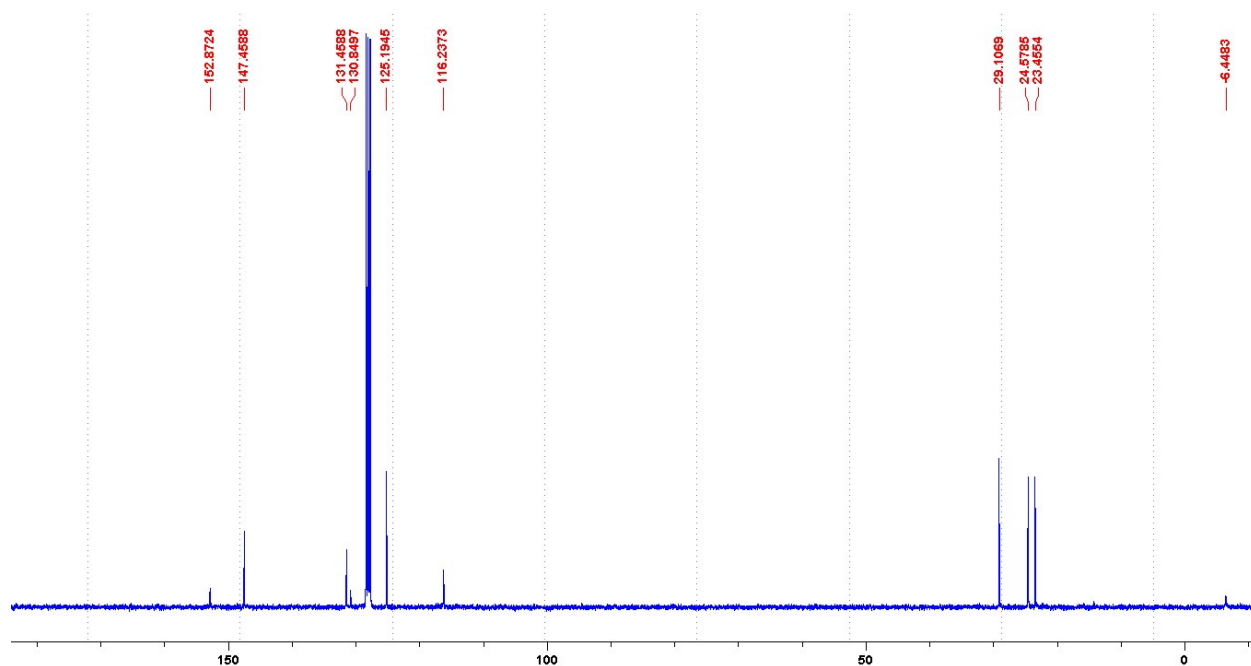


Product 5 ((iPrN)₂-AlMe) in C₆D₆

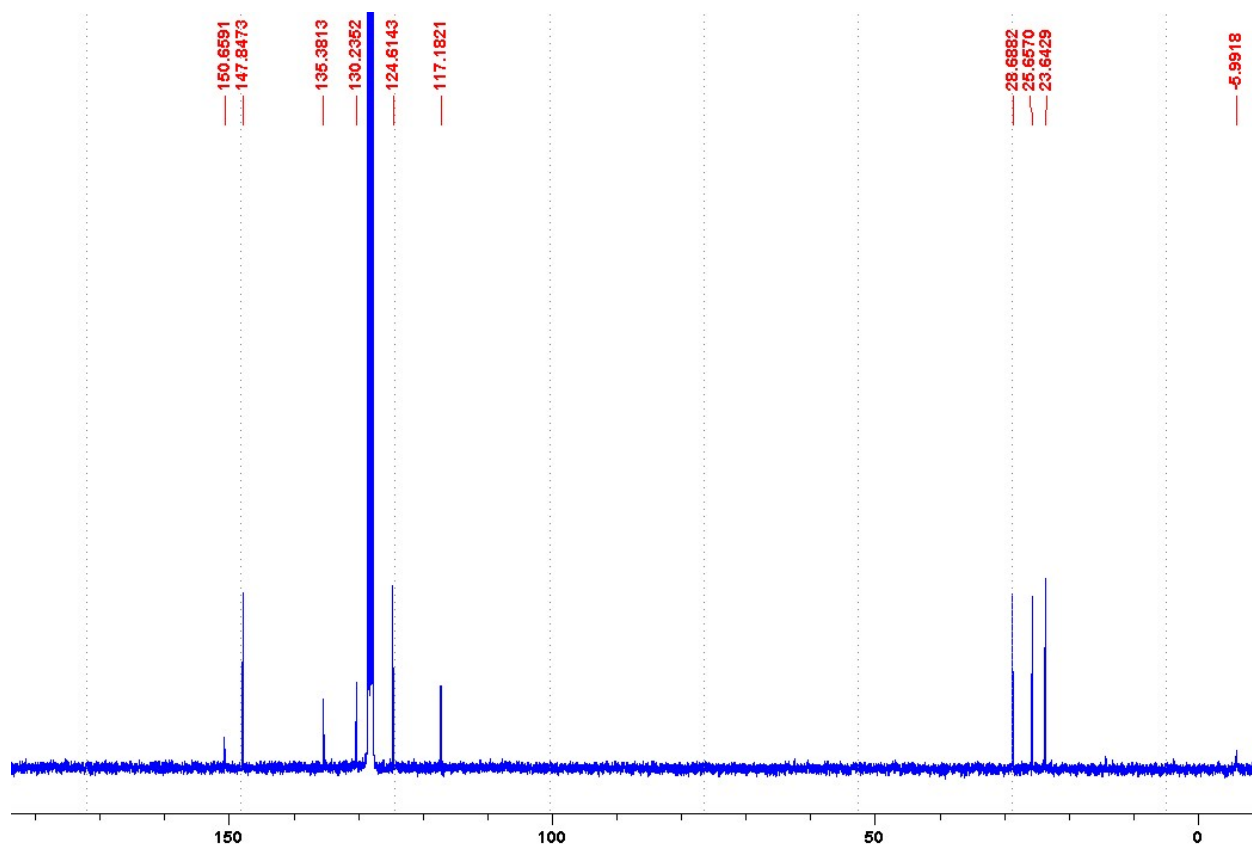


^{13}C NMR Spectra for compounds 2, 3 and 5

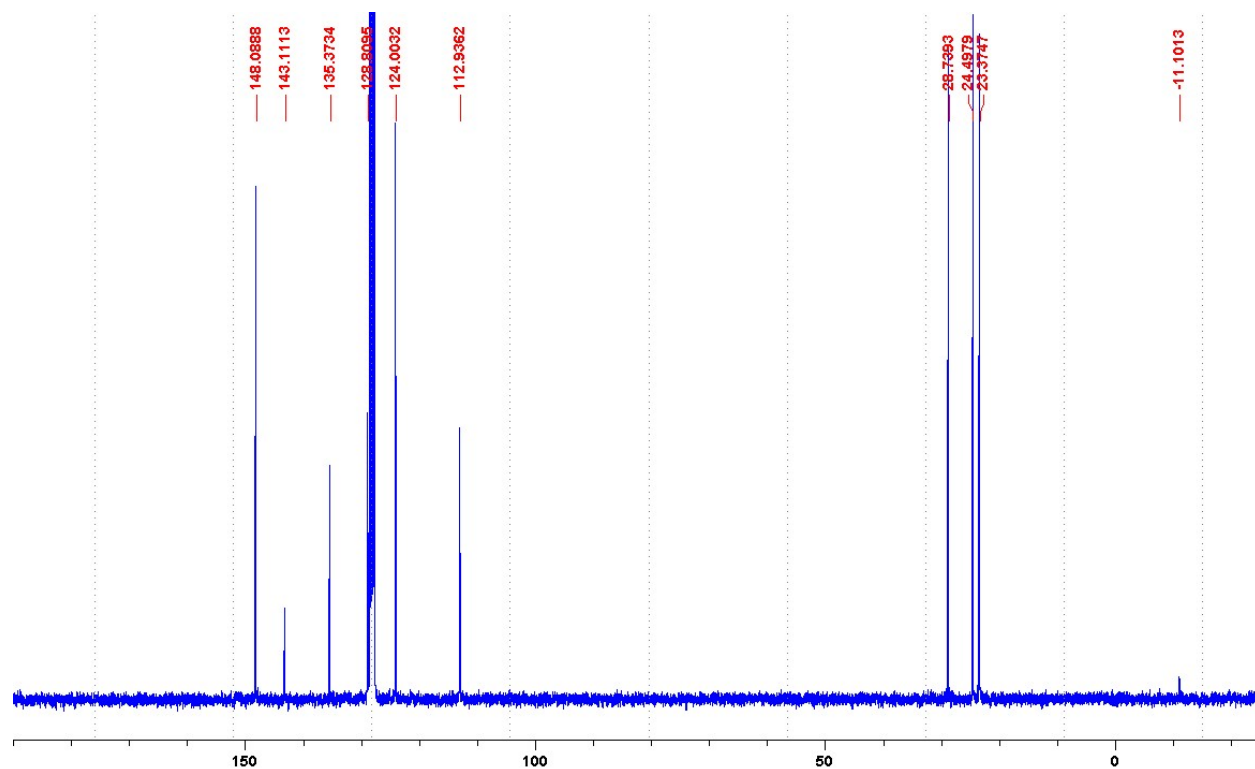
Product 2 (iPr-NH-AlMe₃)



Product 3 ((iPrN-AlMe₂)₂)



Product 5 ((iPrN)₂-AlMe)



Crystallography tables for compound 2

Table 1. Crystal data and structure refinement for 2.

Identification code	2014_11_15_IMAlMe3_0m	
Empirical formula	C ₆₇ H ₁₀₀ Al ₂ N ₆	
Formula weight	1043.48	
Temperature	125(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.3542(18) Å	α = 90.186(3)°.
	b = 9.5893(18) Å	β = 96.123(2)°.
	c = 19.621(4) Å	γ = 111.258(2)°.
Volume	1629.2(5) Å ³	
Z	1	
Density (calculated)	1.064 Mg/m ³	
Absorption coefficient	0.086 mm ⁻¹	
F(000)	570	
Crystal size	0.41 x 0.37 x 0.23 mm ³	
Theta range for data collection	2.090 to 24.999°.	
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -23 ≤ l ≤ 22	
Reflections collected	10772	
Independent reflections	5605 [R(int) = 0.0275]	
Completeness to theta = 24.999°	97.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.5922	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5605 / 36 / 344	
Goodness-of-fit on F ²	1.148	
Final R indices [I > 2σ(I)]	R1 = 0.0536, wR2 = 0.1424	
R indices (all data)	R1 = 0.0697, wR2 = 0.1544	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.406 and -0.477 e.Å ⁻³	

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.

	x	y	z	$U(\text{eq})$
Al(1)	5168(1)	5886(1)	2557(1)	28(1)
N(1)	4979(2)	3935(2)	2159(1)	29(1)
N(2)	6166(2)	2320(2)	2712(1)	25(1)
N(3)	5061(2)	1700(2)	1662(1)	26(1)
C(1)	5383(2)	2759(2)	2181(1)	25(1)
C(2)	6290(2)	967(2)	2516(1)	30(1)
C(3)	5624(2)	591(2)	1873(1)	30(1)
C(4)	4787(3)	5849(2)	3527(1)	37(1)
C(5)	7203(2)	7355(3)	2359(1)	39(1)
C(6)	3453(3)	6129(3)	1931(1)	42(1)
C(7)	6485(2)	2923(2)	3409(1)	24(1)
C(8)	5357(2)	2301(2)	3852(1)	27(1)
C(9)	5679(2)	2876(2)	4524(1)	32(1)
C(10)	7075(2)	3999(2)	4747(1)	35(1)
C(11)	8183(2)	4572(2)	4301(1)	33(1)
C(12)	7916(2)	4054(2)	3622(1)	26(1)
C(13)	3838(2)	1025(2)	3617(1)	34(1)
C(14)	2470(2)	1536(3)	3595(1)	48(1)
C(15)	3618(3)	-317(3)	4068(2)	53(1)
C(16)	9148(2)	4612(2)	3133(1)	32(1)
C(17)	10290(3)	6212(3)	3317(1)	44(1)
C(18)	10046(3)	3557(3)	3121(1)	49(1)
C(19)	4311(2)	1792(2)	991(1)	27(1)
C(20)	2704(2)	1435(2)	912(1)	31(1)
C(21)	2022(3)	1556(3)	261(1)	38(1)
C(22)	2892(3)	1999(3)	-280(1)	41(1)
C(23)	4475(3)	2354(3)	-187(1)	38(1)
C(24)	5229(2)	2270(2)	456(1)	31(1)
C(25)	1741(2)	880(3)	1504(1)	37(1)
C(26)	1245(3)	-819(3)	1540(1)	47(1)
C(27)	338(3)	1345(3)	1473(1)	47(1)

C(28)	6982(2)	2768(3)	576(1)	36(1)
C(29)	7711(3)	4461(3)	728(2)	72(1)
C(30)	7665(3)	2309(3)	-15(1)	47(1)
C(31)	9363(4)	10030(4)	4717(2)	46(1)
C(32)	9785(4)	8803(3)	4861(2)	46(1)
C(33)	11013(4)	8945(3)	5356(2)	46(1)
C(34)	11820(4)	10313(4)	5708(2)	46(1)
C(35)	11399(4)	11539(3)	5565(2)	46(1)
C(36)	10171(4)	11398(3)	5069(2)	46(1)
C(37)	8102(7)	9979(9)	4181(3)	67(2)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **2**.

Al(1)-N(1)	1.9648(19)
Al(1)-C(4)	1.971(2)
Al(1)-C(5)	1.994(2)
Al(1)-C(6)	1.997(2)
N(1)-C(1)	1.313(3)
N(1)-H(1)	0.86(2)
N(2)-C(1)	1.366(2)
N(2)-C(2)	1.400(3)
N(2)-C(7)	1.441(3)
N(3)-C(1)	1.366(3)
N(3)-C(3)	1.394(2)
N(3)-C(19)	1.442(2)
C(2)-C(3)	1.332(3)
C(2)-H(2)	0.9500
C(3)-H(3)	0.9500
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-C(8)	1.402(3)
C(7)-C(12)	1.403(3)
C(8)-C(9)	1.388(3)
C(8)-C(13)	1.525(3)
C(9)-C(10)	1.382(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.388(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.385(3)
C(11)-H(11)	0.9500

C(12)-C(16)	1.525(3)
C(13)-C(14)	1.523(3)
C(13)-C(15)	1.530(3)
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.533(3)
C(16)-C(18)	1.533(3)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(24)	1.401(3)
C(19)-C(20)	1.406(3)
C(20)-C(21)	1.391(3)
C(20)-C(25)	1.523(3)
C(21)-C(22)	1.379(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.385(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.395(3)
C(23)-H(23)	0.9500
C(24)-C(28)	1.524(3)
C(25)-C(26)	1.528(3)
C(25)-C(27)	1.528(3)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800

C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(30)	1.518(3)
C(28)-C(29)	1.530(3)
C(28)-H(28)	1.0000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.3900
C(31)-C(36)	1.3900
C(31)-C(37)	1.482(5)
C(31)-C(36)#1	1.624(6)
C(32)-C(33)	1.3900
C(32)-H(32)	0.9500
C(33)-C(34)	1.3900
C(33)-H(33)	0.9500
C(34)-C(35)	1.3900
C(34)-H(34)	0.9500
C(35)-C(36)	1.3900
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
N(1)-Al(1)-C(4)	114.13(9)
N(1)-Al(1)-C(5)	106.84(9)
C(4)-Al(1)-C(5)	115.19(10)
N(1)-Al(1)-C(6)	96.25(10)
C(4)-Al(1)-C(6)	112.20(10)
C(5)-Al(1)-C(6)	110.57(10)
C(1)-N(1)-Al(1)	149.51(15)

C(1)-N(1)-H(1)	107.2(15)
Al(1)-N(1)-H(1)	102.3(15)
C(1)-N(2)-C(2)	108.73(17)
C(1)-N(2)-C(7)	125.82(16)
C(2)-N(2)-C(7)	123.89(15)
C(1)-N(3)-C(3)	109.79(16)
C(1)-N(3)-C(19)	123.60(16)
C(3)-N(3)-C(19)	126.55(17)
N(1)-C(1)-N(2)	128.38(19)
N(1)-C(1)-N(3)	125.57(17)
N(2)-C(1)-N(3)	106.04(16)
C(3)-C(2)-N(2)	108.32(17)
C(3)-C(2)-H(2)	125.8
N(2)-C(2)-H(2)	125.8
C(2)-C(3)-N(3)	107.09(18)
C(2)-C(3)-H(3)	126.5
N(3)-C(3)-H(3)	126.5
Al(1)-C(4)-H(4A)	109.5
Al(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
Al(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
Al(1)-C(5)-H(5A)	109.5
Al(1)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
Al(1)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
Al(1)-C(6)-H(6A)	109.5
Al(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
Al(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(8)-C(7)-C(12)	123.00(18)

C(8)-C(7)-N(2)	117.74(17)
C(12)-C(7)-N(2)	119.21(16)
C(9)-C(8)-C(7)	117.44(18)
C(9)-C(8)-C(13)	120.45(18)
C(7)-C(8)-C(13)	122.10(19)
C(10)-C(9)-C(8)	120.82(19)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(9)-C(10)-C(11)	120.5(2)
C(9)-C(10)-H(10)	119.8
C(11)-C(10)-H(10)	119.8
C(12)-C(11)-C(10)	121.20(19)
C(12)-C(11)-H(11)	119.4
C(10)-C(11)-H(11)	119.4
C(11)-C(12)-C(7)	117.05(18)
C(11)-C(12)-C(16)	121.97(18)
C(7)-C(12)-C(16)	120.89(18)
C(14)-C(13)-C(8)	111.60(19)
C(14)-C(13)-C(15)	111.32(19)
C(8)-C(13)-C(15)	110.84(17)
C(14)-C(13)-H(13)	107.6
C(8)-C(13)-H(13)	107.6
C(15)-C(13)-H(13)	107.6
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(12)-C(16)-C(17)	113.40(19)

C(12)-C(16)-C(18)	109.84(17)
C(17)-C(16)-C(18)	109.06(18)
C(12)-C(16)-H(16)	108.1
C(17)-C(16)-H(16)	108.1
C(18)-C(16)-H(16)	108.1
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(24)-C(19)-C(20)	123.42(18)
C(24)-C(19)-N(3)	118.14(17)
C(20)-C(19)-N(3)	118.41(17)
C(21)-C(20)-C(19)	116.84(19)
C(21)-C(20)-C(25)	121.37(18)
C(19)-C(20)-C(25)	121.74(18)
C(22)-C(21)-C(20)	121.1(2)
C(22)-C(21)-H(21)	119.4
C(20)-C(21)-H(21)	119.4
C(21)-C(22)-C(23)	120.9(2)
C(21)-C(22)-H(22)	119.6
C(23)-C(22)-H(22)	119.6
C(22)-C(23)-C(24)	120.8(2)
C(22)-C(23)-H(23)	119.6
C(24)-C(23)-H(23)	119.6
C(23)-C(24)-C(19)	116.96(18)
C(23)-C(24)-C(28)	121.25(18)
C(19)-C(24)-C(28)	121.69(18)
C(20)-C(25)-C(26)	110.52(19)

C(20)-C(25)-C(27)	113.35(18)
C(26)-C(25)-C(27)	110.45(19)
C(20)-C(25)-H(25)	107.4
C(26)-C(25)-H(25)	107.4
C(27)-C(25)-H(25)	107.4
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(30)-C(28)-C(24)	112.97(19)
C(30)-C(28)-C(29)	110.7(2)
C(24)-C(28)-C(29)	110.3(2)
C(30)-C(28)-H(28)	107.5
C(24)-C(28)-H(28)	107.5
C(29)-C(28)-H(28)	107.5
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(36)	120.0

C(32)-C(31)-C(37)	123.1(4)
C(36)-C(31)-C(37)	116.9(4)
C(36)-C(31)-C(36)#1	118.4(2)
C(37)-C(31)-C(36)#1	124.7(4)
C(33)-C(32)-C(31)	120.0
C(33)-C(32)-H(32)	120.0
C(31)-C(32)-H(32)	120.0
C(34)-C(33)-C(32)	120.0
C(34)-C(33)-H(33)	120.0
C(32)-C(33)-H(33)	120.0
C(35)-C(34)-C(33)	120.0
C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0
C(34)-C(35)-C(36)	120.0
C(34)-C(35)-H(35)	120.0
C(36)-C(35)-H(35)	120.0
C(35)-C(36)-C(31)	120.0
C(35)-C(36)-H(36)	120.0
C(31)-C(36)-H(36)	120.0
C(31)-C(37)-H(37A)	109.5
C(31)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(31)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+1

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	29(1)	26(1)	31(1)	2(1)	6(1)	10(1)
N(1)	31(1)	30(1)	25(1)	-1(1)	-3(1)	12(1)
N(2)	22(1)	26(1)	24(1)	-1(1)	1(1)	8(1)
N(3)	26(1)	26(1)	23(1)	-2(1)	0(1)	7(1)
C(1)	20(1)	28(1)	24(1)	2(1)	4(1)	6(1)
C(2)	31(1)	29(1)	30(1)	-1(1)	1(1)	14(1)
C(3)	32(1)	26(1)	32(1)	-3(1)	4(1)	11(1)
C(4)	40(1)	36(1)	37(1)	-1(1)	8(1)	14(1)
C(5)	36(1)	33(1)	46(1)	2(1)	7(1)	9(1)
C(6)	40(1)	41(1)	50(2)	14(1)	11(1)	20(1)
C(7)	24(1)	26(1)	23(1)	-1(1)	0(1)	10(1)
C(8)	25(1)	27(1)	30(1)	3(1)	3(1)	9(1)
C(9)	36(1)	36(1)	27(1)	5(1)	8(1)	14(1)
C(10)	44(1)	39(1)	23(1)	-4(1)	-1(1)	17(1)
C(11)	30(1)	30(1)	33(1)	-4(1)	-7(1)	8(1)
C(12)	23(1)	25(1)	29(1)	0(1)	0(1)	9(1)
C(13)	26(1)	35(1)	36(1)	0(1)	4(1)	6(1)
C(14)	27(1)	48(2)	66(2)	4(1)	5(1)	9(1)
C(15)	42(1)	34(1)	70(2)	9(1)	2(1)	0(1)
C(16)	24(1)	34(1)	35(1)	1(1)	4(1)	5(1)
C(17)	31(1)	39(1)	51(2)	2(1)	4(1)	1(1)
C(18)	35(1)	46(1)	66(2)	2(1)	19(1)	12(1)
C(19)	31(1)	25(1)	21(1)	-3(1)	-1(1)	8(1)
C(20)	31(1)	32(1)	28(1)	-4(1)	-1(1)	10(1)
C(21)	35(1)	43(1)	33(1)	-4(1)	-6(1)	14(1)
C(22)	47(1)	44(1)	28(1)	-1(1)	-6(1)	16(1)
C(23)	45(1)	41(1)	25(1)	1(1)	4(1)	11(1)
C(24)	35(1)	28(1)	27(1)	-3(1)	2(1)	9(1)
C(25)	29(1)	47(1)	30(1)	-4(1)	0(1)	9(1)
C(26)	39(1)	53(2)	51(2)	12(1)	14(1)	17(1)
C(27)	39(1)	53(2)	48(2)	-8(1)	6(1)	16(1)

C(28)	34(1)	37(1)	32(1)	0(1)	6(1)	7(1)
C(29)	41(2)	52(2)	110(3)	-26(2)	24(2)	-5(1)
C(30)	47(1)	58(2)	42(2)	2(1)	8(1)	26(1)
C(31)	50(1)	45(1)	43(1)	2(1)	11(1)	16(1)
C(32)	50(1)	45(1)	43(1)	2(1)	11(1)	16(1)
C(33)	50(1)	45(1)	43(1)	2(1)	11(1)	16(1)
C(34)	50(1)	45(1)	43(1)	2(1)	11(1)	16(1)
C(35)	50(1)	45(1)	43(1)	2(1)	11(1)	16(1)
C(36)	50(1)	45(1)	43(1)	2(1)	11(1)	16(1)
C(37)	46(3)	98(5)	57(4)	9(4)	0(3)	28(3)

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

	x	y	z	U(eq)
H(1)	4520(20)	3930(20)	1754(12)	33(6)
H(2)	6768	411	2794	35
H(3)	5547	-271	1609	36
H(4A)	3795	5056	3580	56
H(4B)	4762	6818	3671	56
H(4C)	5616	5654	3812	56
H(5A)	7824	6817	2197	59
H(5B)	7745	7955	2778	59
H(5C)	7038	8015	2003	59
H(6A)	3640	6042	1453	62
H(6B)	3407	7116	2023	62
H(6C)	2472	5347	2010	62
H(9)	4932	2493	4835	39
H(10)	7277	4381	5209	42
H(11)	9141	5335	4464	39
H(13)	3892	697	3139	41
H(14A)	2403	1887	4056	73
H(14B)	1517	695	3436	73
H(14C)	2612	2353	3280	73
H(15A)	4476	-666	4045	80
H(15B)	2643	-1127	3905	80
H(15C)	3595	-19	4544	80
H(16)	8617	4595	2662	39
H(17A)	9718	6870	3383	65
H(17B)	10932	6569	2944	65
H(17C)	10949	6219	3741	65
H(18A)	10548	3531	3583	73
H(18B)	10832	3919	2805	73
H(18C)	9333	2547	2968	73
H(21)	940	1329	186	46

H(22)	2399	2061	-721	49
H(23)	5054	2659	-565	46
H(25)	2417	1336	1938	44
H(26A)	650	-1155	1929	71
H(26B)	2163	-1092	1599	71
H(26C)	605	-1301	1114	71
H(27A)	667	2429	1422	70
H(27B)	-147	1082	1897	70
H(27C)	-406	822	1080	70
H(28)	7244	2270	993	43
H(29A)	8837	4765	809	109
H(29B)	7329	4723	1138	109
H(29C)	7435	4981	336	109
H(30A)	7177	1224	-107	70
H(30B)	8779	2580	106	70
H(30C)	7480	2827	-425	70
H(32)	9233	7868	4620	55
H(33)	11301	8107	5455	55
H(34)	12660	10410	6047	55
H(35)	11951	12474	5805	55
H(36)	9883	12236	4971	55
H(37A)	7683	10739	4295	101
H(37B)	7282	8985	4157	101
H(37C)	8506	10179	3736	101

Table 6. Torsion angles [°] for 2.

Al(1)-N(1)-C(1)-N(2)	13.8(4)
Al(1)-N(1)-C(1)-N(3)	-167.41(19)
C(2)-N(2)-C(1)-N(1)	177.76(18)
C(7)-N(2)-C(1)-N(1)	11.6(3)
C(2)-N(2)-C(1)-N(3)	-1.19(19)
C(7)-N(2)-C(1)-N(3)	-167.34(16)
C(3)-N(3)-C(1)-N(1)	-178.11(17)
C(19)-N(3)-C(1)-N(1)	4.5(3)
C(3)-N(3)-C(1)-N(2)	0.88(19)
C(19)-N(3)-C(1)-N(2)	-176.55(16)
C(1)-N(2)-C(2)-C(3)	1.1(2)
C(7)-N(2)-C(2)-C(3)	167.57(17)
N(2)-C(2)-C(3)-N(3)	-0.5(2)
C(1)-N(3)-C(3)-C(2)	-0.2(2)
C(19)-N(3)-C(3)-C(2)	177.12(17)
C(1)-N(2)-C(7)-C(8)	86.3(2)
C(2)-N(2)-C(7)-C(8)	-77.8(2)
C(1)-N(2)-C(7)-C(12)	-96.2(2)
C(2)-N(2)-C(7)-C(12)	99.7(2)
C(12)-C(7)-C(8)-C(9)	1.9(3)
N(2)-C(7)-C(8)-C(9)	179.27(17)
C(12)-C(7)-C(8)-C(13)	-177.24(18)
N(2)-C(7)-C(8)-C(13)	0.2(3)
C(7)-C(8)-C(9)-C(10)	-1.2(3)
C(13)-C(8)-C(9)-C(10)	177.90(19)
C(8)-C(9)-C(10)-C(11)	-0.1(3)
C(9)-C(10)-C(11)-C(12)	0.9(3)
C(10)-C(11)-C(12)-C(7)	-0.3(3)
C(10)-C(11)-C(12)-C(16)	-176.85(18)
C(8)-C(7)-C(12)-C(11)	-1.1(3)
N(2)-C(7)-C(12)-C(11)	-178.49(16)
C(8)-C(7)-C(12)-C(16)	175.50(17)
N(2)-C(7)-C(12)-C(16)	-1.9(3)
C(9)-C(8)-C(13)-C(14)	69.1(2)

C(7)-C(8)-C(13)-C(14)	-111.8(2)
C(9)-C(8)-C(13)-C(15)	-55.6(3)
C(7)-C(8)-C(13)-C(15)	123.5(2)
C(11)-C(12)-C(16)-C(17)	-28.3(3)
C(7)-C(12)-C(16)-C(17)	155.24(18)
C(11)-C(12)-C(16)-C(18)	94.0(2)
C(7)-C(12)-C(16)-C(18)	-82.5(2)
C(1)-N(3)-C(19)-C(24)	101.1(2)
C(3)-N(3)-C(19)-C(24)	-75.9(2)
C(1)-N(3)-C(19)-C(20)	-77.3(2)
C(3)-N(3)-C(19)-C(20)	105.7(2)
C(24)-C(19)-C(20)-C(21)	0.8(3)
N(3)-C(19)-C(20)-C(21)	179.16(18)
C(24)-C(19)-C(20)-C(25)	178.4(2)
N(3)-C(19)-C(20)-C(25)	-3.3(3)
C(19)-C(20)-C(21)-C(22)	0.3(3)
C(25)-C(20)-C(21)-C(22)	-177.2(2)
C(20)-C(21)-C(22)-C(23)	-0.8(4)
C(21)-C(22)-C(23)-C(24)	0.1(4)
C(22)-C(23)-C(24)-C(19)	0.9(3)
C(22)-C(23)-C(24)-C(28)	-175.4(2)
C(20)-C(19)-C(24)-C(23)	-1.4(3)
N(3)-C(19)-C(24)-C(23)	-179.78(18)
C(20)-C(19)-C(24)-C(28)	174.9(2)
N(3)-C(19)-C(24)-C(28)	-3.4(3)
C(21)-C(20)-C(25)-C(26)	90.6(2)
C(19)-C(20)-C(25)-C(26)	-86.8(3)
C(21)-C(20)-C(25)-C(27)	-34.0(3)
C(19)-C(20)-C(25)-C(27)	148.5(2)
C(23)-C(24)-C(28)-C(30)	-40.4(3)
C(19)-C(24)-C(28)-C(30)	143.5(2)
C(23)-C(24)-C(28)-C(29)	84.2(3)
C(19)-C(24)-C(28)-C(29)	-92.0(3)
C(36)-C(31)-C(32)-C(33)	0.0
C(37)-C(31)-C(32)-C(33)	177.9(5)
C(36)#1-C(31)-C(32)-C(33)	-63(4)

C(31)-C(32)-C(33)-C(34)	0.0
C(32)-C(33)-C(34)-C(35)	0.0
C(33)-C(34)-C(35)-C(36)	0.0
C(34)-C(35)-C(36)-C(31)	0.0
C(32)-C(31)-C(36)-C(35)	0.0
C(37)-C(31)-C(36)-C(35)	-178.1(5)
C(36)#1-C(31)-C(36)-C(35)	3.4(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+1

Crystallography tables for compound 3

Table 1. Crystal data and structure refinement for 3.

Identification code	BM103_0m	
Empirical formula	C ₅₆ H ₇₉ Al N ₆	
Formula weight	863.23	
Temperature	125(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 12.9094(10) Å	α = 90°.
	b = 18.6830(14) Å	β = 90.0500(10)°.
	c = 21.6167(16) Å	γ = 90°.
Volume	5213.7(7) Å ³	
Z	4	
Density (calculated)	1.100 Mg/m ³	
Absorption coefficient	0.080 mm ⁻¹	
F(000)	1880	
Crystal size	0.260 x 0.160 x 0.080 mm ³	
Theta range for data collection	1.838 to 25.000°.	
Index ranges	-15 ≤ h ≤ 15, -22 ≤ k ≤ 22, -25 ≤ l ≤ 25	
Reflections collected	50368	
Independent reflections	9160 [R(int) = 0.0893]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6942	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9160 / 0 / 590	
Goodness-of-fit on F ²	1.009	
Final R indices [I > 2σ(I)]	R1 = 0.0490, wR2 = 0.0998	
R indices (all data)	R1 = 0.0945, wR2 = 0.1207	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.223 and -0.249 e.Å ⁻³	

Table 2. 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.

	x	y	z	$U(\text{eq})$
Al(1)	-90(1)	3240(1)	1467(1)	25(1)
N(1)	-569(1)	2815(1)	2169(1)	25(1)
N(2)	-2376(1)	2607(1)	2422(1)	27(1)
N(3)	-1210(1)	2305(1)	3120(1)	26(1)
N(4)	955(1)	2513(1)	1261(1)	24(1)
N(5)	2700(1)	2116(1)	1131(1)	24(1)
N(6)	2070(1)	2783(1)	393(1)	23(1)
C(1)	-999(2)	3393(1)	748(1)	40(1)
C(2)	735(2)	4107(1)	1665(1)	42(1)
C(3)	-1289(2)	2612(1)	2519(1)	24(1)
C(4)	-2890(2)	2304(1)	2925(1)	31(1)
C(5)	-2189(2)	2128(1)	3348(1)	30(1)
C(6)	1828(2)	2479(1)	952(1)	21(1)
C(7)	3477(2)	2201(1)	692(1)	32(1)
C(8)	3093(2)	2608(1)	239(1)	31(1)
C(9)	-2886(2)	2866(1)	1877(1)	27(1)
C(10)	-3049(2)	3603(1)	1816(1)	29(1)
C(11)	-3604(2)	3834(1)	1298(1)	35(1)
C(12)	-3953(2)	3356(2)	857(1)	38(1)
C(13)	-3762(2)	2636(1)	925(1)	37(1)
C(14)	-3226(2)	2374(1)	1436(1)	31(1)
C(15)	-2655(2)	4128(1)	2296(1)	36(1)
C(16)	-2272(2)	4833(1)	2023(1)	49(1)
C(17)	-3465(2)	4265(2)	2791(1)	56(1)
C(18)	-3013(2)	1580(1)	1501(1)	42(1)
C(19)	-2130(3)	1357(2)	1078(2)	85(1)
C(20)	-3970(3)	1125(2)	1381(2)	92(1)
C(21)	-301(2)	2328(1)	3505(1)	27(1)
C(22)	289(2)	1704(1)	3573(1)	28(1)
C(23)	1144(2)	1733(1)	3969(1)	35(1)
C(24)	1395(2)	2355(2)	4280(1)	40(1)

C(25)	801(2)	2959(1)	4211(1)	37(1)
C(26)	-65(2)	2964(1)	3824(1)	32(1)
C(27)	-2(2)	1028(1)	3226(1)	30(1)
C(28)	256(2)	1094(1)	2535(1)	36(1)
C(29)	505(2)	349(1)	3487(1)	40(1)
C(30)	-703(2)	3639(1)	3738(1)	36(1)
C(31)	-197(2)	4116(1)	3252(1)	41(1)
C(32)	-867(2)	4063(1)	4339(1)	50(1)
C(33)	2794(2)	1660(1)	1666(1)	27(1)
C(34)	2682(2)	923(1)	1579(1)	31(1)
C(35)	2885(2)	486(1)	2084(1)	37(1)
C(36)	3160(2)	775(1)	2651(1)	37(1)
C(37)	3222(2)	1506(1)	2726(1)	34(1)
C(38)	3043(2)	1973(1)	2234(1)	28(1)
C(39)	2300(2)	608(1)	968(1)	37(1)
C(40)	1154(2)	413(2)	1011(1)	54(1)
C(41)	2941(2)	-31(2)	750(1)	57(1)
C(42)	3131(2)	2780(1)	2314(1)	30(1)
C(43)	2481(2)	3043(1)	2857(1)	44(1)
C(44)	4263(2)	3003(2)	2392(1)	51(1)
C(45)	1399(2)	3147(1)	-45(1)	24(1)
C(46)	658(2)	2741(1)	-369(1)	27(1)
C(47)	106(2)	3093(1)	-830(1)	34(1)
C(48)	277(2)	3808(1)	-962(1)	38(1)
C(49)	999(2)	4193(1)	-630(1)	33(1)
C(50)	1584(2)	3872(1)	-162(1)	26(1)
C(51)	487(2)	1952(1)	-240(1)	33(1)
C(52)	-595(2)	1690(2)	-424(1)	56(1)
C(53)	1300(2)	1496(2)	-559(1)	54(1)
C(54)	2397(2)	4312(1)	176(1)	30(1)
C(55)	1986(2)	5050(1)	354(1)	44(1)
C(56)	3384(2)	4399(2)	-216(1)	47(1)

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

Al(1)-N(1)	1.8218(19)
Al(1)-N(4)	1.9648(19)
Al(1)-C(1)	1.967(2)
Al(1)-C(2)	1.985(3)
N(1)-C(3)	1.257(3)
N(2)-C(4)	1.394(3)
N(2)-C(3)	1.419(3)
N(2)-C(9)	1.434(3)
N(3)-C(5)	1.397(3)
N(3)-C(3)	1.424(3)
N(3)-C(21)	1.439(3)
N(4)-C(6)	1.313(3)
N(4)-H(1)	0.86(2)
N(5)-C(6)	1.369(3)
N(5)-C(7)	1.390(3)
N(5)-C(33)	1.442(3)
N(6)-C(6)	1.372(3)
N(6)-C(8)	1.401(3)
N(6)-C(45)	1.451(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(4)-C(5)	1.329(3)
C(4)-H(4)	0.9500
C(5)-H(5)	0.9500
C(7)-C(8)	1.333(3)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(14)	1.394(3)
C(9)-C(10)	1.401(3)
C(10)-C(11)	1.397(3)

C(10)-C(15)	1.517(3)
C(11)-C(12)	1.380(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.376(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.392(3)
C(13)-H(13)	0.9500
C(14)-C(18)	1.515(3)
C(15)-C(17)	1.518(4)
C(15)-C(16)	1.525(3)
C(15)-H(15)	1.0000
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.520(4)
C(18)-C(20)	1.522(4)
C(18)-H(18)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.401(3)
C(21)-C(26)	1.406(3)
C(22)-C(23)	1.397(3)
C(22)-C(27)	1.515(3)
C(23)-C(24)	1.381(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.373(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.396(3)
C(25)-H(25)	0.9500

C(26)-C(30)	1.516(3)
C(27)-C(29)	1.535(3)
C(27)-C(28)	1.536(3)
C(27)-H(27)	1.0000
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.525(3)
C(30)-C(32)	1.537(3)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(38)	1.397(3)
C(33)-C(34)	1.399(3)
C(34)-C(35)	1.388(3)
C(34)-C(39)	1.526(3)
C(35)-C(36)	1.386(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.378(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.395(3)
C(37)-H(37)	0.9500
C(38)-C(42)	1.523(3)
C(39)-C(40)	1.526(4)
C(39)-C(41)	1.528(3)
C(39)-H(39)	1.0000
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800

C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-C(43)	1.524(3)
C(42)-C(44)	1.529(3)
C(42)-H(42)	1.0000
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(50)	1.397(3)
C(45)-C(46)	1.408(3)
C(46)-C(47)	1.389(3)
C(46)-C(51)	1.517(3)
C(47)-C(48)	1.384(3)
C(47)-H(47)	0.9500
C(48)-C(49)	1.377(3)
C(48)-H(48)	0.9500
C(49)-C(50)	1.399(3)
C(49)-H(49)	0.9500
C(50)-C(54)	1.521(3)
C(51)-C(53)	1.518(4)
C(51)-C(52)	1.532(3)
C(51)-H(51)	1.0000
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-C(55)	1.525(3)
C(54)-C(56)	1.539(3)
C(54)-H(54)	1.0000
C(55)-H(55A)	0.9800

C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
N(1)-Al(1)-N(4)	96.95(9)
N(1)-Al(1)-C(1)	121.23(10)
N(4)-Al(1)-C(1)	109.34(10)
N(1)-Al(1)-C(2)	111.01(10)
N(4)-Al(1)-C(2)	104.16(10)
C(1)-Al(1)-C(2)	111.77(12)
C(3)-N(1)-Al(1)	152.17(17)
C(4)-N(2)-C(3)	111.10(18)
C(4)-N(2)-C(9)	124.03(18)
C(3)-N(2)-C(9)	124.86(18)
C(5)-N(3)-C(3)	110.73(18)
C(5)-N(3)-C(21)	122.70(18)
C(3)-N(3)-C(21)	125.00(18)
C(6)-N(4)-Al(1)	137.63(16)
C(6)-N(4)-H(1)	111.1(16)
Al(1)-N(4)-H(1)	104.4(16)
C(6)-N(5)-C(7)	110.14(18)
C(6)-N(5)-C(33)	126.00(18)
C(7)-N(5)-C(33)	123.66(18)
C(6)-N(6)-C(8)	109.10(17)
C(6)-N(6)-C(45)	129.17(18)
C(8)-N(6)-C(45)	121.20(17)
Al(1)-C(1)-H(1A)	109.5
Al(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Al(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
Al(1)-C(2)-H(2A)	109.5
Al(1)-C(2)-H(2B)	109.5

H(2A)-C(2)-H(2B)	109.5
Al(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
N(1)-C(3)-N(2)	130.2(2)
N(1)-C(3)-N(3)	128.1(2)
N(2)-C(3)-N(3)	101.63(18)
C(5)-C(4)-N(2)	108.2(2)
C(5)-C(4)-H(4)	125.9
N(2)-C(4)-H(4)	125.9
C(4)-C(5)-N(3)	108.3(2)
C(4)-C(5)-H(5)	125.9
N(3)-C(5)-H(5)	125.9
N(4)-C(6)-N(5)	125.9(2)
N(4)-C(6)-N(6)	128.70(19)
N(5)-C(6)-N(6)	105.42(18)
C(8)-C(7)-N(5)	107.3(2)
C(8)-C(7)-H(7)	126.3
N(5)-C(7)-H(7)	126.3
C(7)-C(8)-N(6)	108.0(2)
C(7)-C(8)-H(8)	126.0
N(6)-C(8)-H(8)	126.0
C(14)-C(9)-C(10)	122.5(2)
C(14)-C(9)-N(2)	119.0(2)
C(10)-C(9)-N(2)	118.5(2)
C(11)-C(10)-C(9)	117.2(2)
C(11)-C(10)-C(15)	121.4(2)
C(9)-C(10)-C(15)	121.4(2)
C(12)-C(11)-C(10)	121.3(2)
C(12)-C(11)-H(11)	119.4
C(10)-C(11)-H(11)	119.4
C(13)-C(12)-C(11)	120.1(2)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	121.1(2)
C(12)-C(13)-H(13)	119.4

C(14)-C(13)-H(13)	119.4
C(13)-C(14)-C(9)	117.8(2)
C(13)-C(14)-C(18)	120.5(2)
C(9)-C(14)-C(18)	121.6(2)
C(10)-C(15)-C(17)	111.1(2)
C(10)-C(15)-C(16)	113.6(2)
C(17)-C(15)-C(16)	110.6(2)
C(10)-C(15)-H(15)	107.0
C(17)-C(15)-H(15)	107.0
C(16)-C(15)-H(15)	107.0
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(14)-C(18)-C(19)	110.4(2)
C(14)-C(18)-C(20)	112.6(2)
C(19)-C(18)-C(20)	110.7(3)
C(14)-C(18)-H(18)	107.6
C(19)-C(18)-H(18)	107.6
C(20)-C(18)-H(18)	107.6
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5

H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(26)	122.3(2)
C(22)-C(21)-N(3)	118.6(2)
C(26)-C(21)-N(3)	119.0(2)
C(23)-C(22)-C(21)	117.4(2)
C(23)-C(22)-C(27)	122.1(2)
C(21)-C(22)-C(27)	120.5(2)
C(24)-C(23)-C(22)	121.1(2)
C(24)-C(23)-H(23)	119.5
C(22)-C(23)-H(23)	119.5
C(25)-C(24)-C(23)	120.5(2)
C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7
C(24)-C(25)-C(26)	121.2(2)
C(24)-C(25)-H(25)	119.4
C(26)-C(25)-H(25)	119.4
C(25)-C(26)-C(21)	117.4(2)
C(25)-C(26)-C(30)	120.9(2)
C(21)-C(26)-C(30)	121.7(2)
C(22)-C(27)-C(29)	113.65(19)
C(22)-C(27)-C(28)	111.11(19)
C(29)-C(27)-C(28)	109.3(2)
C(22)-C(27)-H(27)	107.5
C(29)-C(27)-H(27)	107.5
C(28)-C(27)-H(27)	107.5
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5

H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(26)-C(30)-C(31)	109.7(2)
C(26)-C(30)-C(32)	113.6(2)
C(31)-C(30)-C(32)	109.9(2)
C(26)-C(30)-H(30)	107.8
C(31)-C(30)-H(30)	107.8
C(32)-C(30)-H(30)	107.8
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(38)-C(33)-C(34)	123.6(2)
C(38)-C(33)-N(5)	118.5(2)
C(34)-C(33)-N(5)	117.8(2)
C(35)-C(34)-C(33)	117.0(2)
C(35)-C(34)-C(39)	121.0(2)
C(33)-C(34)-C(39)	122.0(2)
C(36)-C(35)-C(34)	121.0(2)
C(36)-C(35)-H(35)	119.5
C(34)-C(35)-H(35)	119.5
C(37)-C(36)-C(35)	120.3(2)
C(37)-C(36)-H(36)	119.8
C(35)-C(36)-H(36)	119.8
C(36)-C(37)-C(38)	121.4(2)
C(36)-C(37)-H(37)	119.3

C(38)-C(37)-H(37)	119.3
C(37)-C(38)-C(33)	116.6(2)
C(37)-C(38)-C(42)	121.3(2)
C(33)-C(38)-C(42)	122.1(2)
C(40)-C(39)-C(34)	110.6(2)
C(40)-C(39)-C(41)	111.0(2)
C(34)-C(39)-C(41)	113.2(2)
C(40)-C(39)-H(39)	107.2
C(34)-C(39)-H(39)	107.2
C(41)-C(39)-H(39)	107.2
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(39)-C(41)-H(41A)	109.5
C(39)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(39)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(38)-C(42)-C(43)	111.5(2)
C(38)-C(42)-C(44)	110.7(2)
C(43)-C(42)-C(44)	110.7(2)
C(38)-C(42)-H(42)	107.9
C(43)-C(42)-H(42)	107.9
C(44)-C(42)-H(42)	107.9
C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(42)-C(44)-H(44A)	109.5
C(42)-C(44)-H(44B)	109.5

H(44A)-C(44)-H(44B)	109.5
C(42)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(50)-C(45)-C(46)	123.2(2)
C(50)-C(45)-N(6)	118.02(19)
C(46)-C(45)-N(6)	118.5(2)
C(47)-C(46)-C(45)	116.8(2)
C(47)-C(46)-C(51)	121.2(2)
C(45)-C(46)-C(51)	122.0(2)
C(48)-C(47)-C(46)	121.5(2)
C(48)-C(47)-H(47)	119.2
C(46)-C(47)-H(47)	119.2
C(49)-C(48)-C(47)	120.3(2)
C(49)-C(48)-H(48)	119.8
C(47)-C(48)-H(48)	119.8
C(48)-C(49)-C(50)	121.2(2)
C(48)-C(49)-H(49)	119.4
C(50)-C(49)-H(49)	119.4
C(45)-C(50)-C(49)	117.0(2)
C(45)-C(50)-C(54)	123.8(2)
C(49)-C(50)-C(54)	119.2(2)
C(46)-C(51)-C(53)	111.1(2)
C(46)-C(51)-C(52)	113.3(2)
C(53)-C(51)-C(52)	109.5(2)
C(46)-C(51)-H(51)	107.6
C(53)-C(51)-H(51)	107.6
C(52)-C(51)-H(51)	107.6
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(51)-C(53)-H(53A)	109.5
C(51)-C(53)-H(53B)	109.5

H(53A)-C(53)-H(53B)	109.5
C(51)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(50)-C(54)-C(55)	111.7(2)
C(50)-C(54)-C(56)	111.3(2)
C(55)-C(54)-C(56)	109.4(2)
C(50)-C(54)-H(54)	108.1
C(55)-C(54)-H(54)	108.1
C(56)-C(54)-H(54)	108.1
C(54)-C(55)-H(55A)	109.5
C(54)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(54)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(54)-C(56)-H(56A)	109.5
C(54)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(54)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	26(1)	23(1)	25(1)	3(1)	3(1)	2(1)
N(1)	27(1)	24(1)	24(1)	2(1)	2(1)	1(1)
N(2)	25(1)	30(1)	26(1)	10(1)	0(1)	-1(1)
N(3)	25(1)	29(1)	24(1)	7(1)	-1(1)	-4(1)
N(4)	25(1)	25(1)	20(1)	6(1)	0(1)	3(1)
N(5)	24(1)	27(1)	23(1)	5(1)	0(1)	6(1)
N(6)	22(1)	27(1)	21(1)	3(1)	1(1)	4(1)
C(1)	33(2)	49(2)	37(2)	13(1)	6(1)	11(1)
C(2)	52(2)	35(2)	38(2)	-1(1)	18(1)	-7(1)
C(3)	29(1)	20(1)	23(1)	2(1)	-2(1)	2(1)
C(4)	28(1)	37(2)	28(1)	7(1)	4(1)	-3(1)
C(5)	32(1)	32(1)	25(1)	7(1)	3(1)	-4(1)
C(6)	23(1)	19(1)	21(1)	-2(1)	-2(1)	2(1)
C(7)	24(1)	39(2)	33(1)	6(1)	1(1)	8(1)
C(8)	25(1)	38(2)	30(1)	4(1)	5(1)	3(1)
C(9)	25(1)	32(1)	24(1)	7(1)	-1(1)	1(1)
C(10)	24(1)	36(2)	29(1)	7(1)	4(1)	2(1)
C(11)	32(1)	37(2)	37(2)	13(1)	6(1)	9(1)
C(12)	29(1)	54(2)	31(2)	12(1)	-1(1)	1(1)
C(13)	38(2)	44(2)	28(1)	4(1)	-2(1)	-5(1)
C(14)	29(1)	34(2)	31(1)	3(1)	1(1)	-2(1)
C(15)	37(2)	32(2)	40(2)	5(1)	-2(1)	5(1)
C(16)	61(2)	35(2)	52(2)	1(1)	8(2)	-2(1)
C(17)	73(2)	60(2)	35(2)	-5(2)	6(2)	-7(2)
C(18)	55(2)	36(2)	36(2)	1(1)	-6(1)	-5(1)
C(19)	108(3)	43(2)	105(3)	5(2)	26(2)	26(2)
C(20)	93(3)	47(2)	136(4)	16(2)	-24(3)	-27(2)
C(21)	26(1)	34(1)	22(1)	6(1)	0(1)	-6(1)
C(22)	28(1)	32(1)	23(1)	7(1)	-1(1)	-4(1)
C(23)	34(2)	40(2)	32(1)	9(1)	-4(1)	-2(1)
C(24)	37(2)	53(2)	29(2)	6(1)	-7(1)	-10(1)

C(25)	47(2)	39(2)	26(1)	-2(1)	-2(1)	-13(1)
C(26)	39(2)	35(2)	22(1)	3(1)	3(1)	-9(1)
C(27)	30(1)	28(1)	33(1)	5(1)	-3(1)	-1(1)
C(28)	44(2)	30(1)	35(2)	1(1)	-4(1)	1(1)
C(29)	43(2)	32(2)	45(2)	10(1)	-2(1)	-1(1)
C(30)	43(2)	30(2)	34(2)	0(1)	4(1)	-5(1)
C(31)	55(2)	33(2)	34(2)	1(1)	4(1)	-1(1)
C(32)	66(2)	42(2)	41(2)	-3(1)	18(2)	-9(2)
C(33)	24(1)	32(1)	24(1)	6(1)	-1(1)	8(1)
C(34)	34(1)	27(1)	32(1)	1(1)	-1(1)	11(1)
C(35)	43(2)	28(1)	41(2)	5(1)	-1(1)	10(1)
C(36)	39(2)	37(2)	36(2)	10(1)	-5(1)	9(1)
C(37)	32(1)	40(2)	29(1)	1(1)	-9(1)	4(1)
C(38)	24(1)	32(1)	28(1)	4(1)	-4(1)	4(1)
C(39)	50(2)	29(1)	33(2)	-1(1)	-5(1)	7(1)
C(40)	61(2)	54(2)	48(2)	-14(2)	-11(2)	-4(2)
C(41)	79(2)	46(2)	44(2)	-10(2)	1(2)	21(2)
C(42)	32(1)	33(1)	26(1)	1(1)	-4(1)	-1(1)
C(43)	47(2)	38(2)	48(2)	-5(1)	10(1)	-1(1)
C(44)	40(2)	53(2)	59(2)	-5(2)	1(1)	-9(1)
C(45)	24(1)	30(1)	19(1)	2(1)	2(1)	5(1)
C(46)	27(1)	33(1)	20(1)	-2(1)	0(1)	1(1)
C(47)	36(2)	42(2)	26(1)	-1(1)	-9(1)	1(1)
C(48)	42(2)	45(2)	28(1)	5(1)	-9(1)	9(1)
C(49)	39(2)	34(2)	27(1)	7(1)	-1(1)	3(1)
C(50)	29(1)	30(1)	20(1)	3(1)	2(1)	1(1)
C(51)	41(2)	32(2)	25(1)	-4(1)	-4(1)	-3(1)
C(52)	54(2)	46(2)	69(2)	-3(2)	-15(2)	-13(2)
C(53)	70(2)	40(2)	53(2)	-6(1)	10(2)	2(2)
C(54)	37(2)	30(1)	24(1)	6(1)	-3(1)	-4(1)
C(55)	60(2)	32(2)	40(2)	4(1)	-11(1)	-6(1)
C(56)	42(2)	54(2)	44(2)	7(1)	-2(1)	-12(1)

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

	x	y	z	U(eq)
H(1)	970(18)	2236(13)	1580(11)	35(7)
H(1A)	-604	3621	415	59
H(1B)	-1578	3703	867	59
H(1C)	-1268	2932	604	59
H(2A)	1188	4222	1315	63
H(2B)	1157	4017	2034	63
H(2C)	267	4510	1743	63
H(4)	-3617	2234	2958	37
H(5)	-2329	1918	3740	36
H(7)	4156	2006	711	38
H(8)	3451	2753	-123	37
H(11)	-3744	4330	1247	42
H(12)	-4326	3525	507	46
H(13)	-4000	2312	617	44
H(15)	-2049	3898	2505	43
H(16A)	-1759	4734	1700	74
H(16B)	-1954	5123	2349	74
H(16C)	-2858	5094	1843	74
H(17A)	-4066	4503	2605	84
H(17B)	-3171	4571	3114	84
H(17C)	-3682	3808	2973	84
H(18)	-2787	1491	1937	51
H(19A)	-2326	1446	646	128
H(19B)	-1986	847	1135	128
H(19C)	-1509	1636	1179	128
H(20A)	-4222	1213	960	138
H(20B)	-4511	1251	1679	138
H(20C)	-3792	618	1427	138
H(23)	1560	1318	4024	42
H(24)	1983	2364	4544	48

H(25)	983	3381	4430	45
H(27)	-769	968	3262	36
H(28A)	5	669	2316	54
H(28B)	1008	1134	2483	54
H(28C)	-80	1522	2366	54
H(29A)	222	-72	3277	60
H(29B)	363	315	3932	60
H(29C)	1255	371	3421	60
H(30)	-1399	3494	3579	43
H(31A)	-107	3845	2867	61
H(31B)	480	4277	3402	61
H(31C)	-640	4532	3174	61
H(32A)	-200	4251	4484	74
H(32B)	-1162	3748	4655	74
H(32C)	-1342	4462	4261	74
H(35)	2836	-18	2040	45
H(36)	3307	468	2990	45
H(37)	3389	1697	3121	41
H(39)	2368	990	647	45
H(40A)	915	233	610	82
H(40B)	754	840	1123	82
H(40C)	1058	43	1327	82
H(41A)	2713	-174	335	85
H(41B)	2847	-432	1037	85
H(41C)	3675	102	737	85
H(42)	2860	3012	1929	36
H(43A)	2515	3567	2878	67
H(43B)	2750	2839	3242	67
H(43C)	1760	2894	2799	67
H(44A)	4657	2861	2025	76
H(44B)	4554	2766	2758	76
H(44C)	4303	3523	2445	76
H(47)	-400	2837	-1060	41
H(48)	-105	4035	-1282	46
H(49)	1101	4685	-721	40
H(51)	564	1878	216	40

H(52A)	-658	1690	-875	85
H(52B)	-1119	2009	-246	85
H(52C)	-700	1203	-267	85
H(53A)	1243	1557	-1008	81
H(53B)	1191	992	-452	81
H(53C)	1991	1645	-422	81
H(54)	2588	4053	565	36
H(55A)	1952	5353	-15	66
H(55B)	2451	5268	659	66
H(55C)	1292	5001	533	66
H(56A)	3207	4623	-612	70
H(56B)	3691	3927	-291	70
H(56C)	3881	4701	6	70

Crystallography tables for compound 4

Table 1. Crystal data and structure refinement for 4.

Identification code	BM105_0m	
Empirical formula	C ₅₈ H ₈₄ Al ₂ N ₆	
Formula weight	919.27	
Temperature	125(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.064(2) Å	α = 62.143(2)°.
	b = 22.957(4) Å	β = 75.811(2)°.
	c = 24.196(4) Å	γ = 89.463(2)°.
Volume	5700.7(17) Å ³	
Z	4	
Density (calculated)	1.071 Mg/m ³	
Absorption coefficient	0.091 mm ⁻¹	
F(000)	2000	
Crystal size	0.300 x 0.240 x 0.200 mm ³	
Theta range for data collection	1.900 to 24.999°.	
Index ranges	-14 ≤ h ≤ 14, -27 ≤ k ≤ 27, -28 ≤ l ≤ 28	
Reflections collected	55016	
Independent reflections	19990 [R(int) = 0.0496]	
Completeness to theta = 24.999°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6363	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	19990 / 0 / 1230	
Goodness-of-fit on F ²	1.112	
Final R indices [I > 2σ(I)]	R1 = 0.0641, wR2 = 0.1718	
R indices (all data)	R1 = 0.0917, wR2 = 0.1927	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.596 and -0.470 e.Å ⁻³	

Table 2. 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	$U(\text{eq})$
Al(1)	9411(1)	6487(1)	1851(1)	25(1)
Al(2)	8163(1)	6183(1)	3110(1)	25(1)
Al(3)	3950(1)	1155(1)	3159(1)	25(1)
Al(4)	3781(1)	1446(1)	1928(1)	27(1)
N(1)	9638(2)	7792(1)	2587(1)	26(1)
N(2)	9540(2)	8131(1)	1591(1)	27(1)
N(3)	9045(2)	6953(1)	2343(1)	23(1)
N(4)	7303(2)	4692(1)	3075(1)	24(1)
N(5)	9038(2)	4753(1)	2483(1)	24(1)
N(6)	8567(2)	5711(1)	2625(1)	23(1)
N(7)	4946(2)	-321(1)	3061(1)	23(1)
N(8)	3790(2)	-240(1)	2464(1)	23(1)
N(9)	3975(2)	671(1)	2689(1)	24(1)
N(10)	2857(2)	2771(1)	2630(1)	27(1)
N(11)	3878(2)	3082(1)	1633(1)	28(1)
N(12)	3729(2)	1919(1)	2408(1)	24(1)
C(1)	9367(2)	7556(1)	2193(1)	21(1)
C(2)	9973(3)	8473(2)	2234(2)	32(1)
C(3)	9913(3)	8681(2)	1630(2)	33(1)
C(4)	9851(3)	7408(2)	3216(1)	29(1)
C(5)	10927(3)	7174(2)	3235(2)	36(1)
C(6)	11170(4)	6870(2)	3835(2)	49(1)
C(7)	10390(4)	6809(2)	4378(2)	54(1)
C(8)	9339(4)	7046(2)	4356(2)	48(1)
C(9)	9032(3)	7360(2)	3763(2)	34(1)
C(10)	11829(3)	7273(2)	2626(2)	40(1)
C(11)	12504(4)	6686(2)	2727(2)	64(1)
C(12)	12672(4)	7893(2)	2369(2)	65(1)
C(13)	7902(3)	7646(2)	3722(2)	39(1)
C(14)	7974(3)	8325(2)	3697(2)	45(1)
C(15)	6883(4)	7179(2)	4285(2)	61(1)

C(16)	9274(3)	8208(1)	1011(1)	28(1)
C(17)	8117(3)	8167(2)	1008(2)	35(1)
C(18)	7904(4)	8275(2)	425(2)	49(1)
C(19)	8792(4)	8427(2)	-120(2)	54(1)
C(20)	9915(4)	8486(2)	-109(2)	48(1)
C(21)	10196(3)	8377(2)	456(2)	36(1)
C(22)	7154(3)	8034(2)	1603(2)	48(1)
C(23)	7031(4)	8642(3)	1702(3)	87(2)
C(24)	5978(4)	7806(2)	1580(3)	69(1)
C(25)	11446(3)	8471(2)	435(2)	46(1)
C(26)	11894(4)	9214(2)	87(2)	61(1)
C(27)	12216(4)	8124(3)	103(2)	72(1)
C(28)	8322(2)	5114(1)	2722(1)	21(1)
C(29)	7403(3)	4100(2)	3038(2)	31(1)
C(30)	8451(3)	4137(2)	2681(2)	30(1)
C(31)	6214(3)	4805(1)	3398(1)	25(1)
C(32)	5904(3)	4496(2)	4081(2)	28(1)
C(33)	4790(3)	4534(2)	4393(2)	32(1)
C(34)	4030(3)	4860(2)	4040(2)	35(1)
C(35)	4371(3)	5177(2)	3367(2)	32(1)
C(36)	5468(3)	5152(1)	3032(2)	27(1)
C(37)	6742(3)	4135(2)	4474(2)	32(1)
C(38)	6528(4)	3380(2)	4746(2)	49(1)
C(39)	6689(3)	4300(2)	5026(2)	42(1)
C(40)	5853(3)	5502(2)	2287(2)	32(1)
C(41)	5155(3)	6072(2)	1973(2)	39(1)
C(42)	5802(4)	5017(2)	2025(2)	50(1)
C(43)	10269(3)	4893(1)	2212(2)	24(1)
C(44)	10718(3)	5074(1)	1550(2)	27(1)
C(45)	11919(3)	5171(2)	1311(2)	31(1)
C(46)	12622(3)	5108(2)	1705(2)	31(1)
C(47)	12155(3)	4920(1)	2356(2)	28(1)
C(48)	10967(3)	4789(1)	2629(2)	26(1)
C(49)	9958(3)	5150(2)	1113(2)	34(1)
C(50)	10369(3)	5771(2)	444(2)	41(1)
C(51)	9895(4)	4532(2)	1026(2)	50(1)

C(52)	10446(3)	4500(2)	3361(2)	29(1)
C(53)	11174(3)	4700(2)	3693(2)	41(1)
C(54)	10257(4)	3737(2)	3679(2)	45(1)
C(55)	11112(3)	6567(2)	1573(2)	37(1)
C(56)	8585(3)	6633(2)	1192(2)	33(1)
C(57)	8791(3)	5759(2)	3870(2)	41(1)
C(58)	6554(3)	6386(2)	3274(2)	40(1)
C(59)	4218(2)	100(1)	2739(1)	22(1)
C(60)	4973(3)	-882(2)	2973(2)	28(1)
C(61)	4277(3)	-832(1)	2612(2)	26(1)
C(62)	5656(3)	-235(2)	3426(2)	25(1)
C(63)	5234(3)	-554(1)	4106(2)	28(1)
C(64)	5998(3)	-541(2)	4452(2)	32(1)
C(65)	7105(3)	-238(2)	4142(2)	36(1)
C(66)	7491(3)	90(2)	3468(2)	32(1)
C(67)	6769(3)	102(2)	3094(2)	27(1)
C(68)	4009(3)	-897(2)	4451(2)	32(1)
C(69)	3910(3)	-1628(2)	4613(2)	41(1)
C(70)	3501(3)	-850(2)	5075(2)	43(1)
C(71)	7175(3)	467(2)	2356(2)	34(1)
C(72)	7563(3)	-1(2)	2071(2)	44(1)
C(73)	8145(3)	1033(2)	2083(2)	41(1)
C(74)	2809(3)	-112(1)	2207(1)	23(1)
C(75)	2971(3)	74(1)	1547(1)	24(1)
C(76)	1991(3)	157(2)	1318(2)	28(1)
C(77)	906(3)	68(2)	1724(2)	31(1)
C(78)	772(3)	-126(2)	2378(2)	28(1)
C(79)	1701(3)	-237(1)	2635(1)	25(1)
C(80)	4154(3)	178(2)	1088(2)	30(1)
C(81)	4324(3)	819(2)	438(2)	39(1)
C(82)	4346(3)	-413(2)	956(2)	42(1)
C(83)	1538(3)	-514(2)	3362(2)	31(1)
C(84)	1518(3)	-1274(2)	3688(2)	44(1)
C(85)	457(3)	-333(2)	3699(2)	42(1)
C(86)	3516(3)	2524(1)	2243(1)	23(1)
C(87)	2819(3)	3447(2)	2259(2)	33(1)

C(88)	3432(3)	3638(2)	1658(2)	34(1)
C(89)	2213(3)	2418(1)	3303(2)	28(1)
C(90)	2700(3)	2451(2)	3762(2)	32(1)
C(91)	2014(4)	2176(2)	4402(2)	45(1)
C(92)	922(4)	1891(2)	4567(2)	55(1)
C(93)	460(3)	1846(2)	4124(2)	53(1)
C(94)	1103(3)	2117(2)	3464(2)	37(1)
C(95)	3880(3)	2796(2)	3589(2)	35(1)
C(96)	3818(4)	3496(2)	3511(2)	54(1)
C(97)	4573(4)	2417(2)	4072(2)	48(1)
C(98)	603(3)	2092(2)	2959(2)	51(1)
C(99)	23(5)	2716(2)	2632(3)	75(2)
C(100)	-271(4)	1478(2)	3235(3)	76(2)
C(101)	4721(3)	3148(2)	1059(2)	31(1)
C(102)	5879(3)	3130(2)	1055(2)	38(1)
C(103)	6659(3)	3231(2)	477(2)	51(1)
C(104)	6297(4)	3363(2)	-69(2)	57(1)
C(105)	5168(4)	3396(2)	-51(2)	50(1)
C(106)	4333(3)	3294(2)	509(2)	39(1)
C(107)	6279(3)	3022(2)	1640(2)	48(1)
C(108)	7457(4)	2771(2)	1635(3)	75(2)
C(109)	6296(5)	3660(2)	1693(3)	78(2)
C(110)	3099(4)	3358(2)	491(2)	50(1)
C(111)	2689(5)	2958(3)	203(2)	80(2)
C(112)	2925(4)	4097(2)	106(2)	72(1)
C(113)	2644(3)	748(2)	3947(2)	40(1)
C(114)	5446(3)	1364(2)	3272(2)	38(1)
C(115)	2266(3)	1503(2)	1744(2)	40(1)
C(116)	5213(3)	1593(2)	1252(2)	37(1)

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

Al(1)-N(3)	1.919(2)
Al(1)-N(6)	1.923(3)
Al(1)-C(55)	1.978(3)
Al(1)-C(56)	1.979(3)
Al(1)-Al(2)	2.7954(13)
Al(2)-N(6)	1.920(2)
Al(2)-N(3)	1.924(3)
Al(2)-C(57)	1.975(4)
Al(2)-C(58)	1.980(4)
Al(3)-N(9)	1.921(2)
Al(3)-N(12)	1.923(3)
Al(3)-C(113)	1.970(3)
Al(3)-C(114)	1.985(4)
Al(3)-Al(4)	2.7923(13)
Al(4)-N(12)	1.918(2)
Al(4)-N(9)	1.936(3)
Al(4)-C(116)	1.970(3)
Al(4)-C(115)	1.974(4)
N(1)-C(2)	1.391(4)
N(1)-C(1)	1.395(4)
N(1)-C(4)	1.447(4)
N(2)-C(3)	1.396(4)
N(2)-C(1)	1.403(4)
N(2)-C(16)	1.445(4)
N(3)-C(1)	1.292(4)
N(4)-C(28)	1.384(4)
N(4)-C(29)	1.404(4)
N(4)-C(31)	1.443(4)
N(5)-C(30)	1.396(4)
N(5)-C(28)	1.398(4)
N(5)-C(43)	1.440(4)
N(6)-C(28)	1.302(4)
N(7)-C(59)	1.388(4)
N(7)-C(60)	1.399(4)

N(7)-C(62)	1.447(4)
N(8)-C(61)	1.397(4)
N(8)-C(59)	1.406(4)
N(8)-C(74)	1.435(4)
N(9)-C(59)	1.297(4)
N(10)-C(87)	1.390(4)
N(10)-C(86)	1.397(4)
N(10)-C(89)	1.439(4)
N(11)-C(86)	1.392(4)
N(11)-C(88)	1.401(4)
N(11)-C(101)	1.450(4)
N(12)-C(86)	1.296(4)
C(2)-C(3)	1.329(4)
C(2)-H(2)	0.9500
C(3)-H(3)	0.9500
C(4)-C(9)	1.403(4)
C(4)-C(5)	1.403(5)
C(5)-C(6)	1.393(5)
C(5)-C(10)	1.520(5)
C(6)-C(7)	1.362(6)
C(6)-H(6)	0.9500
C(7)-C(8)	1.380(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.415(5)
C(8)-H(8)	0.9500
C(9)-C(13)	1.513(5)
C(10)-C(11)	1.519(5)
C(10)-C(12)	1.528(5)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.534(5)

C(13)-C(15)	1.534(5)
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.402(5)
C(16)-C(21)	1.409(5)
C(17)-C(18)	1.403(5)
C(17)-C(22)	1.513(5)
C(18)-C(19)	1.376(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.371(6)
C(19)-H(19)	0.9500
C(20)-C(21)	1.395(5)
C(20)-H(20)	0.9500
C(21)-C(25)	1.511(5)
C(22)-C(23)	1.523(6)
C(22)-C(24)	1.539(6)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(27)	1.536(5)
C(25)-C(26)	1.538(5)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800

C(27)-H(27C)	0.9800
C(29)-C(30)	1.322(4)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-C(36)	1.396(4)
C(31)-C(32)	1.407(4)
C(32)-C(33)	1.395(4)
C(32)-C(37)	1.527(5)
C(33)-C(34)	1.381(5)
C(33)-H(33)	0.9500
C(34)-C(35)	1.386(5)
C(34)-H(34)	0.9500
C(35)-C(36)	1.388(4)
C(35)-H(35)	0.9500
C(36)-C(40)	1.534(4)
C(37)-C(38)	1.537(5)
C(37)-C(39)	1.538(5)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(42)	1.523(5)
C(40)-C(41)	1.537(5)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(48)	1.404(4)
C(43)-C(44)	1.411(4)
C(44)-C(45)	1.400(4)

C(44)-C(49)	1.513(5)
C(45)-C(46)	1.382(5)
C(45)-H(45)	0.9500
C(46)-C(47)	1.386(4)
C(46)-H(46)	0.9500
C(47)-C(48)	1.393(4)
C(47)-H(47)	0.9500
C(48)-C(52)	1.528(4)
C(49)-C(51)	1.533(5)
C(49)-C(50)	1.538(5)
C(49)-H(49)	1.0000
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-C(53)	1.526(5)
C(52)-C(54)	1.542(4)
C(52)-H(52)	1.0000
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
C(58)-H(58A)	0.9800

C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(60)-C(61)	1.321(4)
C(60)-H(60)	0.9500
C(61)-H(61)	0.9500
C(62)-C(67)	1.399(4)
C(62)-C(63)	1.404(4)
C(63)-C(64)	1.397(4)
C(63)-C(68)	1.518(5)
C(64)-C(65)	1.367(5)
C(64)-H(64)	0.9500
C(65)-C(66)	1.390(5)
C(65)-H(65)	0.9500
C(66)-C(67)	1.393(4)
C(66)-H(66)	0.9500
C(67)-C(71)	1.520(4)
C(68)-C(69)	1.535(4)
C(68)-C(70)	1.537(4)
C(68)-H(68)	1.0000
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800
C(71)-C(73)	1.530(5)
C(71)-C(72)	1.540(5)
C(71)-H(71)	1.0000
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
C(73)-H(73A)	0.9800
C(73)-H(73B)	0.9800
C(73)-H(73C)	0.9800
C(74)-C(75)	1.408(4)
C(74)-C(79)	1.412(4)

C(75)-C(76)	1.401(4)
C(75)-C(80)	1.519(4)
C(76)-C(77)	1.381(5)
C(76)-H(76)	0.9500
C(77)-C(78)	1.394(4)
C(77)-H(77)	0.9500
C(78)-C(79)	1.377(4)
C(78)-H(78)	0.9500
C(79)-C(83)	1.524(4)
C(80)-C(82)	1.536(4)
C(80)-C(81)	1.538(4)
C(80)-H(80)	1.0000
C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(83)-C(85)	1.525(5)
C(83)-C(84)	1.540(5)
C(83)-H(83)	1.0000
C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800
C(84)-H(84C)	0.9800
C(85)-H(85A)	0.9800
C(85)-H(85B)	0.9800
C(85)-H(85C)	0.9800
C(87)-C(88)	1.317(4)
C(87)-H(87)	0.9500
C(88)-H(88)	0.9500
C(89)-C(94)	1.389(5)
C(89)-C(90)	1.411(5)
C(90)-C(91)	1.395(5)
C(90)-C(95)	1.499(5)
C(91)-C(92)	1.355(6)
C(91)-H(91)	0.9500

C(92)-C(93)	1.366(6)
C(92)-H(92)	0.9500
C(93)-C(94)	1.419(5)
C(93)-H(93)	0.9500
C(94)-C(98)	1.513(5)
C(95)-C(97)	1.529(5)
C(95)-C(96)	1.533(5)
C(95)-H(95)	1.0000
C(96)-H(96A)	0.9800
C(96)-H(96B)	0.9800
C(96)-H(96C)	0.9800
C(97)-H(97A)	0.9800
C(97)-H(97B)	0.9800
C(97)-H(97C)	0.9800
C(98)-C(100)	1.533(6)
C(98)-C(99)	1.536(6)
C(98)-H(98)	1.0000
C(99)-H(99A)	0.9800
C(99)-H(99B)	0.9800
C(99)-H(99C)	0.9800
C(100)-H(10A)	0.9800
C(100)-H(10B)	0.9800
C(100)-H(10C)	0.9800
C(101)-C(102)	1.395(5)
C(101)-C(106)	1.409(5)
C(102)-C(103)	1.397(5)
C(102)-C(107)	1.517(5)
C(103)-C(104)	1.392(6)
C(103)-H(103)	0.9500
C(104)-C(105)	1.355(6)
C(104)-H(104)	0.9500
C(105)-C(106)	1.394(5)
C(105)-H(105)	0.9500
C(106)-C(110)	1.504(6)
C(107)-C(109)	1.529(5)
C(107)-C(108)	1.528(6)

C(107)-H(107)	1.0000
C(108)-H(10D)	0.9800
C(108)-H(10E)	0.9800
C(108)-H(10F)	0.9800
C(109)-H(10G)	0.9800
C(109)-H(10H)	0.9800
C(109)-H(10I)	0.9800
C(110)-C(111)	1.533(6)
C(110)-C(112)	1.549(6)
C(110)-H(110)	1.0000
C(111)-H(11D)	0.9800
C(111)-H(11E)	0.9800
C(111)-H(11F)	0.9800
C(112)-H(11G)	0.9800
C(112)-H(11H)	0.9800
C(112)-H(11I)	0.9800
C(113)-H(11J)	0.9800
C(113)-H(11K)	0.9800
C(113)-H(11L)	0.9800
C(114)-H(11M)	0.9800
C(114)-H(11N)	0.9800
C(114)-H(11O)	0.9800
C(115)-H(11P)	0.9800
C(115)-H(11Q)	0.9800
C(115)-H(11R)	0.9800
C(116)-H(11S)	0.9800
C(116)-H(11T)	0.9800
C(116)-H(11U)	0.9800
N(3)-Al(1)-N(6)	86.64(10)
N(3)-Al(1)-C(55)	106.10(13)
N(6)-Al(1)-C(55)	119.63(14)
N(3)-Al(1)-C(56)	119.00(13)
N(6)-Al(1)-C(56)	105.15(13)
C(55)-Al(1)-C(56)	117.12(15)
N(3)-Al(1)-Al(2)	43.39(7)

N(6)-Al(1)-Al(2)	43.28(7)
C(55)-Al(1)-Al(2)	123.11(12)
C(56)-Al(1)-Al(2)	119.77(11)
N(6)-Al(2)-N(3)	86.62(10)
N(6)-Al(2)-C(57)	107.57(13)
N(3)-Al(2)-C(57)	118.70(14)
N(6)-Al(2)-C(58)	117.37(13)
N(3)-Al(2)-C(58)	106.66(14)
C(57)-Al(2)-C(58)	116.63(17)
N(6)-Al(2)-Al(1)	43.37(7)
N(3)-Al(2)-Al(1)	43.27(7)
C(57)-Al(2)-Al(1)	123.59(12)
C(58)-Al(2)-Al(1)	119.77(12)
N(9)-Al(3)-N(12)	87.14(11)
N(9)-Al(3)-C(113)	108.48(13)
N(12)-Al(3)-C(113)	117.90(14)
N(9)-Al(3)-C(114)	116.58(13)
N(12)-Al(3)-C(114)	106.96(14)
C(113)-Al(3)-C(114)	116.53(16)
N(9)-Al(3)-Al(4)	43.84(8)
N(12)-Al(3)-Al(4)	43.31(7)
C(113)-Al(3)-Al(4)	123.54(12)
C(114)-Al(3)-Al(4)	119.93(12)
N(12)-Al(4)-N(9)	86.86(11)
N(12)-Al(4)-C(116)	117.63(13)
N(9)-Al(4)-C(116)	103.66(13)
N(12)-Al(4)-C(115)	104.43(13)
N(9)-Al(4)-C(115)	118.36(14)
C(116)-Al(4)-C(115)	121.28(16)
N(12)-Al(4)-Al(3)	43.45(8)
N(9)-Al(4)-Al(3)	43.42(7)
C(116)-Al(4)-Al(3)	118.11(12)
C(115)-Al(4)-Al(3)	120.61(12)
C(2)-N(1)-C(1)	110.5(2)
C(2)-N(1)-C(4)	120.2(2)
C(1)-N(1)-C(4)	127.5(2)

C(3)-N(2)-C(1)	110.1(2)
C(3)-N(2)-C(16)	121.0(2)
C(1)-N(2)-C(16)	128.6(2)
C(1)-N(3)-Al(1)	130.7(2)
C(1)-N(3)-Al(2)	135.9(2)
Al(1)-N(3)-Al(2)	93.34(11)
C(28)-N(4)-C(29)	109.7(2)
C(28)-N(4)-C(31)	129.8(2)
C(29)-N(4)-C(31)	120.2(2)
C(30)-N(5)-C(28)	110.2(2)
C(30)-N(5)-C(43)	121.4(2)
C(28)-N(5)-C(43)	126.8(2)
C(28)-N(6)-Al(2)	136.3(2)
C(28)-N(6)-Al(1)	130.1(2)
Al(2)-N(6)-Al(1)	93.35(11)
C(59)-N(7)-C(60)	110.7(2)
C(59)-N(7)-C(62)	129.3(2)
C(60)-N(7)-C(62)	120.0(2)
C(61)-N(8)-C(59)	110.0(2)
C(61)-N(8)-C(74)	121.6(2)
C(59)-N(8)-C(74)	126.8(2)
C(59)-N(9)-Al(3)	138.9(2)
C(59)-N(9)-Al(4)	127.4(2)
Al(3)-N(9)-Al(4)	92.74(11)
C(87)-N(10)-C(86)	110.2(2)
C(87)-N(10)-C(89)	120.6(2)
C(86)-N(10)-C(89)	129.1(2)
C(86)-N(11)-C(88)	110.0(2)
C(86)-N(11)-C(101)	128.2(2)
C(88)-N(11)-C(101)	121.2(2)
C(86)-N(12)-Al(4)	128.4(2)
C(86)-N(12)-Al(3)	138.2(2)
Al(4)-N(12)-Al(3)	93.23(11)
N(3)-C(1)-N(1)	128.5(3)
N(3)-C(1)-N(2)	128.2(3)
N(1)-C(1)-N(2)	103.3(2)

C(3)-C(2)-N(1)	108.1(3)
C(3)-C(2)-H(2)	125.9
N(1)-C(2)-H(2)	125.9
C(2)-C(3)-N(2)	108.0(3)
C(2)-C(3)-H(3)	126.0
N(2)-C(3)-H(3)	126.0
C(9)-C(4)-C(5)	123.4(3)
C(9)-C(4)-N(1)	118.1(3)
C(5)-C(4)-N(1)	118.0(3)
C(6)-C(5)-C(4)	117.4(3)
C(6)-C(5)-C(10)	120.3(3)
C(4)-C(5)-C(10)	122.2(3)
C(7)-C(6)-C(5)	120.8(4)
C(7)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(6)-C(7)-C(8)	121.6(4)
C(6)-C(7)-H(7)	119.2
C(8)-C(7)-H(7)	119.2
C(7)-C(8)-C(9)	120.7(4)
C(7)-C(8)-H(8)	119.6
C(9)-C(8)-H(8)	119.6
C(4)-C(9)-C(8)	116.1(3)
C(4)-C(9)-C(13)	122.2(3)
C(8)-C(9)-C(13)	121.7(3)
C(11)-C(10)-C(5)	113.8(3)
C(11)-C(10)-C(12)	108.9(3)
C(5)-C(10)-C(12)	109.8(3)
C(11)-C(10)-H(10)	108.1
C(5)-C(10)-H(10)	108.1
C(12)-C(10)-H(10)	108.1
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(9)-C(13)-C(14)	110.6(3)
C(9)-C(13)-C(15)	112.4(3)
C(14)-C(13)-C(15)	110.1(3)
C(9)-C(13)-H(13)	107.8
C(14)-C(13)-H(13)	107.8
C(15)-C(13)-H(13)	107.8
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-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)	122.8(3)
C(17)-C(16)-N(2)	119.0(3)
C(21)-C(16)-N(2)	118.0(3)
C(16)-C(17)-C(18)	116.8(3)
C(16)-C(17)-C(22)	121.0(3)
C(18)-C(17)-C(22)	122.1(3)
C(19)-C(18)-C(17)	121.4(4)
C(19)-C(18)-H(18)	119.3
C(17)-C(18)-H(18)	119.3
C(20)-C(19)-C(18)	120.4(4)
C(20)-C(19)-H(19)	119.8
C(18)-C(19)-H(19)	119.8

C(19)-C(20)-C(21)	121.6(4)
C(19)-C(20)-H(20)	119.2
C(21)-C(20)-H(20)	119.2
C(20)-C(21)-C(16)	117.0(4)
C(20)-C(21)-C(25)	119.3(3)
C(16)-C(21)-C(25)	123.7(3)
C(17)-C(22)-C(23)	111.9(3)
C(17)-C(22)-C(24)	113.0(4)
C(23)-C(22)-C(24)	108.1(3)
C(17)-C(22)-H(22)	107.9
C(23)-C(22)-H(22)	107.9
C(24)-C(22)-H(22)	107.9
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(21)-C(25)-C(27)	112.5(4)
C(21)-C(25)-C(26)	110.4(3)
C(27)-C(25)-C(26)	109.7(3)
C(21)-C(25)-H(25)	108.0
C(27)-C(25)-H(25)	108.0
C(26)-C(25)-H(25)	108.0
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(6)-C(28)-N(4)	128.7(3)
N(6)-C(28)-N(5)	127.4(3)
N(4)-C(28)-N(5)	103.9(2)
C(30)-C(29)-N(4)	108.5(3)
C(30)-C(29)-H(29)	125.8
N(4)-C(29)-H(29)	125.8
C(29)-C(30)-N(5)	107.7(3)
C(29)-C(30)-H(30)	126.2
N(5)-C(30)-H(30)	126.2
C(36)-C(31)-C(32)	122.7(3)
C(36)-C(31)-N(4)	119.2(3)
C(32)-C(31)-N(4)	117.8(3)
C(33)-C(32)-C(31)	117.4(3)
C(33)-C(32)-C(37)	120.5(3)
C(31)-C(32)-C(37)	122.1(3)
C(34)-C(33)-C(32)	120.6(3)
C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7
C(33)-C(34)-C(35)	120.7(3)
C(33)-C(34)-H(34)	119.7
C(35)-C(34)-H(34)	119.7
C(34)-C(35)-C(36)	120.9(3)
C(34)-C(35)-H(35)	119.5
C(36)-C(35)-H(35)	119.5
C(35)-C(36)-C(31)	117.5(3)
C(35)-C(36)-C(40)	121.3(3)
C(31)-C(36)-C(40)	121.1(3)
C(32)-C(37)-C(38)	111.7(3)
C(32)-C(37)-C(39)	111.5(3)
C(38)-C(37)-C(39)	110.2(3)

C(32)-C(37)-H(37)	107.7
C(38)-C(37)-H(37)	107.7
C(39)-C(37)-H(37)	107.7
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(42)-C(40)-C(36)	111.8(3)
C(42)-C(40)-C(41)	109.0(3)
C(36)-C(40)-C(41)	113.1(3)
C(42)-C(40)-H(40)	107.5
C(36)-C(40)-H(40)	107.5
C(41)-C(40)-H(40)	107.5
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(48)-C(43)-C(44)	123.1(3)
C(48)-C(43)-N(5)	118.6(3)
C(44)-C(43)-N(5)	118.1(3)

C(45)-C(44)-C(43)	116.6(3)
C(45)-C(44)-C(49)	120.7(3)
C(43)-C(44)-C(49)	122.7(3)
C(46)-C(45)-C(44)	121.2(3)
C(46)-C(45)-H(45)	119.4
C(44)-C(45)-H(45)	119.4
C(45)-C(46)-C(47)	120.8(3)
C(45)-C(46)-H(46)	119.6
C(47)-C(46)-H(46)	119.6
C(46)-C(47)-C(48)	120.7(3)
C(46)-C(47)-H(47)	119.7
C(48)-C(47)-H(47)	119.7
C(47)-C(48)-C(43)	117.5(3)
C(47)-C(48)-C(52)	121.2(3)
C(43)-C(48)-C(52)	121.2(3)
C(44)-C(49)-C(51)	110.4(3)
C(44)-C(49)-C(50)	112.6(3)
C(51)-C(49)-C(50)	109.6(3)
C(44)-C(49)-H(49)	108.0
C(51)-C(49)-H(49)	108.0
C(50)-C(49)-H(49)	108.0
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(48)-C(52)-C(53)	114.0(3)
C(48)-C(52)-C(54)	109.2(2)
C(53)-C(52)-C(54)	109.2(3)

C(48)-C(52)-H(52)	108.1
C(53)-C(52)-H(52)	108.1
C(54)-C(52)-H(52)	108.1
C(52)-C(53)-H(53A)	109.5
C(52)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(52)-C(54)-H(54A)	109.5
C(52)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(52)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
Al(1)-C(55)-H(55A)	109.5
Al(1)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
Al(1)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
Al(1)-C(56)-H(56A)	109.5
Al(1)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
Al(1)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
Al(2)-C(57)-H(57A)	109.5
Al(2)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
Al(2)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
Al(2)-C(58)-H(58A)	109.5
Al(2)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5

Al(2)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
N(9)-C(59)-N(7)	129.9(3)
N(9)-C(59)-N(8)	126.9(3)
N(7)-C(59)-N(8)	103.2(2)
C(61)-C(60)-N(7)	107.9(3)
C(61)-C(60)-H(60)	126.0
N(7)-C(60)-H(60)	126.0
C(60)-C(61)-N(8)	108.3(3)
C(60)-C(61)-H(61)	125.9
N(8)-C(61)-H(61)	125.9
C(67)-C(62)-C(63)	123.2(3)
C(67)-C(62)-N(7)	118.6(3)
C(63)-C(62)-N(7)	117.9(3)
C(64)-C(63)-C(62)	116.7(3)
C(64)-C(63)-C(68)	121.4(3)
C(62)-C(63)-C(68)	121.9(3)
C(65)-C(64)-C(63)	121.4(3)
C(65)-C(64)-H(64)	119.3
C(63)-C(64)-H(64)	119.3
C(64)-C(65)-C(66)	120.6(3)
C(64)-C(65)-H(65)	119.7
C(66)-C(65)-H(65)	119.7
C(65)-C(66)-C(67)	120.8(3)
C(65)-C(66)-H(66)	119.6
C(67)-C(66)-H(66)	119.6
C(66)-C(67)-C(62)	117.1(3)
C(66)-C(67)-C(71)	121.3(3)
C(62)-C(67)-C(71)	121.5(3)
C(63)-C(68)-C(69)	112.3(3)
C(63)-C(68)-C(70)	112.6(3)
C(69)-C(68)-C(70)	109.2(3)
C(63)-C(68)-H(68)	107.5
C(69)-C(68)-H(68)	107.5
C(70)-C(68)-H(68)	107.5

C(68)-C(69)-H(69A)	109.5
C(68)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(68)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(68)-C(70)-H(70A)	109.5
C(68)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(68)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
C(67)-C(71)-C(73)	113.3(3)
C(67)-C(71)-C(72)	112.5(3)
C(73)-C(71)-C(72)	108.8(3)
C(67)-C(71)-H(71)	107.3
C(73)-C(71)-H(71)	107.3
C(72)-C(71)-H(71)	107.3
C(71)-C(72)-H(72A)	109.5
C(71)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(71)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(71)-C(73)-H(73A)	109.5
C(71)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5
C(71)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
C(75)-C(74)-C(79)	121.9(3)
C(75)-C(74)-N(8)	118.8(3)
C(79)-C(74)-N(8)	119.0(3)
C(76)-C(75)-C(74)	117.6(3)
C(76)-C(75)-C(80)	119.9(3)
C(74)-C(75)-C(80)	122.5(3)

C(77)-C(76)-C(75)	121.1(3)
C(77)-C(76)-H(76)	119.5
C(75)-C(76)-H(76)	119.5
C(76)-C(77)-C(78)	120.0(3)
C(76)-C(77)-H(77)	120.0
C(78)-C(77)-H(77)	120.0
C(79)-C(78)-C(77)	121.5(3)
C(79)-C(78)-H(78)	119.2
C(77)-C(78)-H(78)	119.2
C(78)-C(79)-C(74)	117.8(3)
C(78)-C(79)-C(83)	121.3(3)
C(74)-C(79)-C(83)	120.9(3)
C(75)-C(80)-C(82)	111.0(3)
C(75)-C(80)-C(81)	111.8(3)
C(82)-C(80)-C(81)	109.1(3)
C(75)-C(80)-H(80)	108.3
C(82)-C(80)-H(80)	108.3
C(81)-C(80)-H(80)	108.3
C(80)-C(81)-H(81A)	109.5
C(80)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(80)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(80)-C(82)-H(82A)	109.5
C(80)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(80)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(85)-C(83)-C(79)	113.7(3)
C(85)-C(83)-C(84)	109.8(3)
C(79)-C(83)-C(84)	109.6(3)
C(85)-C(83)-H(83)	107.9
C(79)-C(83)-H(83)	107.9
C(84)-C(83)-H(83)	107.9

C(83)-C(84)-H(84A)	109.5
C(83)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5
C(83)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5
C(83)-C(85)-H(85A)	109.5
C(83)-C(85)-H(85B)	109.5
H(85A)-C(85)-H(85B)	109.5
C(83)-C(85)-H(85C)	109.5
H(85A)-C(85)-H(85C)	109.5
H(85B)-C(85)-H(85C)	109.5
N(12)-C(86)-N(11)	128.2(3)
N(12)-C(86)-N(10)	128.4(3)
N(11)-C(86)-N(10)	103.4(2)
C(88)-C(87)-N(10)	108.3(3)
C(88)-C(87)-H(87)	125.8
N(10)-C(87)-H(87)	125.8
C(87)-C(88)-N(11)	108.0(3)
C(87)-C(88)-H(88)	126.0
N(11)-C(88)-H(88)	126.0
C(94)-C(89)-C(90)	122.9(3)
C(94)-C(89)-N(10)	119.0(3)
C(90)-C(89)-N(10)	117.8(3)
C(91)-C(90)-C(89)	117.4(3)
C(91)-C(90)-C(95)	119.2(3)
C(89)-C(90)-C(95)	123.3(3)
C(92)-C(91)-C(90)	120.7(4)
C(92)-C(91)-H(91)	119.7
C(90)-C(91)-H(91)	119.7
C(91)-C(92)-C(93)	121.8(4)
C(91)-C(92)-H(92)	119.1
C(93)-C(92)-H(92)	119.1
C(92)-C(93)-C(94)	120.7(4)
C(92)-C(93)-H(93)	119.6
C(94)-C(93)-H(93)	119.6

C(89)-C(94)-C(93)	116.4(3)
C(89)-C(94)-C(98)	121.6(3)
C(93)-C(94)-C(98)	121.9(3)
C(90)-C(95)-C(97)	113.9(3)
C(90)-C(95)-C(96)	111.0(3)
C(97)-C(95)-C(96)	109.3(3)
C(90)-C(95)-H(95)	107.5
C(97)-C(95)-H(95)	107.5
C(96)-C(95)-H(95)	107.5
C(95)-C(96)-H(96A)	109.5
C(95)-C(96)-H(96B)	109.5
H(96A)-C(96)-H(96B)	109.5
C(95)-C(96)-H(96C)	109.5
H(96A)-C(96)-H(96C)	109.5
H(96B)-C(96)-H(96C)	109.5
C(95)-C(97)-H(97A)	109.5
C(95)-C(97)-H(97B)	109.5
H(97A)-C(97)-H(97B)	109.5
C(95)-C(97)-H(97C)	109.5
H(97A)-C(97)-H(97C)	109.5
H(97B)-C(97)-H(97C)	109.5
C(94)-C(98)-C(100)	113.2(4)
C(94)-C(98)-C(99)	110.9(3)
C(100)-C(98)-C(99)	108.8(3)
C(94)-C(98)-H(98)	107.9
C(100)-C(98)-H(98)	107.9
C(99)-C(98)-H(98)	107.9
C(98)-C(99)-H(99A)	109.5
C(98)-C(99)-H(99B)	109.5
H(99A)-C(99)-H(99B)	109.5
C(98)-C(99)-H(99C)	109.5
H(99A)-C(99)-H(99C)	109.5
H(99B)-C(99)-H(99C)	109.5
C(98)-C(100)-H(10A)	109.5
C(98)-C(100)-H(10B)	109.5
H(10A)-C(100)-H(10B)	109.5

C(98)-C(100)-H(10C)	109.5
H(10A)-C(100)-H(10C)	109.5
H(10B)-C(100)-H(10C)	109.5
C(102)-C(101)-C(106)	123.4(3)
C(102)-C(101)-N(11)	118.8(3)
C(106)-C(101)-N(11)	117.5(3)
C(103)-C(102)-C(101)	116.4(4)
C(103)-C(102)-C(107)	121.5(4)
C(101)-C(102)-C(107)	122.1(3)
C(104)-C(103)-C(102)	121.4(4)
C(104)-C(103)-H(103)	119.3
C(102)-C(103)-H(103)	119.3
C(105)-C(104)-C(103)	120.3(4)
C(105)-C(104)-H(104)	119.9
C(103)-C(104)-H(104)	119.9
C(104)-C(105)-C(106)	121.9(4)
C(104)-C(105)-H(105)	119.1
C(106)-C(105)-H(105)	119.1
C(105)-C(106)-C(101)	116.6(4)
C(105)-C(106)-C(110)	119.1(3)
C(101)-C(106)-C(110)	124.2(3)
C(102)-C(107)-C(109)	110.5(3)
C(102)-C(107)-C(108)	113.3(4)
C(109)-C(107)-C(108)	109.9(3)
C(102)-C(107)-H(107)	107.6
C(109)-C(107)-H(107)	107.6
C(108)-C(107)-H(107)	107.6
C(107)-C(108)-H(10D)	109.5
C(107)-C(108)-H(10E)	109.5
H(10D)-C(108)-H(10E)	109.5
C(107)-C(108)-H(10F)	109.5
H(10D)-C(108)-H(10F)	109.5
H(10E)-C(108)-H(10F)	109.5
C(107)-C(109)-H(10G)	109.5
C(107)-C(109)-H(10H)	109.5
H(10G)-C(109)-H(10H)	109.5

C(107)-C(109)-H(10I)	109.5
H(10G)-C(109)-H(10I)	109.5
H(10H)-C(109)-H(10I)	109.5
C(106)-C(110)-C(111)	112.4(4)
C(106)-C(110)-C(112)	110.6(4)
C(111)-C(110)-C(112)	110.1(4)
C(106)-C(110)-H(110)	107.9
C(111)-C(110)-H(110)	107.9
C(112)-C(110)-H(110)	107.9
C(110)-C(111)-H(11D)	109.5
C(110)-C(111)-H(11E)	109.5
H(11D)-C(111)-H(11E)	109.5
C(110)-C(111)-H(11F)	109.5
H(11D)-C(111)-H(11F)	109.5
H(11E)-C(111)-H(11F)	109.5
C(110)-C(112)-H(11G)	109.5
C(110)-C(112)-H(11H)	109.5
H(11G)-C(112)-H(11H)	109.5
C(110)-C(112)-H(11I)	109.5
H(11G)-C(112)-H(11I)	109.5
H(11H)-C(112)-H(11I)	109.5
Al(3)-C(113)-H(11J)	109.5
Al(3)-C(113)-H(11K)	109.5
H(11J)-C(113)-H(11K)	109.5
Al(3)-C(113)-H(11L)	109.5
H(11J)-C(113)-H(11L)	109.5
H(11K)-C(113)-H(11L)	109.5
Al(3)-C(114)-H(11M)	109.5
Al(3)-C(114)-H(11N)	109.5
H(11M)-C(114)-H(11N)	109.5
Al(3)-C(114)-H(11O)	109.5
H(11M)-C(114)-H(11O)	109.5
H(11N)-C(114)-H(11O)	109.5
Al(4)-C(115)-H(11P)	109.5
Al(4)-C(115)-H(11Q)	109.5
H(11P)-C(115)-H(11Q)	109.5

Al(4)-C(115)-H(11R)	109.5
H(11P)-C(115)-H(11R)	109.5
H(11Q)-C(115)-H(11R)	109.5
Al(4)-C(116)-H(11S)	109.5
Al(4)-C(116)-H(11T)	109.5
H(11S)-C(116)-H(11T)	109.5
Al(4)-C(116)-H(11U)	109.5
H(11S)-C(116)-H(11U)	109.5
H(11T)-C(116)-H(11U)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. 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}
Al(1)	34(1)	21(1)	21(1)	-13(1)	-3(1)	2(1)
Al(2)	33(1)	22(1)	22(1)	-14(1)	-2(1)	0(1)
Al(3)	36(1)	22(1)	22(1)	-15(1)	-9(1)	6(1)
Al(4)	38(1)	23(1)	24(1)	-14(1)	-10(1)	6(1)
N(1)	40(2)	20(1)	19(1)	-11(1)	-6(1)	1(1)
N(2)	38(2)	24(1)	18(1)	-10(1)	-5(1)	1(1)
N(3)	29(1)	21(1)	20(1)	-13(1)	-4(1)	3(1)
N(4)	28(1)	21(1)	24(1)	-15(1)	-2(1)	1(1)
N(5)	27(1)	22(1)	26(1)	-15(1)	-3(1)	1(1)
N(6)	26(1)	21(1)	24(1)	-14(1)	-5(1)	2(1)
N(7)	32(1)	21(1)	23(1)	-14(1)	-11(1)	5(1)
N(8)	31(1)	22(1)	23(1)	-15(1)	-9(1)	5(1)
N(9)	29(1)	22(1)	23(1)	-14(1)	-6(1)	4(1)
N(10)	43(2)	22(1)	19(1)	-13(1)	-8(1)	7(1)
N(11)	44(2)	23(1)	20(1)	-12(1)	-7(1)	8(1)
N(12)	33(2)	20(1)	24(1)	-13(1)	-9(1)	4(1)
C(1)	26(2)	20(2)	18(1)	-12(1)	-1(1)	2(1)
C(2)	51(2)	21(2)	26(2)	-14(1)	-7(2)	-3(2)
C(3)	51(2)	20(2)	25(2)	-12(1)	-5(2)	-2(1)
C(4)	46(2)	22(2)	21(2)	-12(1)	-9(1)	-2(1)
C(5)	48(2)	23(2)	38(2)	-14(2)	-15(2)	-1(2)
C(6)	62(3)	44(2)	46(2)	-20(2)	-27(2)	8(2)
C(7)	77(3)	47(2)	37(2)	-13(2)	-30(2)	9(2)
C(8)	72(3)	45(2)	26(2)	-18(2)	-8(2)	-4(2)
C(9)	49(2)	30(2)	22(2)	-14(1)	-4(2)	-8(2)
C(10)	36(2)	40(2)	47(2)	-23(2)	-11(2)	4(2)
C(11)	58(3)	51(3)	89(3)	-40(3)	-17(3)	19(2)
C(12)	52(3)	52(3)	87(3)	-38(3)	0(2)	-3(2)
C(13)	45(2)	42(2)	28(2)	-22(2)	4(2)	-8(2)
C(14)	47(2)	47(2)	46(2)	-28(2)	-9(2)	4(2)
C(15)	66(3)	67(3)	48(2)	-41(2)	19(2)	-18(2)

C(16)	43(2)	20(2)	24(2)	-12(1)	-13(1)	7(1)
C(17)	47(2)	21(2)	41(2)	-14(2)	-17(2)	9(2)
C(18)	61(3)	31(2)	64(3)	-17(2)	-41(2)	10(2)
C(19)	96(4)	36(2)	39(2)	-16(2)	-39(2)	5(2)
C(20)	82(3)	38(2)	23(2)	-14(2)	-14(2)	4(2)
C(21)	57(2)	26(2)	21(2)	-10(1)	-9(2)	4(2)
C(22)	39(2)	46(2)	62(3)	-28(2)	-16(2)	15(2)
C(23)	53(3)	96(4)	149(5)	-97(4)	-11(3)	18(3)
C(24)	46(3)	43(2)	111(4)	-33(3)	-21(3)	9(2)
C(25)	49(2)	50(2)	28(2)	-15(2)	1(2)	2(2)
C(26)	59(3)	65(3)	44(2)	-22(2)	0(2)	-13(2)
C(27)	70(3)	84(3)	42(2)	-25(2)	4(2)	22(3)
C(28)	26(2)	22(2)	18(1)	-12(1)	-6(1)	4(1)
C(29)	34(2)	21(2)	40(2)	-18(2)	-6(2)	1(1)
C(30)	35(2)	22(2)	37(2)	-21(2)	-5(2)	4(1)
C(31)	26(2)	22(2)	27(2)	-15(1)	-2(1)	-3(1)
C(32)	35(2)	22(2)	28(2)	-15(1)	-7(1)	-2(1)
C(33)	33(2)	35(2)	29(2)	-20(2)	0(2)	-2(2)
C(34)	31(2)	41(2)	40(2)	-29(2)	-4(2)	3(2)
C(35)	28(2)	32(2)	41(2)	-22(2)	-11(2)	3(1)
C(36)	33(2)	22(2)	28(2)	-15(1)	-7(1)	1(1)
C(37)	38(2)	26(2)	27(2)	-11(1)	-7(1)	3(1)
C(38)	59(3)	30(2)	52(2)	-13(2)	-21(2)	8(2)
C(39)	52(2)	50(2)	29(2)	-20(2)	-14(2)	12(2)
C(40)	31(2)	35(2)	28(2)	-14(2)	-8(1)	3(1)
C(41)	48(2)	33(2)	36(2)	-15(2)	-18(2)	4(2)
C(42)	78(3)	50(2)	31(2)	-25(2)	-19(2)	23(2)
C(43)	26(2)	18(2)	30(2)	-15(1)	-3(1)	2(1)
C(44)	34(2)	21(2)	27(2)	-14(1)	-6(1)	3(1)
C(45)	35(2)	27(2)	29(2)	-14(1)	-1(2)	3(1)
C(46)	29(2)	25(2)	35(2)	-15(2)	0(2)	3(1)
C(47)	31(2)	22(2)	33(2)	-15(1)	-8(1)	4(1)
C(48)	33(2)	18(2)	29(2)	-14(1)	-7(1)	5(1)
C(49)	35(2)	39(2)	27(2)	-18(2)	-4(2)	0(2)
C(50)	49(2)	47(2)	29(2)	-19(2)	-11(2)	4(2)
C(51)	64(3)	52(2)	42(2)	-32(2)	-9(2)	-4(2)

C(52)	33(2)	32(2)	27(2)	-18(1)	-6(1)	5(1)
C(53)	50(2)	40(2)	35(2)	-20(2)	-10(2)	2(2)
C(54)	65(3)	35(2)	26(2)	-11(2)	-5(2)	-8(2)
C(55)	33(2)	29(2)	44(2)	-21(2)	4(2)	-1(2)
C(56)	50(2)	25(2)	25(2)	-13(1)	-9(2)	5(2)
C(57)	65(3)	27(2)	32(2)	-15(2)	-13(2)	-1(2)
C(58)	35(2)	37(2)	51(2)	-31(2)	1(2)	-1(2)
C(59)	25(2)	22(2)	21(2)	-14(1)	-2(1)	1(1)
C(60)	39(2)	21(2)	29(2)	-16(1)	-10(2)	8(1)
C(61)	35(2)	22(2)	29(2)	-17(1)	-9(1)	6(1)
C(62)	32(2)	25(2)	30(2)	-20(1)	-14(1)	10(1)
C(63)	41(2)	21(2)	26(2)	-13(1)	-15(1)	9(1)
C(64)	47(2)	30(2)	26(2)	-16(2)	-15(2)	10(2)
C(65)	44(2)	38(2)	41(2)	-26(2)	-24(2)	13(2)
C(66)	33(2)	31(2)	41(2)	-23(2)	-14(2)	7(1)
C(67)	32(2)	23(2)	29(2)	-15(1)	-9(1)	8(1)
C(68)	42(2)	29(2)	24(2)	-10(1)	-12(2)	5(2)
C(69)	50(2)	31(2)	39(2)	-13(2)	-16(2)	-1(2)
C(70)	49(2)	50(2)	28(2)	-19(2)	-7(2)	4(2)
C(71)	33(2)	39(2)	31(2)	-18(2)	-8(2)	9(2)
C(72)	46(2)	51(2)	38(2)	-30(2)	-1(2)	-4(2)
C(73)	47(2)	34(2)	36(2)	-13(2)	-6(2)	2(2)
C(74)	32(2)	16(1)	26(2)	-14(1)	-8(1)	2(1)
C(75)	32(2)	18(2)	26(2)	-13(1)	-7(1)	2(1)
C(76)	39(2)	25(2)	25(2)	-14(1)	-10(1)	3(1)
C(77)	36(2)	26(2)	36(2)	-14(2)	-16(2)	3(1)
C(78)	29(2)	25(2)	32(2)	-16(1)	-4(1)	-1(1)
C(79)	34(2)	19(2)	26(2)	-13(1)	-9(1)	2(1)
C(80)	37(2)	33(2)	23(2)	-16(1)	-9(1)	8(2)
C(81)	44(2)	41(2)	29(2)	-15(2)	-7(2)	9(2)
C(82)	57(2)	42(2)	34(2)	-25(2)	-8(2)	14(2)
C(83)	34(2)	31(2)	26(2)	-13(1)	-5(1)	-2(1)
C(84)	49(2)	38(2)	30(2)	-9(2)	-1(2)	13(2)
C(85)	52(2)	39(2)	31(2)	-18(2)	-4(2)	3(2)
C(86)	32(2)	23(2)	19(2)	-14(1)	-8(1)	4(1)
C(87)	55(2)	21(2)	25(2)	-13(1)	-8(2)	13(2)

C(88)	57(2)	21(2)	24(2)	-10(1)	-9(2)	14(2)
C(89)	37(2)	18(2)	27(2)	-12(1)	-2(1)	5(1)
C(90)	46(2)	27(2)	22(2)	-13(1)	-6(2)	9(2)
C(91)	61(3)	42(2)	27(2)	-17(2)	-2(2)	2(2)
C(92)	66(3)	48(2)	35(2)	-20(2)	14(2)	-2(2)
C(93)	39(2)	33(2)	68(3)	-20(2)	6(2)	-4(2)
C(94)	38(2)	26(2)	54(2)	-25(2)	-9(2)	6(2)
C(95)	46(2)	32(2)	31(2)	-17(2)	-15(2)	9(2)
C(96)	52(2)	38(2)	81(3)	-31(2)	-33(2)	12(2)
C(97)	62(3)	52(2)	45(2)	-30(2)	-28(2)	22(2)
C(98)	40(2)	49(2)	84(3)	-44(2)	-25(2)	12(2)
C(99)	82(4)	60(3)	106(4)	-44(3)	-58(3)	13(3)
C(100)	65(3)	54(3)	137(5)	-61(3)	-45(3)	13(2)
C(101)	43(2)	23(2)	26(2)	-14(1)	-2(2)	3(1)
C(102)	40(2)	21(2)	44(2)	-15(2)	-1(2)	0(2)
C(103)	43(2)	26(2)	64(3)	-16(2)	7(2)	1(2)
C(104)	76(3)	31(2)	37(2)	-12(2)	21(2)	0(2)
C(105)	76(3)	41(2)	27(2)	-16(2)	0(2)	10(2)
C(106)	60(2)	32(2)	24(2)	-14(2)	-6(2)	1(2)
C(107)	43(2)	36(2)	68(3)	-24(2)	-22(2)	2(2)
C(108)	54(3)	47(3)	114(4)	-25(3)	-35(3)	5(2)
C(109)	83(4)	72(3)	119(4)	-65(3)	-57(3)	19(3)
C(110)	61(3)	65(3)	26(2)	-22(2)	-14(2)	8(2)
C(111)	100(4)	103(4)	42(3)	-35(3)	-27(3)	-16(3)
C(112)	78(3)	83(3)	42(2)	-17(2)	-25(2)	29(3)
C(113)	62(2)	26(2)	26(2)	-12(2)	-4(2)	11(2)
C(114)	52(2)	39(2)	47(2)	-32(2)	-27(2)	16(2)
C(115)	55(2)	28(2)	51(2)	-24(2)	-29(2)	11(2)
C(116)	55(2)	27(2)	28(2)	-17(2)	-2(2)	4(2)

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

	x	y	z	U(eq)
H(2)	10205	8744	2396	39
H(3)	10092	9125	1286	39
H(6)	11888	6703	3866	59
H(7)	10576	6597	4782	65
H(8)	8815	6998	4743	58
H(10)	11427	7346	2288	48
H(11A)	12969	6634	3024	97
H(11B)	13011	6764	2309	97
H(11C)	11968	6282	2915	97
H(12A)	12244	8276	2297	98
H(12B)	13215	7975	1959	98
H(12C)	13096	7826	2687	98
H(13)	7756	7713	3308	47
H(14A)	8190	8280	4079	68
H(14B)	7223	8491	3695	68
H(14C)	8555	8638	3302	68
H(15A)	6898	6733	4328	92
H(15B)	6160	7344	4196	92
H(15C)	6941	7162	4689	92
H(18)	7131	8243	406	59
H(19)	8625	8490	-508	65
H(20)	10515	8605	-494	58
H(22)	7345	7672	1991	58
H(23A)	7747	8768	1765	130
H(23B)	6393	8539	2087	130
H(23C)	6874	9011	1320	130
H(24A)	5696	8183	1260	103
H(24B)	5427	7635	2009	103
H(24C)	6062	7456	1455	103
H(25)	11499	8274	892	55

H(26A)	11843	9419	-362	91
H(26B)	12699	9268	88	91
H(26C)	11427	9430	314	91
H(27A)	11844	7675	265	107
H(27B)	12963	8096	201	107
H(27C)	12333	8378	-368	107
H(29)	6817	3735	3235	37
H(30)	8750	3805	2579	36
H(33)	4551	4332	4854	39
H(34)	3265	4866	4260	42
H(35)	3847	5414	3131	38
H(37)	7539	4292	4174	38
H(38A)	5747	3213	5037	73
H(38B)	7088	3165	4989	73
H(38C)	6614	3279	4387	73
H(39A)	6762	4782	4852	64
H(39B)	7320	4122	5221	64
H(39C)	5951	4099	5357	64
H(40)	6675	5697	2146	38
H(41A)	4372	5888	2043	58
H(41B)	5526	6328	1506	58
H(41C)	5120	6362	2171	58
H(42A)	6277	4664	2207	75
H(42B)	6093	5254	1551	75
H(42C)	5003	4822	2150	75
H(45)	12258	5282	871	38
H(46)	13434	5195	1526	37
H(47)	12651	4880	2619	34
H(49)	9163	5191	1328	40
H(50A)	10448	6163	501	62
H(50B)	9805	5825	198	62
H(50C)	11116	5722	206	62
H(51A)	10672	4466	839	75
H(51B)	9415	4592	734	75
H(51C)	9557	4143	1449	75
H(52)	9678	4660	3434	35

H(53A)	11868	4474	3705	62
H(53B)	10725	4574	4138	62
H(53C)	11397	5182	3451	62
H(54A)	9753	3606	3484	67
H(54B)	9896	3550	4146	67
H(54C)	11000	3569	3610	67
H(55A)	11391	6240	1931	55
H(55B)	11435	7015	1449	55
H(55C)	11353	6487	1199	55
H(56A)	8490	6222	1170	49
H(56B)	9031	6985	767	49
H(56C)	7827	6764	1313	49
H(57A)	8644	5275	4065	61
H(57B)	8417	5897	4191	61
H(57C)	9623	5895	3732	61
H(58A)	6252	6453	2910	59
H(58B)	6535	6791	3316	59
H(58C)	6081	6016	3676	59
H(60)	5414	-1237	3144	33
H(61)	4133	-1144	2477	32
H(64)	5742	-749	4913	39
H(65)	7614	-250	4390	43
H(66)	8257	307	3260	38
H(68)	3523	-666	4149	38
H(69A)	4137	-1657	4209	61
H(69B)	3112	-1833	4847	61
H(69C)	4419	-1862	4885	61
H(70A)	3829	-1161	5419	65
H(70B)	2663	-962	5211	65
H(70C)	3688	-397	4992	65
H(71)	6504	669	2195	41
H(72A)	8154	-251	2264	65
H(72B)	7882	261	1599	65
H(72C)	6901	-310	2169	65
H(73A)	7965	1289	2317	62
H(73B)	8220	1324	1620	62

H(73C)	8870	848	2138	62
H(76)	2073	278	876	34
H(77)	252	138	1559	38
H(78)	23	-182	2652	34
H(80)	4748	215	1298	36
H(81A)	3824	768	196	59
H(81B)	5130	907	183	59
H(81C)	4126	1191	521	59
H(82A)	4270	-820	1367	64
H(82B)	5120	-339	667	64
H(82C)	3772	-456	748	64
H(83)	2219	-326	3420	37
H(84A)	839	-1472	3653	65
H(84B)	1485	-1447	4147	65
H(84C)	2216	-1387	3470	65
H(85A)	426	146	3457	62
H(85B)	477	-453	4142	62
H(85C)	-226	-575	3716	62
H(87)	2419	3724	2413	40
H(88)	3550	4075	1304	41
H(91)	2316	2188	4724	54
H(92)	466	1717	5004	66
H(93)	-301	1632	4260	63
H(95)	4315	2843	3158	41
H(96A)	3431	3753	3175	80
H(96B)	4599	3717	3385	80
H(96C)	3384	3468	3925	80
H(97A)	4258	2441	4474	72
H(97B)	5380	2615	3884	72
H(97C)	4524	1951	4169	72
H(98)	1251	2081	2617	61
H(99A)	-605	2744	2960	112
H(99B)	-287	2692	2304	112
H(99C)	591	3111	2424	112
H(10A)	49	1081	3500	113
H(10B)	-439	1438	2877	113

H(10C)	-984	1522	3505	113
H(103)	7454	3210	456	61
H(104)	6844	3429	-457	69
H(105)	4938	3492	-430	61
H(107)	5706	2678	2037	57
H(10D)	7475	2400	1540	112
H(10E)	7595	2621	2061	112
H(10F)	8057	3131	1301	112
H(10G)	6788	4020	1289	116
H(10H)	6599	3590	2057	116
H(10I)	5511	3778	1767	116
H(110)	2610	3180	948	60
H(11D)	3064	3169	-265	120
H(11E)	1852	2944	276	120
H(11F)	2889	2505	414	120
H(11G)	3094	4337	327	107
H(11H)	2125	4127	83	107
H(11I)	3445	4294	-334	107
H(11J)	1920	800	3823	60
H(11K)	2657	966	4210	60
H(11L)	2706	274	4200	60
H(11M)	5564	998	3670	57
H(11N)	5440	1774	3304	57
H(11O)	6071	1422	2898	57
H(11P)	1666	1234	2149	60
H(11Q)	2269	1336	1438	60
H(11R)	2110	1966	1555	60
H(11S)	5140	1932	829	56
H(11T)	5352	1177	1240	56
H(11U)	5860	1744	1352	56

Table 6. Torsion angles [°] for 4.

Al(1)-N(3)-C(1)-N(1)	-142.2(3)
Al(2)-N(3)-C(1)-N(1)	32.6(5)
Al(1)-N(3)-C(1)-N(2)	37.1(5)
Al(2)-N(3)-C(1)-N(2)	-148.2(3)
C(2)-N(1)-C(1)-N(3)	178.5(3)
C(4)-N(1)-C(1)-N(3)	13.8(5)
C(2)-N(1)-C(1)-N(2)	-0.9(3)
C(4)-N(1)-C(1)-N(2)	-165.6(3)
C(3)-N(2)-C(1)-N(3)	-178.6(3)
C(16)-N(2)-C(1)-N(3)	8.1(5)
C(3)-N(2)-C(1)-N(1)	0.8(3)
C(16)-N(2)-C(1)-N(1)	-172.5(3)
C(1)-N(1)-C(2)-C(3)	0.7(4)
C(4)-N(1)-C(2)-C(3)	166.7(3)
N(1)-C(2)-C(3)-N(2)	-0.2(4)
C(1)-N(2)-C(3)-C(2)	-0.4(4)
C(16)-N(2)-C(3)-C(2)	173.5(3)
C(2)-N(1)-C(4)-C(9)	86.3(4)
C(1)-N(1)-C(4)-C(9)	-110.3(3)
C(2)-N(1)-C(4)-C(5)	-85.9(4)
C(1)-N(1)-C(4)-C(5)	77.5(4)
C(9)-C(4)-C(5)-C(6)	1.2(5)
N(1)-C(4)-C(5)-C(6)	173.0(3)
C(9)-C(4)-C(5)-C(10)	-175.8(3)
N(1)-C(4)-C(5)-C(10)	-4.0(4)
C(4)-C(5)-C(6)-C(7)	-0.5(5)
C(10)-C(5)-C(6)-C(7)	176.6(3)
C(5)-C(6)-C(7)-C(8)	-0.3(6)
C(6)-C(7)-C(8)-C(9)	0.3(6)
C(5)-C(4)-C(9)-C(8)	-1.1(5)
N(1)-C(4)-C(9)-C(8)	-172.9(3)
C(5)-C(4)-C(9)-C(13)	177.0(3)
N(1)-C(4)-C(9)-C(13)	5.3(4)
C(7)-C(8)-C(9)-C(4)	0.4(5)

C(7)-C(8)-C(9)-C(13)	-177.8(3)
C(6)-C(5)-C(10)-C(11)	40.6(5)
C(4)-C(5)-C(10)-C(11)	-142.5(3)
C(6)-C(5)-C(10)-C(12)	-81.8(4)
C(4)-C(5)-C(10)-C(12)	95.1(4)
C(4)-C(9)-C(13)-C(14)	-98.7(4)
C(8)-C(9)-C(13)-C(14)	79.4(4)
C(4)-C(9)-C(13)-C(15)	137.8(3)
C(8)-C(9)-C(13)-C(15)	-44.2(4)
C(3)-N(2)-C(16)-C(17)	-102.5(4)
C(1)-N(2)-C(16)-C(17)	70.1(4)
C(3)-N(2)-C(16)-C(21)	72.3(4)
C(1)-N(2)-C(16)-C(21)	-115.1(3)
C(21)-C(16)-C(17)-C(18)	2.7(5)
N(2)-C(16)-C(17)-C(18)	177.2(3)
C(21)-C(16)-C(17)-C(22)	-175.4(3)
N(2)-C(16)-C(17)-C(22)	-0.9(4)
C(16)-C(17)-C(18)-C(19)	-1.2(5)
C(22)-C(17)-C(18)-C(19)	176.8(3)
C(17)-C(18)-C(19)-C(20)	-1.0(6)
C(18)-C(19)-C(20)-C(21)	2.0(6)
C(19)-C(20)-C(21)-C(16)	-0.6(5)
C(19)-C(20)-C(21)-C(25)	-178.1(3)
C(17)-C(16)-C(21)-C(20)	-1.8(5)
N(2)-C(16)-C(21)-C(20)	-176.4(3)
C(17)-C(16)-C(21)-C(25)	175.5(3)
N(2)-C(16)-C(21)-C(25)	0.9(5)
C(16)-C(17)-C(22)-C(23)	74.5(5)
C(18)-C(17)-C(22)-C(23)	-103.5(4)
C(16)-C(17)-C(22)-C(24)	-163.1(3)
C(18)-C(17)-C(22)-C(24)	18.9(5)
C(20)-C(21)-C(25)-C(27)	-48.0(5)
C(16)-C(21)-C(25)-C(27)	134.7(3)
C(20)-C(21)-C(25)-C(26)	74.9(4)
C(16)-C(21)-C(25)-C(26)	-102.4(4)
Al(2)-N(6)-C(28)-N(4)	33.9(5)

Al(1)-N(6)-C(28)-N(4)	-139.0(3)
Al(2)-N(6)-C(28)-N(5)	-146.9(3)
Al(1)-N(6)-C(28)-N(5)	40.3(4)
C(29)-N(4)-C(28)-N(6)	178.4(3)
C(31)-N(4)-C(28)-N(6)	4.2(5)
C(29)-N(4)-C(28)-N(5)	-1.0(3)
C(31)-N(4)-C(28)-N(5)	-175.2(3)
C(30)-N(5)-C(28)-N(6)	-178.5(3)
C(43)-N(5)-C(28)-N(6)	15.9(5)
C(30)-N(5)-C(28)-N(4)	0.9(3)
C(43)-N(5)-C(28)-N(4)	-164.7(3)
C(28)-N(4)-C(29)-C(30)	0.7(4)
C(31)-N(4)-C(29)-C(30)	175.6(3)
N(4)-C(29)-C(30)-N(5)	-0.1(4)
C(28)-N(5)-C(30)-C(29)	-0.5(4)
C(43)-N(5)-C(30)-C(29)	166.0(3)
C(28)-N(4)-C(31)-C(36)	79.9(4)
C(29)-N(4)-C(31)-C(36)	-93.8(3)
C(28)-N(4)-C(31)-C(32)	-106.7(3)
C(29)-N(4)-C(31)-C(32)	79.6(4)
C(36)-C(31)-C(32)-C(33)	1.6(4)
N(4)-C(31)-C(32)-C(33)	-171.5(3)
C(36)-C(31)-C(32)-C(37)	-178.2(3)
N(4)-C(31)-C(32)-C(37)	8.6(4)
C(31)-C(32)-C(33)-C(34)	0.2(4)
C(37)-C(32)-C(33)-C(34)	-179.9(3)
C(32)-C(33)-C(34)-C(35)	-2.3(5)
C(33)-C(34)-C(35)-C(36)	2.6(5)
C(34)-C(35)-C(36)-C(31)	-0.8(4)
C(34)-C(35)-C(36)-C(40)	180.0(3)
C(32)-C(31)-C(36)-C(35)	-1.4(4)
N(4)-C(31)-C(36)-C(35)	171.7(3)
C(32)-C(31)-C(36)-C(40)	177.8(3)
N(4)-C(31)-C(36)-C(40)	-9.1(4)
C(33)-C(32)-C(37)-C(38)	80.9(4)
C(31)-C(32)-C(37)-C(38)	-99.3(4)

C(33)-C(32)-C(37)-C(39)	-43.0(4)
C(31)-C(32)-C(37)-C(39)	136.9(3)
C(35)-C(36)-C(40)-C(42)	-100.8(4)
C(31)-C(36)-C(40)-C(42)	80.0(4)
C(35)-C(36)-C(40)-C(41)	22.7(4)
C(31)-C(36)-C(40)-C(41)	-156.5(3)
C(30)-N(5)-C(43)-C(48)	-93.6(3)
C(28)-N(5)-C(43)-C(48)	70.5(4)
C(30)-N(5)-C(43)-C(44)	81.1(4)
C(28)-N(5)-C(43)-C(44)	-114.7(3)
C(48)-C(43)-C(44)-C(45)	-2.1(4)
N(5)-C(43)-C(44)-C(45)	-176.6(3)
C(48)-C(43)-C(44)-C(49)	176.7(3)
N(5)-C(43)-C(44)-C(49)	2.2(4)
C(43)-C(44)-C(45)-C(46)	-1.6(4)
C(49)-C(44)-C(45)-C(46)	179.5(3)
C(44)-C(45)-C(46)-C(47)	2.7(5)
C(45)-C(46)-C(47)-C(48)	0.0(5)
C(46)-C(47)-C(48)-C(43)	-3.6(4)
C(46)-C(47)-C(48)-C(52)	172.4(3)
C(44)-C(43)-C(48)-C(47)	4.7(4)
N(5)-C(43)-C(48)-C(47)	179.2(2)
C(44)-C(43)-C(48)-C(52)	-171.3(3)
N(5)-C(43)-C(48)-C(52)	3.2(4)
C(45)-C(44)-C(49)-C(51)	78.2(4)
C(43)-C(44)-C(49)-C(51)	-100.6(3)
C(45)-C(44)-C(49)-C(50)	-44.7(4)
C(43)-C(44)-C(49)-C(50)	136.5(3)
C(47)-C(48)-C(52)-C(53)	30.4(4)
C(43)-C(48)-C(52)-C(53)	-153.8(3)
C(47)-C(48)-C(52)-C(54)	-92.1(3)
C(43)-C(48)-C(52)-C(54)	83.7(4)
Al(3)-N(9)-C(59)-N(7)	-25.3(5)
Al(4)-N(9)-C(59)-N(7)	140.0(3)
Al(3)-N(9)-C(59)-N(8)	155.1(2)
Al(4)-N(9)-C(59)-N(8)	-39.5(4)

C(60)-N(7)-C(59)-N(9)	-178.5(3)
C(62)-N(7)-C(59)-N(9)	-1.0(5)
C(60)-N(7)-C(59)-N(8)	1.1(3)
C(62)-N(7)-C(59)-N(8)	178.6(3)
C(61)-N(8)-C(59)-N(9)	178.4(3)
C(74)-N(8)-C(59)-N(9)	-15.9(5)
C(61)-N(8)-C(59)-N(7)	-1.2(3)
C(74)-N(8)-C(59)-N(7)	164.4(3)
C(59)-N(7)-C(60)-C(61)	-0.6(3)
C(62)-N(7)-C(60)-C(61)	-178.4(3)
N(7)-C(60)-C(61)-N(8)	-0.2(3)
C(59)-N(8)-C(61)-C(60)	0.9(3)
C(74)-N(8)-C(61)-C(60)	-165.6(3)
C(59)-N(7)-C(62)-C(67)	-87.3(4)
C(60)-N(7)-C(62)-C(67)	90.0(3)
C(59)-N(7)-C(62)-C(63)	99.0(4)
C(60)-N(7)-C(62)-C(63)	-83.7(3)
C(67)-C(62)-C(63)-C(64)	-2.1(4)
N(7)-C(62)-C(63)-C(64)	171.3(3)
C(67)-C(62)-C(63)-C(68)	177.9(3)
N(7)-C(62)-C(63)-C(68)	-8.7(4)
C(62)-C(63)-C(64)-C(65)	-0.5(5)
C(68)-C(63)-C(64)-C(65)	179.4(3)
C(63)-C(64)-C(65)-C(66)	2.3(5)
C(64)-C(65)-C(66)-C(67)	-1.5(5)
C(65)-C(66)-C(67)-C(62)	-1.0(4)
C(65)-C(66)-C(67)-C(71)	179.1(3)
C(63)-C(62)-C(67)-C(66)	2.8(4)
N(7)-C(62)-C(67)-C(66)	-170.5(3)
C(63)-C(62)-C(67)-C(71)	-177.2(3)
N(7)-C(62)-C(67)-C(71)	9.4(4)
C(64)-C(63)-C(68)-C(69)	-90.3(4)
C(62)-C(63)-C(68)-C(69)	89.6(3)
C(64)-C(63)-C(68)-C(70)	33.5(4)
C(62)-C(63)-C(68)-C(70)	-146.6(3)
C(66)-C(67)-C(71)-C(73)	-25.3(4)

C(62)-C(67)-C(71)-C(73)	154.7(3)
C(66)-C(67)-C(71)-C(72)	98.6(4)
C(62)-C(67)-C(71)-C(72)	-81.3(4)
C(61)-N(8)-C(74)-C(75)	-76.9(3)
C(59)-N(8)-C(74)-C(75)	119.0(3)
C(61)-N(8)-C(74)-C(79)	97.1(3)
C(59)-N(8)-C(74)-C(79)	-67.1(4)
C(79)-C(74)-C(75)-C(76)	2.5(4)
N(8)-C(74)-C(75)-C(76)	176.3(2)
C(79)-C(74)-C(75)-C(80)	-177.0(3)
N(8)-C(74)-C(75)-C(80)	-3.2(4)
C(74)-C(75)-C(76)-C(77)	0.7(4)
C(80)-C(75)-C(76)-C(77)	-179.8(3)
C(75)-C(76)-C(77)-C(78)	-1.7(5)
C(76)-C(77)-C(78)-C(79)	-0.6(5)
C(77)-C(78)-C(79)-C(74)	3.6(4)
C(77)-C(78)-C(79)-C(83)	-173.9(3)
C(75)-C(74)-C(79)-C(78)	-4.6(4)
N(8)-C(74)-C(79)-C(78)	-178.4(3)
C(75)-C(74)-C(79)-C(83)	172.9(3)
N(8)-C(74)-C(79)-C(83)	-0.9(4)
C(76)-C(75)-C(80)-C(82)	-75.8(4)
C(74)-C(75)-C(80)-C(82)	103.7(3)
C(76)-C(75)-C(80)-C(81)	46.2(4)
C(74)-C(75)-C(80)-C(81)	-134.2(3)
C(78)-C(79)-C(83)-C(85)	-28.8(4)
C(74)-C(79)-C(83)-C(85)	153.8(3)
C(78)-C(79)-C(83)-C(84)	94.5(3)
C(74)-C(79)-C(83)-C(84)	-82.9(3)
Al(4)-N(12)-C(86)-N(11)	-39.3(5)
Al(3)-N(12)-C(86)-N(11)	147.8(3)
Al(4)-N(12)-C(86)-N(10)	139.6(3)
Al(3)-N(12)-C(86)-N(10)	-33.3(5)
C(88)-N(11)-C(86)-N(12)	178.3(3)
C(101)-N(11)-C(86)-N(12)	-10.5(5)
C(88)-N(11)-C(86)-N(10)	-0.9(3)

C(101)-N(11)-C(86)-N(10)	170.4(3)
C(87)-N(10)-C(86)-N(12)	-178.3(3)
C(89)-N(10)-C(86)-N(12)	-2.3(5)
C(87)-N(10)-C(86)-N(11)	0.8(3)
C(89)-N(10)-C(86)-N(11)	176.8(3)
C(86)-N(10)-C(87)-C(88)	-0.5(4)
C(89)-N(10)-C(87)-C(88)	-176.9(3)
N(10)-C(87)-C(88)-N(11)	0.0(4)
C(86)-N(11)-C(88)-C(87)	0.6(4)
C(101)-N(11)-C(88)-C(87)	-171.4(3)
C(87)-N(10)-C(89)-C(94)	91.6(4)
C(86)-N(10)-C(89)-C(94)	-84.0(4)
C(87)-N(10)-C(89)-C(90)	-82.2(4)
C(86)-N(10)-C(89)-C(90)	102.2(4)
C(94)-C(89)-C(90)-C(91)	-1.0(5)
N(10)-C(89)-C(90)-C(91)	172.5(3)
C(94)-C(89)-C(90)-C(95)	-177.7(3)
N(10)-C(89)-C(90)-C(95)	-4.2(4)
C(89)-C(90)-C(91)-C(92)	-0.2(5)
C(95)-C(90)-C(91)-C(92)	176.6(3)
C(90)-C(91)-C(92)-C(93)	1.6(6)
C(91)-C(92)-C(93)-C(94)	-1.8(6)
C(90)-C(89)-C(94)-C(93)	0.9(5)
N(10)-C(89)-C(94)-C(93)	-172.6(3)
C(90)-C(89)-C(94)-C(98)	179.7(3)
N(10)-C(89)-C(94)-C(98)	6.2(5)
C(92)-C(93)-C(94)-C(89)	0.6(5)
C(92)-C(93)-C(94)-C(98)	-178.3(3)
C(91)-C(90)-C(95)-C(97)	45.2(4)
C(89)-C(90)-C(95)-C(97)	-138.1(3)
C(91)-C(90)-C(95)-C(96)	-78.6(4)
C(89)-C(90)-C(95)-C(96)	98.1(4)
C(89)-C(94)-C(98)-C(100)	149.6(3)
C(93)-C(94)-C(98)-C(100)	-31.6(5)
C(89)-C(94)-C(98)-C(99)	-87.8(4)
C(93)-C(94)-C(98)-C(99)	91.0(5)

C(86)-N(11)-C(101)-C(102)	-69.1(4)
C(88)-N(11)-C(101)-C(102)	101.3(4)
C(86)-N(11)-C(101)-C(106)	117.1(4)
C(88)-N(11)-C(101)-C(106)	-72.5(4)
C(106)-C(101)-C(102)-C(103)	-3.3(5)
N(11)-C(101)-C(102)-C(103)	-176.7(3)
C(106)-C(101)-C(102)-C(107)	175.3(3)
N(11)-C(101)-C(102)-C(107)	1.9(5)
C(101)-C(102)-C(103)-C(104)	1.8(5)
C(107)-C(102)-C(103)-C(104)	-176.7(3)
C(102)-C(103)-C(104)-C(105)	0.1(6)
C(103)-C(104)-C(105)-C(106)	-0.8(6)
C(104)-C(105)-C(106)-C(101)	-0.5(5)
C(104)-C(105)-C(106)-C(110)	178.3(4)
C(102)-C(101)-C(106)-C(105)	2.7(5)
N(11)-C(101)-C(106)-C(105)	176.2(3)
C(102)-C(101)-C(106)-C(110)	-176.1(3)
N(11)-C(101)-C(106)-C(110)	-2.6(5)
C(103)-C(102)-C(107)-C(109)	101.4(4)
C(101)-C(102)-C(107)-C(109)	-77.1(4)
C(103)-C(102)-C(107)-C(108)	-22.5(5)
C(101)-C(102)-C(107)-C(108)	159.1(3)
C(105)-C(106)-C(110)-C(111)	49.8(5)
C(101)-C(106)-C(110)-C(111)	-131.4(4)
C(105)-C(106)-C(110)-C(112)	-73.7(4)
C(101)-C(106)-C(110)-C(112)	105.1(4)

Symmetry transformations used to generate equivalent atoms:

Crystallography tables for compound 5

Table 1. Crystal data and structure refinement for 5.

Identification code	2014_12_19_AT97_0ma	
Empirical formula	C ₅₅ H ₇₅ Al N ₆	
Formula weight	847.19	
Temperature	125(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 22.0069(19) Å	α = 90°.
	b = 11.7183(10) Å	β = 99.4460(10)°.
	c = 20.0358(17) Å	γ = 90°.
Volume	5096.8(8) Å ³	
Z	4	
Density (calculated)	1.104 Mg/m ³	
Absorption coefficient	0.081 mm ⁻¹	
F(000)	1840	
Crystal size	0.365 x 0.357 x 0.134 mm ³	
Theta range for data collection	2.020 to 24.996°.	
Index ranges	-26 ≤ h ≤ 26, -10 ≤ k ≤ 13, -23 ≤ l ≤ 23	
Reflections collected	32942	
Independent reflections	8897 [R(int) = 0.0290]	
Completeness to theta = 24.996°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6905	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	8897 / 0 / 576	
Goodness-of-fit on F ²	1.024	
Final R indices [I > 2σ(I)]	R1 = 0.0418, wR2 = 0.0996	
R indices (all data)	R1 = 0.0566, wR2 = 0.1083	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.708 and -0.296 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Al(1)	2627(1)	10040(1)	3641(1)	22(1)
N(1)	3179(1)	10454(1)	3145(1)	24(1)
N(2)	4091(1)	9274(1)	3253(1)	22(1)
N(3)	4133(1)	10978(1)	2799(1)	21(1)
N(4)	1906(1)	9521(1)	3246(1)	24(1)
N(5)	1016(1)	10694(1)	3326(1)	22(1)
N(6)	856(1)	9021(1)	2838(1)	24(1)
C(1)	2832(1)	10242(2)	4618(1)	41(1)
C(2)	3732(1)	10262(1)	3080(1)	21(1)
C(3)	4672(1)	9400(2)	3065(1)	25(1)
C(4)	4695(1)	10430(2)	2787(1)	24(1)
C(5)	3850(1)	8262(1)	3517(1)	24(1)
C(6)	4028(1)	7985(2)	4203(1)	27(1)
C(7)	3778(1)	6999(2)	4440(1)	34(1)
C(8)	3366(1)	6336(2)	4022(1)	37(1)
C(9)	3194(1)	6620(2)	3346(1)	34(1)
C(10)	3434(1)	7581(2)	3077(1)	27(1)
C(11)	4494(1)	8693(2)	4673(1)	30(1)
C(12)	5142(1)	8190(2)	4702(1)	39(1)
C(13)	4344(1)	8779(2)	5393(1)	38(1)
C(14)	3266(1)	7881(2)	2328(1)	29(1)
C(15)	3774(1)	7492(2)	1936(1)	38(1)
C(16)	2644(1)	7398(2)	2000(1)	41(1)
C(17)	3944(1)	12010(1)	2435(1)	22(1)
C(18)	3684(1)	11932(2)	1748(1)	25(1)
C(19)	3515(1)	12945(2)	1402(1)	29(1)
C(20)	3592(1)	13988(2)	1725(1)	29(1)
C(21)	3844(1)	14044(2)	2408(1)	28(1)
C(22)	4028(1)	13058(2)	2774(1)	24(1)
C(23)	4271(1)	13114(2)	3530(1)	26(1)
C(24)	3723(1)	13111(2)	3915(1)	33(1)

C(25)	4692(1)	14135(2)	3736(1)	36(1)
C(26)	3559(1)	10787(2)	1396(1)	30(1)
C(27)	3791(1)	10739(2)	718(1)	46(1)
C(28)	2868(1)	10518(2)	1300(1)	40(1)
C(29)	1334(1)	9725(1)	3151(1)	21(1)
C(30)	285(1)	9551(2)	2822(1)	26(1)
C(31)	382(1)	10566(2)	3122(1)	25(1)
C(32)	963(1)	7961(1)	2523(1)	24(1)
C(33)	929(1)	7932(2)	1818(1)	27(1)
C(34)	1062(1)	6902(2)	1525(1)	30(1)
C(35)	1226(1)	5945(2)	1917(1)	32(1)
C(36)	1244(1)	5989(2)	2609(1)	31(1)
C(37)	1109(1)	6994(2)	2927(1)	27(1)
C(38)	762(1)	8977(2)	1379(1)	33(1)
C(39)	245(1)	8718(2)	793(1)	56(1)
C(40)	1326(1)	9451(2)	1125(1)	65(1)
C(41)	1109(1)	7017(2)	3686(1)	33(1)
C(42)	647(1)	6140(2)	3881(1)	63(1)
C(43)	1743(1)	6798(2)	4088(1)	53(1)
C(44)	1319(1)	11633(1)	3700(1)	23(1)
C(45)	1255(1)	11767(2)	4384(1)	28(1)
C(46)	1565(1)	12676(2)	4733(1)	36(1)
C(47)	1928(1)	13407(2)	4427(1)	41(1)
C(48)	1984(1)	13256(2)	3753(1)	34(1)
C(49)	1675(1)	12378(2)	3370(1)	25(1)
C(50)	877(1)	10924(2)	4723(1)	34(1)
C(51)	1221(1)	9802(2)	4880(1)	44(1)
C(52)	675(1)	11384(2)	5367(1)	50(1)
C(53)	1703(1)	12228(2)	2619(1)	27(1)
C(54)	2222(1)	12896(2)	2376(1)	38(1)
C(55)	1084(1)	12554(2)	2186(1)	36(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **5**.

Al(1)-N(1)	1.7589(14)
Al(1)-N(4)	1.7618(14)
Al(1)-C(1)	1.9499(18)
N(1)-C(2)	1.266(2)
N(2)-C(3)	1.398(2)
N(2)-C(2)	1.413(2)
N(2)-C(5)	1.435(2)
N(3)-C(4)	1.397(2)
N(3)-C(2)	1.400(2)
N(3)-C(17)	1.437(2)
N(4)-C(29)	1.265(2)
N(5)-C(31)	1.396(2)
N(5)-C(29)	1.408(2)
N(5)-C(44)	1.432(2)
N(6)-C(30)	1.397(2)
N(6)-C(29)	1.401(2)
N(6)-C(32)	1.430(2)
C(3)-C(4)	1.333(2)
C(5)-C(6)	1.404(2)
C(5)-C(10)	1.410(2)
C(6)-C(7)	1.396(2)
C(6)-C(11)	1.519(2)
C(7)-C(8)	1.371(3)
C(8)-C(9)	1.386(3)
C(9)-C(10)	1.390(2)
C(10)-C(14)	1.525(2)
C(11)-C(13)	1.536(2)
C(11)-C(12)	1.536(2)
C(14)-C(16)	1.527(2)
C(14)-C(15)	1.538(2)
C(17)-C(22)	1.401(2)
C(17)-C(18)	1.406(2)
C(18)-C(19)	1.394(2)
C(18)-C(26)	1.518(2)

C(19)-C(20)	1.381(3)
C(20)-C(21)	1.390(2)
C(21)-C(22)	1.393(2)
C(22)-C(23)	1.522(2)
C(23)-C(25)	1.528(2)
C(23)-C(24)	1.534(2)
C(26)-C(27)	1.529(2)
C(26)-C(28)	1.533(3)
C(30)-C(31)	1.334(2)
C(32)-C(37)	1.399(2)
C(32)-C(33)	1.403(2)
C(33)-C(34)	1.394(2)
C(33)-C(38)	1.516(2)
C(34)-C(35)	1.382(3)
C(35)-C(36)	1.382(2)
C(36)-C(37)	1.394(2)
C(37)-C(41)	1.521(2)
C(38)-C(40)	1.523(3)
C(38)-C(39)	1.525(3)
C(41)-C(43)	1.513(3)
C(41)-C(42)	1.541(3)
C(44)-C(49)	1.408(2)
C(44)-C(45)	1.409(2)
C(45)-C(46)	1.392(3)
C(45)-C(50)	1.521(3)
C(46)-C(47)	1.380(3)
C(47)-C(48)	1.388(3)
C(48)-C(49)	1.392(2)
C(49)-C(53)	1.526(2)
C(50)-C(51)	1.525(3)
C(50)-C(52)	1.530(3)
C(53)-C(54)	1.528(2)
C(53)-C(55)	1.537(2)
N(1)-Al(1)-N(4)	119.72(7)
N(1)-Al(1)-C(1)	117.77(8)

N(4)-Al(1)-C(1)	122.45(7)
C(2)-N(1)-Al(1)	140.75(12)
C(3)-N(2)-C(2)	110.22(13)
C(3)-N(2)-C(5)	126.63(13)
C(2)-N(2)-C(5)	122.85(13)
C(4)-N(3)-C(2)	110.43(13)
C(4)-N(3)-C(17)	124.12(13)
C(2)-N(3)-C(17)	124.02(13)
C(29)-N(4)-Al(1)	143.43(13)
C(31)-N(5)-C(29)	110.66(13)
C(31)-N(5)-C(44)	126.34(13)
C(29)-N(5)-C(44)	122.90(13)
C(30)-N(6)-C(29)	110.72(14)
C(30)-N(6)-C(32)	126.07(13)
C(29)-N(6)-C(32)	122.94(13)
N(1)-C(2)-N(3)	127.97(15)
N(1)-C(2)-N(2)	128.92(15)
N(3)-C(2)-N(2)	103.08(12)
C(4)-C(3)-N(2)	107.92(14)
C(3)-C(4)-N(3)	108.32(14)
C(6)-C(5)-C(10)	121.97(16)
C(6)-C(5)-N(2)	119.46(15)
C(10)-C(5)-N(2)	118.56(14)
C(7)-C(6)-C(5)	117.57(16)
C(7)-C(6)-C(11)	120.30(15)
C(5)-C(6)-C(11)	122.08(15)
C(8)-C(7)-C(6)	121.25(17)
C(7)-C(8)-C(9)	120.58(17)
C(8)-C(9)-C(10)	120.88(17)
C(9)-C(10)-C(5)	117.73(16)
C(9)-C(10)-C(14)	121.43(16)
C(5)-C(10)-C(14)	120.83(15)
C(6)-C(11)-C(13)	113.01(15)
C(6)-C(11)-C(12)	109.98(15)
C(13)-C(11)-C(12)	109.33(14)
C(10)-C(14)-C(16)	113.19(15)

C(10)-C(14)-C(15)	110.73(14)
C(16)-C(14)-C(15)	110.21(15)
C(22)-C(17)-C(18)	122.17(15)
C(22)-C(17)-N(3)	119.24(14)
C(18)-C(17)-N(3)	118.60(14)
C(19)-C(18)-C(17)	117.64(15)
C(19)-C(18)-C(26)	120.56(14)
C(17)-C(18)-C(26)	121.72(15)
C(20)-C(19)-C(18)	121.27(15)
C(19)-C(20)-C(21)	120.06(16)
C(20)-C(21)-C(22)	120.96(16)
C(21)-C(22)-C(17)	117.89(15)
C(21)-C(22)-C(23)	120.85(15)
C(17)-C(22)-C(23)	121.13(14)
C(22)-C(23)-C(25)	113.63(14)
C(22)-C(23)-C(24)	108.85(13)
C(25)-C(23)-C(24)	110.99(14)
C(18)-C(26)-C(27)	112.52(15)
C(18)-C(26)-C(28)	109.88(15)
C(27)-C(26)-C(28)	110.49(16)
N(4)-C(29)-N(6)	127.62(15)
N(4)-C(29)-N(5)	129.62(15)
N(6)-C(29)-N(5)	102.76(13)
C(31)-C(30)-N(6)	108.00(14)
C(30)-C(31)-N(5)	107.86(14)
C(37)-C(32)-C(33)	122.17(15)
C(37)-C(32)-N(6)	119.21(14)
C(33)-C(32)-N(6)	118.62(15)
C(34)-C(33)-C(32)	117.62(16)
C(34)-C(33)-C(38)	120.23(15)
C(32)-C(33)-C(38)	122.15(15)
C(35)-C(34)-C(33)	121.13(16)
C(36)-C(35)-C(34)	120.14(17)
C(35)-C(36)-C(37)	121.07(17)
C(36)-C(37)-C(32)	117.81(15)
C(36)-C(37)-C(41)	120.44(16)

C(32)-C(37)-C(41)	121.73(15)
C(33)-C(38)-C(40)	110.80(16)
C(33)-C(38)-C(39)	111.39(16)
C(40)-C(38)-C(39)	111.13(18)
C(43)-C(41)-C(37)	112.20(16)
C(43)-C(41)-C(42)	109.94(17)
C(37)-C(41)-C(42)	110.49(15)
C(49)-C(44)-C(45)	122.66(15)
C(49)-C(44)-N(5)	118.60(14)
C(45)-C(44)-N(5)	118.73(15)
C(46)-C(45)-C(44)	117.08(16)
C(46)-C(45)-C(50)	122.13(15)
C(44)-C(45)-C(50)	120.76(15)
C(47)-C(46)-C(45)	121.52(17)
C(46)-C(47)-C(48)	120.28(17)
C(47)-C(48)-C(49)	121.14(18)
C(48)-C(49)-C(44)	117.28(15)
C(48)-C(49)-C(53)	122.28(16)
C(44)-C(49)-C(53)	120.43(15)
C(45)-C(50)-C(51)	111.26(15)
C(45)-C(50)-C(52)	113.79(17)
C(51)-C(50)-C(52)	109.42(16)
C(49)-C(53)-C(54)	114.08(15)
C(49)-C(53)-C(55)	110.67(14)
C(54)-C(53)-C(55)	109.38(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5. 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)	21(1)	23(1)	24(1)	2(1)	5(1)	0(1)
N(1)	23(1)	21(1)	29(1)	2(1)	6(1)	1(1)
N(2)	22(1)	19(1)	26(1)	4(1)	7(1)	1(1)
N(3)	21(1)	20(1)	23(1)	3(1)	6(1)	1(1)
N(4)	24(1)	23(1)	26(1)	1(1)	7(1)	1(1)
N(5)	21(1)	22(1)	23(1)	-1(1)	5(1)	0(1)
N(6)	22(1)	23(1)	26(1)	-2(1)	4(1)	-1(1)
C(1)	31(1)	61(2)	29(1)	-2(1)	2(1)	2(1)
C(2)	24(1)	19(1)	19(1)	0(1)	4(1)	-1(1)
C(3)	20(1)	27(1)	28(1)	1(1)	7(1)	3(1)
C(4)	20(1)	27(1)	26(1)	1(1)	7(1)	0(1)
C(5)	23(1)	19(1)	30(1)	3(1)	10(1)	3(1)
C(6)	27(1)	25(1)	31(1)	3(1)	10(1)	5(1)
C(7)	41(1)	27(1)	35(1)	10(1)	11(1)	4(1)
C(8)	44(1)	22(1)	47(1)	9(1)	17(1)	-1(1)
C(9)	35(1)	23(1)	45(1)	-1(1)	11(1)	-3(1)
C(10)	26(1)	22(1)	34(1)	0(1)	10(1)	3(1)
C(11)	32(1)	28(1)	30(1)	7(1)	4(1)	2(1)
C(12)	34(1)	46(1)	38(1)	9(1)	6(1)	4(1)
C(13)	40(1)	41(1)	31(1)	4(1)	4(1)	3(1)
C(14)	33(1)	24(1)	31(1)	-3(1)	6(1)	-2(1)
C(15)	41(1)	36(1)	37(1)	-4(1)	12(1)	-2(1)
C(16)	36(1)	46(1)	41(1)	-4(1)	3(1)	-5(1)
C(17)	21(1)	21(1)	25(1)	4(1)	8(1)	0(1)
C(18)	24(1)	26(1)	26(1)	2(1)	9(1)	-1(1)
C(19)	31(1)	32(1)	24(1)	5(1)	6(1)	-1(1)
C(20)	31(1)	26(1)	32(1)	9(1)	7(1)	2(1)
C(21)	30(1)	21(1)	33(1)	0(1)	9(1)	0(1)
C(22)	21(1)	24(1)	27(1)	2(1)	8(1)	0(1)
C(23)	28(1)	24(1)	26(1)	-1(1)	4(1)	2(1)
C(24)	37(1)	36(1)	28(1)	-3(1)	8(1)	-1(1)

C(25)	35(1)	38(1)	33(1)	-4(1)	4(1)	-6(1)
C(26)	38(1)	27(1)	24(1)	1(1)	5(1)	0(1)
C(27)	72(2)	34(1)	35(1)	-3(1)	21(1)	-1(1)
C(28)	43(1)	35(1)	41(1)	-2(1)	-1(1)	-7(1)
C(29)	25(1)	20(1)	18(1)	1(1)	6(1)	-1(1)
C(30)	20(1)	30(1)	30(1)	0(1)	4(1)	-1(1)
C(31)	21(1)	27(1)	28(1)	1(1)	6(1)	1(1)
C(32)	21(1)	22(1)	29(1)	-4(1)	5(1)	-4(1)
C(33)	24(1)	28(1)	28(1)	-2(1)	5(1)	-6(1)
C(34)	32(1)	31(1)	28(1)	-8(1)	7(1)	-7(1)
C(35)	32(1)	26(1)	40(1)	-9(1)	10(1)	-4(1)
C(36)	32(1)	24(1)	39(1)	2(1)	7(1)	0(1)
C(37)	26(1)	26(1)	30(1)	-1(1)	5(1)	-2(1)
C(38)	39(1)	31(1)	28(1)	2(1)	8(1)	-1(1)
C(39)	68(2)	51(2)	42(1)	7(1)	-8(1)	4(1)
C(40)	63(2)	49(2)	90(2)	29(1)	34(1)	0(1)
C(41)	41(1)	30(1)	28(1)	2(1)	8(1)	2(1)
C(42)	59(1)	90(2)	44(1)	4(1)	18(1)	-18(1)
C(43)	55(1)	65(2)	39(1)	6(1)	3(1)	4(1)
C(44)	22(1)	21(1)	25(1)	-1(1)	3(1)	2(1)
C(45)	31(1)	28(1)	26(1)	-1(1)	3(1)	5(1)
C(46)	45(1)	34(1)	28(1)	-7(1)	2(1)	2(1)
C(47)	47(1)	29(1)	42(1)	-9(1)	-4(1)	-5(1)
C(48)	32(1)	26(1)	44(1)	3(1)	2(1)	-4(1)
C(49)	22(1)	22(1)	31(1)	2(1)	2(1)	4(1)
C(50)	37(1)	42(1)	25(1)	0(1)	10(1)	-2(1)
C(51)	60(1)	40(1)	37(1)	8(1)	20(1)	-1(1)
C(52)	58(1)	62(2)	34(1)	1(1)	21(1)	8(1)
C(53)	29(1)	23(1)	31(1)	6(1)	9(1)	3(1)
C(54)	34(1)	34(1)	47(1)	13(1)	16(1)	6(1)
C(55)	34(1)	39(1)	34(1)	11(1)	6(1)	0(1)

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

	x	y	z	U(eq)
H(1A)	2753	9529	4845	61
H(1B)	2578	10853	4761	61
H(1C)	3269	10445	4739	61
H(3)	4993	8850	3125	30
H(4)	5035	10738	2611	29
H(7)	3896	6784	4900	41
H(8)	3197	5675	4197	44
H(9)	2908	6152	3062	40
H(11)	4493	9482	4483	36
H(12A)	5146	7400	4861	59
H(12B)	5438	8642	5013	59
H(12C)	5256	8209	4249	59
H(13A)	3916	9028	5373	56
H(13B)	4620	9333	5654	56
H(13C)	4399	8030	5613	56
H(14)	3239	8732	2294	35
H(15A)	4169	7821	2145	56
H(15B)	3674	7748	1466	56
H(15C)	3803	6657	1948	56
H(16A)	2537	7696	1539	62
H(16B)	2327	7624	2265	62
H(16C)	2668	6563	1986	62
H(19)	3344	12917	935	34
H(20)	3472	14669	1481	35
H(21)	3892	14764	2627	33
H(23)	4516	12405	3657	32
H(24A)	3470	13790	3792	50
H(24B)	3876	13116	4403	50
H(24C)	3475	12424	3796	50
H(25A)	4454	14843	3654	53

H(25B)	5027	14140	3468	53
H(25C)	4865	14078	4218	53
H(26)	3782	10187	1697	36
H(27A)	3564	11294	406	68
H(27B)	3727	9971	527	68
H(27C)	4232	10923	787	68
H(28A)	2733	10504	1742	61
H(28B)	2792	9772	1082	61
H(28C)	2639	11106	1016	61
H(30)	-104	9242	2632	32
H(31)	75	11106	3184	30
H(34)	1041	6857	1048	36
H(35)	1326	5256	1710	39
H(36)	1351	5323	2873	37
H(38)	610	9576	1667	39
H(39A)	384	8136	500	84
H(39B)	136	9415	531	84
H(39C)	-116	8435	971	84
H(40A)	1484	8880	839	98
H(40B)	1646	9633	1511	98
H(40C)	1213	10144	860	98
H(41)	974	7794	3808	39
H(42A)	770	5371	3765	95
H(42B)	234	6308	3634	95
H(42C)	642	6184	4369	95
H(43A)	1729	6882	4572	80
H(43B)	2036	7349	3954	80
H(43C)	1874	6022	3997	80
H(46)	1527	12798	5193	43
H(47)	2139	14015	4679	49
H(48)	2238	13760	3550	41
H(50)	495	10753	4393	41
H(51A)	1369	9526	4473	66
H(51B)	943	9235	5026	66
H(51C)	1573	9923	5241	66
H(52A)	1038	11483	5718	75

H(52B)	390	10843	5524	75
H(52C)	469	12121	5270	75
H(53)	1775	11400	2540	33
H(54A)	2158	13715	2435	56
H(54B)	2222	12733	1896	56
H(54C)	2618	12667	2640	56
H(55A)	1017	13377	2221	53
H(55B)	750	12140	2348	53
H(55C)	1091	12351	1712	53

Crystallography tables for compound 6

Table 1. Crystal data and structure refinement for 6.

Identification code	2015_08_14_AT186_cation_0m	
Empirical formula	C ₆₆ H ₉₁ Al F ₁₂ N ₆ O ₁₄ S ₄	
Formula weight	1575.66	
Temperature	125(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁	
Unit cell dimensions	a = 12.6935(15) Å	α = 90°.
	b = 16.0668(19) Å	β = 102.1980(10)°.
	c = 19.437(2) Å	γ = 90°.
Volume	3874.6(8) Å ³	
Z	2	
Density (calculated)	1.351 Mg/m ³	
Absorption coefficient	0.225 mm ⁻¹	
F(000)	1652	
Crystal size	0.430 x 0.210 x 0.180 mm ³	
Theta range for data collection	2.074 to 26.000°.	
Index ranges	-15 ≤ h ≤ 14, -18 ≤ k ≤ 19, -23 ≤ l ≤ 23	
Reflections collected	27730	
Independent reflections	14581 [R(int) = 0.0256]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6721	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	14581 / 1 / 1003	
Goodness-of-fit on F ²	1.022	
Final R indices [I > 2σ(I)]	R1 = 0.0456, wR2 = 0.1060	
R indices (all data)	R1 = 0.0579, wR2 = 0.1134	
Absolute structure parameter	0.47(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.534 and -0.388 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
S(1)	5372(1)	6078(1)	1606(1)	37(1)
S(2)	5102(1)	3709(1)	4031(1)	28(1)
S(4)	7576(1)	4059(1)	2964(1)	23(1)
Al(2)	5134(1)	4527(1)	2543(1)	21(1)
F(1)	4243(3)	5808(2)	330(2)	61(1)
F(2)	5530(3)	6701(3)	402(2)	79(1)
F(3)	5884(3)	5404(3)	500(2)	84(1)
F(4)	4019(3)	2604(2)	4565(2)	64(1)
F(5)	4808(3)	2120(2)	3769(2)	53(1)
F(6)	3375(2)	2859(2)	3473(2)	62(1)
F(10)	8389(3)	4629(3)	1936(2)	73(1)
F(11)	9554(2)	4300(3)	2879(2)	84(1)
F(12)	8633(3)	5416(2)	2839(2)	71(1)
O(1)	5014(2)	5228(2)	1760(2)	29(1)
O(2)	6490(3)	6224(3)	1879(2)	61(1)
O(3)	4619(3)	6708(2)	1690(2)	45(1)
O(4)	5284(2)	3772(2)	3300(1)	24(1)
O(5)	6058(3)	3483(2)	4524(2)	34(1)
O(6)	4445(3)	4356(2)	4214(2)	47(1)
O(10)	6627(2)	4588(2)	2676(1)	22(1)
O(11)	7910(2)	4099(2)	3705(1)	34(1)
O(12)	7517(3)	3259(2)	2644(2)	48(1)
O(13)	5170(2)	5472(2)	3153(2)	29(1)
O(14)	5123(2)	3595(2)	1920(2)	28(1)
N(1)	-55(3)	4038(2)	8095(2)	27(1)
N(2)	1241(3)	4732(2)	8968(2)	25(1)
N(3)	184(3)	3845(2)	9348(2)	23(1)
N(4)	221(3)	4803(2)	6906(2)	26(1)
N(5)	-1117(3)	4139(2)	6036(2)	22(1)
N(6)	-29(3)	4991(2)	5659(2)	22(1)
C(1)	5249(5)	5993(4)	658(3)	53(2)

C(2)	4282(4)	2778(3)	3955(3)	38(1)
C(4)	8596(4)	4642(4)	2631(3)	47(1)
C(5)	4236(4)	5980(3)	3229(3)	42(1)
C(6)	4730(6)	6728(4)	3647(4)	76(2)
C(7)	5715(6)	6406(5)	4093(4)	81(2)
C(8)	6133(4)	5782(3)	3650(3)	42(1)
C(9)	4831(4)	2734(3)	2059(3)	40(1)
C(10)	4789(6)	2292(4)	1360(3)	61(2)
C(11)	5660(5)	2731(4)	1075(3)	56(2)
C(12)	5505(4)	3631(4)	1257(2)	40(1)
C(13)	411(3)	4190(3)	8751(2)	22(1)
C(14)	1533(4)	4719(3)	9700(2)	28(1)
C(15)	895(3)	4182(3)	9936(2)	28(1)
C(16)	1760(3)	5201(3)	8498(2)	26(1)
C(17)	1438(4)	6033(3)	8356(2)	30(1)
C(18)	1909(4)	6453(3)	7873(2)	39(1)
C(19)	2672(4)	6078(3)	7558(3)	44(1)
C(20)	2986(4)	5264(3)	7723(3)	39(1)
C(21)	2532(4)	4804(3)	8199(2)	33(1)
C(22)	580(5)	6438(3)	8686(2)	40(1)
C(23)	-533(5)	6266(4)	8252(3)	51(1)
C(24)	761(6)	7376(3)	8803(3)	56(2)
C(25)	2883(4)	3917(3)	8387(3)	44(1)
C(26)	3768(6)	3896(5)	9061(4)	81(2)
C(27)	3266(5)	3457(4)	7800(3)	62(2)
C(28)	-601(3)	3200(3)	9341(2)	21(1)
C(29)	-291(4)	2377(3)	9254(2)	27(1)
C(30)	-1074(4)	1767(3)	9233(2)	34(1)
C(31)	-2106(4)	1967(3)	9284(2)	36(1)
C(32)	-2394(4)	2783(3)	9367(2)	32(1)
C(33)	-1636(4)	3425(3)	9404(2)	27(1)
C(34)	850(4)	2152(3)	9201(3)	36(1)
C(35)	1516(4)	1896(4)	9924(3)	51(1)
C(36)	884(5)	1471(4)	8658(3)	54(2)
C(37)	-1933(4)	4316(3)	9536(2)	36(1)
C(38)	-1872(5)	4440(4)	10320(3)	49(1)

C(39)	-3045(6)	4577(5)	9128(3)	76(2)
C(40)	-264(3)	4653(2)	6249(2)	21(1)
C(41)	-1417(3)	4149(3)	5294(2)	24(1)
C(42)	-752(3)	4678(3)	5069(2)	22(1)
C(43)	819(3)	5592(2)	5659(2)	21(1)
C(44)	1798(3)	5317(3)	5520(2)	29(1)
C(45)	2596(4)	5908(3)	5514(2)	36(1)
C(46)	2415(4)	6736(3)	5637(2)	38(1)
C(47)	1443(4)	6996(3)	5771(2)	36(1)
C(48)	614(4)	6428(3)	5788(2)	28(1)
C(49)	1980(4)	4411(3)	5343(3)	37(1)
C(50)	3074(5)	4078(4)	5737(3)	56(2)
C(51)	1889(4)	4306(3)	4562(3)	44(1)
C(52)	-477(4)	6707(3)	5911(3)	36(1)
C(53)	-1251(4)	6897(4)	5215(3)	47(1)
C(54)	-391(5)	7472(4)	6398(3)	57(2)
C(55)	-1639(3)	3669(3)	6508(2)	23(1)
C(56)	-1325(4)	2841(3)	6652(2)	27(1)
C(57)	-1805(4)	2422(3)	7136(2)	36(1)
C(58)	-2566(4)	2804(3)	7437(2)	37(1)
C(59)	-2892(4)	3614(4)	7264(2)	39(1)
C(60)	-2429(3)	4076(3)	6791(2)	30(1)
C(61)	-497(4)	2422(3)	6308(2)	34(1)
C(62)	-697(5)	1493(3)	6195(3)	47(1)
C(63)	652(4)	2585(3)	6720(3)	44(1)
C(64)	-2783(4)	4964(3)	6597(3)	43(1)
C(65)	-3112(6)	5455(4)	7195(3)	65(2)
C(66)	-3717(7)	4969(5)	5965(3)	88(3)
O(7)	3641(2)	4466(2)	2423(2)	30(1)
S(3B)	2669(4)	4759(4)	1949(3)	33(1)
F(7B)	2005(10)	3222(8)	2143(8)	79(4)
F(8B)	1690(20)	4180(20)	2820(14)	99(13)
F(9B)	750(30)	4110(20)	1780(20)	65(10)
O(8B)	2286(8)	5532(8)	1973(6)	56(1)
O(9B)	2785(9)	4407(9)	1251(7)	56(1)
C(3B)	1729(17)	3989(16)	2154(11)	38(5)

S(3A)	2720(2)	4391(2)	1779(1)	25(1)
F(7A)	1621(4)	5090(5)	2597(4)	81(2)
F(8A)	1611(10)	3775(9)	2661(8)	85(6)
F(9A)	686(15)	4379(12)	1741(10)	45(3)
O(8A)	2569(5)	5077(5)	1335(3)	56(1)
O(9A)	2640(4)	3594(4)	1430(3)	56(1)
C(3A)	1609(8)	4395(7)	2230(5)	31(2)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **6**.

S(1)-O(3)	1.425(4)
S(1)-O(2)	1.426(4)
S(1)-O(1)	1.489(3)
S(1)-C(1)	1.821(6)
S(2)-O(5)	1.425(3)
S(2)-O(6)	1.425(3)
S(2)-O(4)	1.490(3)
S(2)-C(2)	1.811(5)
S(4)-O(11)	1.415(3)
S(4)-O(12)	1.424(3)
S(4)-O(10)	1.484(3)
S(4)-C(4)	1.823(5)
Al(2)-O(10)	1.860(3)
Al(2)-O(7)	1.863(3)
Al(2)-O(1)	1.874(3)
Al(2)-O(4)	1.885(3)
Al(2)-O(13)	1.921(3)
Al(2)-O(14)	1.924(3)
F(1)-C(1)	1.335(7)
F(2)-C(1)	1.320(6)
F(3)-C(1)	1.321(7)
F(4)-C(2)	1.327(6)
F(5)-C(2)	1.339(6)
F(6)-C(2)	1.329(6)
F(10)-C(4)	1.321(6)
F(11)-C(4)	1.328(6)
F(12)-C(4)	1.305(8)
O(13)-C(5)	1.471(5)
O(13)-C(8)	1.475(6)
O(14)-C(12)	1.471(5)
O(14)-C(9)	1.472(6)
N(1)-C(13)	1.310(5)
N(2)-C(13)	1.364(5)
N(2)-C(14)	1.394(5)

N(2)-C(16)	1.446(5)
N(3)-C(13)	1.371(5)
N(3)-C(15)	1.406(5)
N(3)-C(28)	1.436(5)
N(4)-C(40)	1.318(5)
N(5)-C(40)	1.355(5)
N(5)-C(41)	1.410(5)
N(5)-C(55)	1.453(5)
N(6)-C(40)	1.358(5)
N(6)-C(42)	1.401(5)
N(6)-C(43)	1.446(5)
C(5)-C(6)	1.511(8)
C(6)-C(7)	1.457(9)
C(7)-C(8)	1.491(8)
C(9)-C(10)	1.523(7)
C(10)-C(11)	1.512(9)
C(11)-C(12)	1.511(8)
C(14)-C(15)	1.329(6)
C(16)-C(21)	1.395(7)
C(16)-C(17)	1.409(7)
C(17)-C(18)	1.389(6)
C(17)-C(22)	1.521(7)
C(18)-C(19)	1.388(8)
C(19)-C(20)	1.385(8)
C(20)-C(21)	1.400(7)
C(21)-C(25)	1.515(7)
C(22)-C(23)	1.510(7)
C(22)-C(24)	1.534(7)
C(25)-C(27)	1.522(8)
C(25)-C(26)	1.535(8)
C(28)-C(33)	1.392(6)
C(28)-C(29)	1.400(6)
C(29)-C(30)	1.391(6)
C(29)-C(34)	1.517(6)
C(30)-C(31)	1.373(7)
C(31)-C(32)	1.380(7)

C(32)-C(33)	1.402(6)
C(33)-C(37)	1.517(7)
C(34)-C(36)	1.528(8)
C(34)-C(35)	1.536(7)
C(37)-C(38)	1.523(7)
C(37)-C(39)	1.524(8)
C(41)-C(42)	1.335(6)
C(43)-C(44)	1.398(6)
C(43)-C(48)	1.402(6)
C(44)-C(45)	1.390(6)
C(44)-C(49)	1.524(7)
C(45)-C(46)	1.380(7)
C(46)-C(47)	1.379(7)
C(47)-C(48)	1.399(6)
C(48)-C(52)	1.522(7)
C(49)-C(51)	1.508(7)
C(49)-C(50)	1.532(7)
C(52)-C(53)	1.525(7)
C(52)-C(54)	1.541(7)
C(55)-C(56)	1.400(6)
C(55)-C(60)	1.404(6)
C(56)-C(57)	1.397(6)
C(56)-C(61)	1.518(7)
C(57)-C(58)	1.375(7)
C(58)-C(59)	1.386(8)
C(59)-C(60)	1.404(7)
C(60)-C(64)	1.518(7)
C(61)-C(62)	1.522(7)
C(61)-C(63)	1.530(7)
C(64)-C(66)	1.516(8)
C(64)-C(65)	1.535(8)
O(7)-S(3B)	1.453(6)
O(7)-S(3A)	1.526(4)
S(3B)-O(8B)	1.339(15)
S(3B)-O(9B)	1.505(14)
S(3B)-C(3B)	1.82(3)

F(7B)-C(3B)	1.28(3)
F(8B)-C(3B)	1.34(4)
F(9B)-C(3B)	1.31(4)
S(3A)-O(8A)	1.388(7)
S(3A)-O(9A)	1.443(8)
S(3A)-C(3A)	1.810(10)
F(7A)-C(3A)	1.324(13)
F(8A)-C(3A)	1.302(16)
F(9A)-C(3A)	1.34(2)

O(3)-S(1)-O(2)	118.6(3)
O(3)-S(1)-O(1)	112.9(2)
O(2)-S(1)-O(1)	113.5(2)
O(3)-S(1)-C(1)	104.7(2)
O(2)-S(1)-C(1)	104.7(3)
O(1)-S(1)-C(1)	99.8(2)
O(5)-S(2)-O(6)	118.5(2)
O(5)-S(2)-O(4)	112.19(18)
O(6)-S(2)-O(4)	113.90(18)
O(5)-S(2)-C(2)	103.7(2)
O(6)-S(2)-C(2)	105.5(2)
O(4)-S(2)-C(2)	100.5(2)
O(11)-S(4)-O(12)	117.5(2)
O(11)-S(4)-O(10)	113.71(17)
O(12)-S(4)-O(10)	112.92(19)
O(11)-S(4)-C(4)	104.8(2)
O(12)-S(4)-C(4)	106.6(3)
O(10)-S(4)-C(4)	98.9(2)
O(10)-Al(2)-O(7)	179.22(14)
O(10)-Al(2)-O(1)	89.24(13)
O(7)-Al(2)-O(1)	91.36(13)
O(10)-Al(2)-O(4)	89.64(13)
O(7)-Al(2)-O(4)	89.78(13)
O(1)-Al(2)-O(4)	176.62(16)
O(10)-Al(2)-O(13)	88.98(13)
O(7)-Al(2)-O(13)	90.53(14)

O(1)-Al(2)-O(13)	90.75(15)
O(4)-Al(2)-O(13)	92.42(13)
O(10)-Al(2)-O(14)	90.02(13)
O(7)-Al(2)-O(14)	90.48(14)
O(1)-Al(2)-O(14)	88.13(14)
O(4)-Al(2)-O(14)	88.68(13)
O(13)-Al(2)-O(14)	178.50(15)
S(1)-O(1)-Al(2)	137.6(2)
S(2)-O(4)-Al(2)	141.0(2)
S(4)-O(10)-Al(2)	138.14(19)
C(5)-O(13)-C(8)	108.8(3)
C(5)-O(13)-Al(2)	125.8(3)
C(8)-O(13)-Al(2)	125.3(3)
C(12)-O(14)-C(9)	109.8(3)
C(12)-O(14)-Al(2)	124.2(3)
C(9)-O(14)-Al(2)	125.8(3)
C(13)-N(2)-C(14)	109.2(3)
C(13)-N(2)-C(16)	124.2(3)
C(14)-N(2)-C(16)	126.5(3)
C(13)-N(3)-C(15)	108.6(3)
C(13)-N(3)-C(28)	123.6(3)
C(15)-N(3)-C(28)	127.6(3)
C(40)-N(5)-C(41)	109.4(3)
C(40)-N(5)-C(55)	124.4(3)
C(41)-N(5)-C(55)	126.2(3)
C(40)-N(6)-C(42)	108.9(3)
C(40)-N(6)-C(43)	124.2(3)
C(42)-N(6)-C(43)	126.8(3)
F(2)-C(1)-F(3)	107.6(4)
F(2)-C(1)-F(1)	108.6(4)
F(3)-C(1)-F(1)	107.4(6)
F(2)-C(1)-S(1)	110.2(5)
F(3)-C(1)-S(1)	111.3(4)
F(1)-C(1)-S(1)	111.7(3)
F(4)-C(2)-F(6)	107.9(4)
F(4)-C(2)-F(5)	108.1(4)

F(6)-C(2)-F(5)	107.1(4)
F(4)-C(2)-S(2)	110.5(4)
F(6)-C(2)-S(2)	111.9(3)
F(5)-C(2)-S(2)	111.2(3)
F(12)-C(4)-F(10)	108.5(5)
F(12)-C(4)-F(11)	108.1(5)
F(10)-C(4)-F(11)	109.5(5)
F(12)-C(4)-S(4)	111.2(4)
F(10)-C(4)-S(4)	110.6(4)
F(11)-C(4)-S(4)	108.9(4)
O(13)-C(5)-C(6)	104.0(4)
C(7)-C(6)-C(5)	104.2(5)
C(6)-C(7)-C(8)	105.0(5)
O(13)-C(8)-C(7)	104.9(4)
O(14)-C(9)-C(10)	103.7(4)
C(11)-C(10)-C(9)	102.7(4)
C(12)-C(11)-C(10)	102.6(5)
O(14)-C(12)-C(11)	104.6(4)
N(1)-C(13)-N(2)	125.5(4)
N(1)-C(13)-N(3)	128.1(4)
N(2)-C(13)-N(3)	106.4(3)
C(15)-C(14)-N(2)	108.2(3)
C(14)-C(15)-N(3)	107.7(4)
C(21)-C(16)-C(17)	123.6(4)
C(21)-C(16)-N(2)	118.6(4)
C(17)-C(16)-N(2)	117.8(4)
C(18)-C(17)-C(16)	116.4(5)
C(18)-C(17)-C(22)	121.7(4)
C(16)-C(17)-C(22)	121.8(4)
C(19)-C(18)-C(17)	121.9(5)
C(20)-C(19)-C(18)	120.0(5)
C(19)-C(20)-C(21)	120.9(5)
C(16)-C(21)-C(20)	117.2(5)
C(16)-C(21)-C(25)	121.8(4)
C(20)-C(21)-C(25)	121.0(5)
C(23)-C(22)-C(17)	110.8(4)

C(23)-C(22)-C(24)	110.8(5)
C(17)-C(22)-C(24)	112.6(5)
C(21)-C(25)-C(27)	113.7(5)
C(21)-C(25)-C(26)	110.5(5)
C(27)-C(25)-C(26)	109.7(5)
C(33)-C(28)-C(29)	123.4(4)
C(33)-C(28)-N(3)	118.6(4)
C(29)-C(28)-N(3)	118.0(4)
C(30)-C(29)-C(28)	116.9(4)
C(30)-C(29)-C(34)	121.1(4)
C(28)-C(29)-C(34)	122.0(4)
C(31)-C(30)-C(29)	121.3(4)
C(30)-C(31)-C(32)	120.8(4)
C(31)-C(32)-C(33)	120.6(4)
C(28)-C(33)-C(32)	117.1(4)
C(28)-C(33)-C(37)	122.2(4)
C(32)-C(33)-C(37)	120.7(4)
C(29)-C(34)-C(36)	112.6(4)
C(29)-C(34)-C(35)	110.5(4)
C(36)-C(34)-C(35)	110.4(4)
C(33)-C(37)-C(38)	109.3(4)
C(33)-C(37)-C(39)	114.0(5)
C(38)-C(37)-C(39)	109.3(4)
N(4)-C(40)-N(5)	126.0(4)
N(4)-C(40)-N(6)	127.2(4)
N(5)-C(40)-N(6)	106.8(3)
C(42)-C(41)-N(5)	106.8(3)
C(41)-C(42)-N(6)	108.1(3)
C(44)-C(43)-C(48)	123.0(4)
C(44)-C(43)-N(6)	118.8(4)
C(48)-C(43)-N(6)	118.2(4)
C(45)-C(44)-C(43)	117.7(4)
C(45)-C(44)-C(49)	120.3(4)
C(43)-C(44)-C(49)	121.9(4)
C(46)-C(45)-C(44)	120.6(5)
C(47)-C(46)-C(45)	120.9(4)

C(46)-C(47)-C(48)	120.9(4)
C(47)-C(48)-C(43)	116.9(4)
C(47)-C(48)-C(52)	121.7(4)
C(43)-C(48)-C(52)	121.3(4)
C(51)-C(49)-C(44)	110.6(4)
C(51)-C(49)-C(50)	109.4(4)
C(44)-C(49)-C(50)	112.7(4)
C(48)-C(52)-C(53)	110.9(4)
C(48)-C(52)-C(54)	112.5(4)
C(53)-C(52)-C(54)	109.6(4)
C(56)-C(55)-C(60)	124.2(4)
C(56)-C(55)-N(5)	118.2(4)
C(60)-C(55)-N(5)	117.6(4)
C(57)-C(56)-C(55)	116.5(4)
C(57)-C(56)-C(61)	121.7(4)
C(55)-C(56)-C(61)	121.8(4)
C(58)-C(57)-C(56)	121.1(5)
C(57)-C(58)-C(59)	121.1(4)
C(58)-C(59)-C(60)	120.8(5)
C(55)-C(60)-C(59)	116.2(5)
C(55)-C(60)-C(64)	122.6(4)
C(59)-C(60)-C(64)	121.1(5)
C(56)-C(61)-C(62)	112.8(4)
C(56)-C(61)-C(63)	111.4(4)
C(62)-C(61)-C(63)	110.8(4)
C(66)-C(64)-C(60)	110.2(5)
C(66)-C(64)-C(65)	108.6(5)
C(60)-C(64)-C(65)	114.1(5)
S(3B)-O(7)-Al(2)	140.1(3)
S(3A)-O(7)-Al(2)	133.6(2)
O(8B)-S(3B)-O(7)	122.9(6)
O(8B)-S(3B)-O(9B)	119.0(8)
O(7)-S(3B)-O(9B)	102.7(6)
O(8B)-S(3B)-C(3B)	111.2(10)
O(7)-S(3B)-C(3B)	98.6(8)
O(9B)-S(3B)-C(3B)	97.8(9)

F(7B)-C(3B)-F(9B)	111(2)
F(7B)-C(3B)-F(8B)	107(2)
F(9B)-C(3B)-F(8B)	106(3)
F(7B)-C(3B)-S(3B)	117.0(15)
F(9B)-C(3B)-S(3B)	111(2)
F(8B)-C(3B)-S(3B)	102.7(18)
O(8A)-S(3A)-O(9A)	115.1(4)
O(8A)-S(3A)-O(7)	115.4(3)
O(9A)-S(3A)-O(7)	114.9(3)
O(8A)-S(3A)-C(3A)	106.2(5)
O(9A)-S(3A)-C(3A)	104.2(5)
O(7)-S(3A)-C(3A)	98.2(4)
F(8A)-C(3A)-F(7A)	107.5(11)
F(8A)-C(3A)-F(9A)	108.9(12)
F(7A)-C(3A)-F(9A)	107.9(11)
F(8A)-C(3A)-S(3A)	114.4(10)
F(7A)-C(3A)-S(3A)	110.0(7)
F(9A)-C(3A)-S(3A)	108.0(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6. 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}
S(1)	28(1)	38(1)	43(1)	19(1)	3(1)	-2(1)
S(2)	28(1)	30(1)	28(1)	8(1)	11(1)	4(1)
S(4)	20(1)	26(1)	22(1)	0(1)	3(1)	2(1)
Al(2)	18(1)	22(1)	22(1)	5(1)	4(1)	1(1)
F(1)	59(2)	85(3)	37(2)	7(2)	7(2)	17(2)
F(2)	99(3)	76(3)	72(2)	48(2)	37(2)	5(2)
F(3)	96(3)	96(3)	81(3)	41(2)	64(2)	53(3)
F(4)	67(2)	68(2)	66(2)	33(2)	32(2)	-5(2)
F(5)	53(2)	32(2)	72(2)	6(2)	12(2)	-7(1)
F(6)	29(2)	72(2)	80(2)	28(2)	-2(2)	-15(2)
F(10)	59(2)	121(3)	47(2)	31(2)	31(2)	16(2)
F(11)	22(2)	135(4)	97(3)	61(3)	20(2)	20(2)
F(12)	51(2)	60(3)	97(3)	22(2)	3(2)	-30(2)
O(1)	24(2)	33(2)	28(2)	10(1)	2(1)	-2(1)
O(2)	34(2)	52(3)	89(3)	36(2)	-6(2)	-13(2)
O(3)	50(2)	39(2)	45(2)	9(2)	8(2)	5(2)
O(4)	26(2)	25(2)	23(1)	5(1)	6(1)	1(1)
O(5)	34(2)	39(2)	27(2)	7(1)	2(1)	4(2)
O(6)	52(2)	47(2)	48(2)	16(2)	28(2)	22(2)
O(10)	20(1)	21(2)	24(1)	1(1)	4(1)	0(1)
O(11)	34(2)	44(2)	22(2)	3(1)	1(1)	4(2)
O(12)	50(2)	34(2)	53(2)	-15(2)	-5(2)	15(2)
O(13)	24(2)	27(2)	35(2)	1(1)	4(1)	5(1)
O(14)	29(2)	28(2)	28(2)	-1(1)	5(1)	-4(1)
N(1)	30(2)	28(2)	21(2)	-2(2)	-1(1)	-14(2)
N(2)	30(2)	24(2)	18(2)	2(1)	0(1)	-12(2)
N(3)	26(2)	22(2)	19(2)	0(1)	2(1)	-8(1)
N(4)	30(2)	29(2)	19(2)	-1(1)	3(1)	-17(2)
N(5)	24(2)	23(2)	17(2)	1(1)	1(1)	-5(2)
N(6)	25(2)	23(2)	16(2)	-2(1)	1(1)	-5(1)
C(1)	61(4)	54(4)	54(3)	33(3)	33(3)	23(3)

C(2)	29(3)	40(3)	46(3)	17(2)	11(2)	-5(2)
C(4)	25(2)	69(4)	47(3)	23(3)	11(2)	4(3)
C(5)	41(3)	34(3)	53(3)	-2(2)	13(2)	20(2)
C(6)	72(5)	60(4)	87(5)	-32(4)	-6(4)	30(4)
C(7)	74(5)	80(5)	82(5)	-47(4)	-3(4)	29(4)
C(8)	40(3)	42(3)	39(3)	-16(2)	0(2)	6(2)
C(9)	50(3)	26(3)	41(3)	-4(2)	6(2)	-8(2)
C(10)	80(5)	52(4)	44(3)	-16(3)	0(3)	-16(3)
C(11)	78(4)	56(4)	35(3)	-19(3)	16(3)	-6(3)
C(12)	46(3)	53(3)	21(2)	-5(2)	6(2)	-2(3)
C(13)	25(2)	22(2)	19(2)	2(2)	1(2)	-3(2)
C(14)	33(2)	27(2)	21(2)	-2(2)	-2(2)	-13(2)
C(15)	36(2)	28(2)	18(2)	-2(2)	-1(2)	-8(2)
C(16)	33(2)	27(2)	17(2)	3(2)	1(2)	-16(2)
C(17)	42(3)	22(2)	21(2)	-1(2)	-1(2)	-14(2)
C(18)	55(3)	28(3)	30(2)	2(2)	2(2)	-18(2)
C(19)	49(3)	50(3)	31(3)	5(2)	6(2)	-27(3)
C(20)	34(3)	49(3)	35(3)	3(2)	7(2)	-14(2)
C(21)	25(2)	37(3)	31(2)	2(2)	-5(2)	-13(2)
C(22)	68(4)	25(3)	27(2)	-2(2)	10(2)	-9(2)
C(23)	56(4)	43(3)	54(3)	-13(3)	12(3)	2(3)
C(24)	98(5)	23(3)	47(3)	-9(2)	15(3)	-9(3)
C(25)	33(3)	44(3)	58(3)	14(2)	13(2)	5(2)
C(26)	72(5)	89(6)	70(4)	10(4)	-13(4)	27(4)
C(27)	66(4)	53(4)	69(4)	6(3)	16(3)	9(3)
C(28)	25(2)	22(2)	16(2)	1(2)	5(2)	-4(2)
C(29)	31(2)	24(2)	26(2)	0(2)	8(2)	-4(2)
C(30)	44(3)	23(2)	37(3)	-3(2)	15(2)	-9(2)
C(31)	38(3)	37(3)	33(2)	-1(2)	11(2)	-20(2)
C(32)	27(2)	40(3)	32(2)	3(2)	10(2)	-4(2)
C(33)	30(2)	29(2)	22(2)	2(2)	4(2)	1(2)
C(34)	35(3)	27(3)	50(3)	6(2)	18(2)	4(2)
C(35)	38(3)	56(4)	55(3)	-12(3)	2(2)	10(3)
C(36)	55(4)	68(4)	44(3)	3(3)	19(3)	20(3)
C(37)	40(3)	29(3)	43(3)	4(2)	19(2)	5(2)
C(38)	58(3)	42(3)	48(3)	-8(3)	9(2)	11(3)

C(39)	94(5)	70(5)	53(4)	-9(3)	-8(3)	46(4)
C(40)	22(2)	17(2)	22(2)	0(2)	4(2)	-4(2)
C(41)	28(2)	23(2)	18(2)	0(2)	0(2)	-2(2)
C(42)	28(2)	22(2)	13(2)	0(2)	2(2)	-6(2)
C(43)	24(2)	18(2)	19(2)	0(2)	1(2)	-5(2)
C(44)	29(2)	31(3)	26(2)	6(2)	6(2)	-4(2)
C(45)	26(2)	42(3)	39(3)	6(2)	6(2)	-1(2)
C(46)	36(3)	37(3)	38(3)	4(2)	2(2)	-23(2)
C(47)	50(3)	24(2)	31(2)	0(2)	4(2)	-11(2)
C(48)	37(3)	27(2)	19(2)	0(2)	3(2)	-2(2)
C(49)	38(3)	28(3)	50(3)	3(2)	20(2)	3(2)
C(50)	61(4)	49(3)	57(3)	6(3)	7(3)	21(3)
C(51)	41(3)	37(3)	56(3)	-7(2)	16(2)	1(2)
C(52)	45(3)	24(2)	43(3)	0(2)	16(2)	2(2)
C(53)	35(3)	49(3)	53(3)	-19(3)	0(2)	7(2)
C(54)	78(4)	54(4)	35(3)	-12(3)	4(3)	27(3)
C(55)	25(2)	24(2)	18(2)	-2(2)	1(2)	-10(2)
C(56)	38(3)	24(2)	18(2)	-2(2)	-1(2)	-10(2)
C(57)	55(3)	24(2)	26(2)	0(2)	4(2)	-16(2)
C(58)	46(3)	43(3)	25(2)	-5(2)	11(2)	-27(2)
C(59)	35(3)	51(3)	34(3)	-9(2)	14(2)	-17(2)
C(60)	23(2)	38(3)	28(2)	-2(2)	1(2)	-8(2)
C(61)	49(3)	26(2)	29(2)	2(2)	9(2)	1(2)
C(62)	64(4)	33(3)	39(3)	-4(2)	2(3)	4(3)
C(63)	48(3)	35(3)	54(3)	-4(2)	19(3)	-2(2)
C(64)	33(3)	47(3)	50(3)	7(2)	13(2)	9(2)
C(65)	74(4)	56(4)	55(4)	-19(3)	-6(3)	11(3)
C(66)	116(6)	77(5)	53(4)	-21(3)	-23(4)	49(5)
O(7)	19(1)	36(2)	34(2)	11(1)	4(1)	0(1)
S(3B)	29(2)	44(3)	21(2)	0(2)	-3(2)	-5(2)
F(7B)	48(7)	58(8)	118(11)	2(7)	-12(7)	-24(6)
F(8B)	31(7)	220(40)	47(8)	23(16)	16(5)	-32(16)
F(9B)	28(11)	100(30)	56(9)	28(13)	-10(7)	-25(13)
O(8B)	36(2)	75(3)	51(2)	6(2)	-8(2)	1(2)
O(9B)	36(2)	75(3)	51(2)	6(2)	-8(2)	1(2)
C(3B)	30(10)	54(16)	29(10)	-4(11)	4(7)	3(10)

S(3A)	18(1)	39(2)	19(1)	3(1)	3(1)	1(1)
F(7A)	42(3)	116(6)	88(4)	-56(5)	18(3)	9(3)
F(8A)	31(4)	121(10)	99(11)	88(9)	6(5)	-8(5)
F(9A)	19(3)	77(9)	39(4)	13(5)	4(3)	2(5)
O(8A)	36(2)	75(3)	51(2)	6(2)	-8(2)	1(2)
O(9A)	36(2)	75(3)	51(2)	6(2)	-8(2)	1(2)
C(3A)	19(4)	48(7)	27(5)	0(5)	7(3)	3(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 6.

	x	y	z	U(eq)
H(5A)	3763	5670	3484	50
H(5B)	3809	6150	2763	50
H(6A)	4895	7171	3332	92
H(6B)	4240	6955	3934	92
H(7A)	5558	6140	4521	98
H(7B)	6245	6858	4238	98
H(8A)	6643	6045	3394	50
H(8B)	6506	5322	3943	50
H(9A)	4121	2713	2193	47
H(9B)	5380	2480	2438	47
H(10A)	4949	1692	1432	73
H(10B)	4075	2360	1041	73
H(11A)	6385	2529	1306	67
H(11B)	5557	2653	559	67
H(12A)	6193	3941	1320	48
H(12B)	4966	3904	883	48
H(14)	2092	5038	9982	33
H(15)	916	4050	10415	34
H(18)	1702	7012	7755	46
H(19)	2980	6381	7230	52
H(20)	3516	5015	7510	47
H(22)	624	6176	9158	48
H(23A)	-596	6503	7780	77
H(23B)	-1074	6520	8479	77
H(23C)	-652	5664	8214	77
H(24A)	667	7657	8347	84
H(24B)	1493	7474	9075	84
H(24C)	238	7595	9063	84
H(25)	2246	3609	8485	53
H(26A)	4399	4205	8984	121

H(26B)	3972	3317	9181	121
H(26C)	3498	4153	9447	121
H(27A)	2745	3539	7355	94
H(27B)	3328	2862	7911	94
H(27C)	3970	3674	7756	94
H(30)	-891	1200	9183	41
H(31)	-2629	1539	9261	43
H(32)	-3112	2911	9401	39
H(34)	1190	2662	9047	43
H(35A)	1207	1391	10084	76
H(35B)	1505	2346	10263	76
H(35C)	2261	1786	9887	76
H(36A)	360	1598	8223	81
H(36B)	705	934	8844	81
H(36C)	1609	1443	8558	81
H(37)	-1388	4691	9392	43
H(38A)	-2032	5022	10410	74
H(38B)	-1146	4300	10582	74
H(38C)	-2399	4077	10474	74
H(39A)	-3063	4552	8622	114
H(39B)	-3197	5147	9258	114
H(39C)	-3591	4200	9241	114
H(41)	-1983	3839	5010	29
H(42)	-765	4817	4593	26
H(45)	3272	5740	5424	43
H(46)	2969	7132	5630	46
H(47)	1335	7570	5853	43
H(49)	1403	4068	5484	44
H(08G)	3091	3472	5684	85
H(08H)	3179	4220	6237	85
H(08I)	3650	4329	5541	85
H(07A)	1171	4484	4311	66
H(07B)	1997	3720	4456	66
H(07C)	2438	4647	4409	66
H(52)	-788	6238	6142	44
H(08A)	-974	7367	4984	71

H(08B)	-1961	7040	5304	71
H(08C)	-1316	6407	4909	71
H(08D)	-217	7965	6147	85
H(08E)	179	7378	6817	85
H(08F)	-1079	7558	6540	85
H(57)	-1601	1864	7260	43
H(58)	-2874	2507	7769	45
H(59)	-3435	3860	7468	47
H(61)	-561	2681	5833	41
H(62A)	-1442	1402	5942	70
H(62B)	-577	1211	6652	70
H(62C)	-201	1269	5917	70
H(63A)	1168	2334	6470	67
H(63B)	746	2339	7190	67
H(63C)	778	3186	6762	67
H(64)	-2165	5261	6461	51
H(65A)	-3191	6045	7066	97
H(65B)	-2556	5393	7626	97
H(65C)	-3800	5241	7274	97
H(66A)	-3885	5544	5812	132
H(66B)	-4350	4715	6095	132
H(66C)	-3522	4650	5581	132
H(1)	-550(40)	3670(30)	8060(20)	32(13)
H(4)	720(40)	5120(30)	6940(20)	15(11)
H(5)	0(60)	4460(50)	7420(40)	100(20)

Crystallography tables for compound 7

Table 1. Crystal data and structure refinement for 7.

Identification code	2015_08_04_AT_Alcation_0m	
Empirical formula	C ₂₈ H ₃₈ F ₃ N ₃ O ₃ S	
Formula weight	553.67	
Temperature	125(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 10.5014(8) Å	α = 90°.
	b = 14.0346(10) Å	β = 90°.
	c = 20.5119(15) Å	γ = 90°.
Volume	3023.1(4) Å ³	
Z	4	
Density (calculated)	1.216 Mg/m ³	
Absorption coefficient	0.157 mm ⁻¹	
F(000)	1176	
Crystal size	0.27 x 0.20 x 0.15 mm ³	
Theta range for data collection	2.179 to 25.000°.	
Index ranges	-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -20 ≤ l ≤ 24	
Reflections collected	20332	
Independent reflections	5314 [R(int) = 0.0282]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6883	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5314 / 0 / 380	
Goodness-of-fit on F ²	1.032	
Final R indices [I > 2σ(I)]	R1 = 0.0343, wR2 = 0.0763	
R indices (all data)	R1 = 0.0399, wR2 = 0.0798	
Absolute structure parameter	0.01(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.435 and -0.245 e.Å ⁻³	

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

	x	y	z	$U(\text{eq})$
N(1)	9224(2)	4877(2)	5534(1)	32(1)
N(2)	8768(2)	5662(2)	6537(1)	27(1)
N(3)	9020(2)	4130(2)	6568(1)	25(1)
C(1)	9000(2)	4888(2)	6174(1)	26(1)
C(2)	8656(3)	5381(2)	7187(1)	30(1)
C(3)	8805(3)	4441(2)	7207(1)	30(1)
C(4)	8643(3)	6627(2)	6299(1)	26(1)
C(5)	9744(3)	7170(2)	6240(1)	32(1)
C(6)	9587(3)	8118(2)	6056(2)	40(1)
C(7)	8379(3)	8481(2)	5936(2)	40(1)
C(8)	7313(3)	7909(2)	5980(2)	34(1)
C(9)	7419(2)	6963(2)	6165(1)	27(1)
C(10)	11063(3)	6734(3)	6352(2)	47(1)
C(11)	11847(3)	6740(3)	5747(2)	50(1)
C(12)	11688(4)	7105(3)	6942(2)	70(1)
C(13)	6253(3)	6321(2)	6213(2)	35(1)
C(14)	5813(3)	6024(3)	5530(2)	58(1)
C(15)	5172(3)	6784(3)	6587(2)	44(1)
C(16)	9273(3)	3162(2)	6367(1)	26(1)
C(17)	10533(3)	2836(2)	6400(1)	28(1)
C(18)	10743(3)	1888(2)	6230(1)	33(1)
C(19)	9746(3)	1306(2)	6042(2)	38(1)
C(20)	8518(3)	1656(2)	6004(2)	38(1)
C(21)	8245(3)	2601(2)	6166(1)	31(1)
C(22)	11632(3)	3474(2)	6604(2)	33(1)
C(23)	12363(3)	3057(3)	7178(2)	48(1)
C(24)	12530(3)	3654(3)	6028(2)	52(1)
C(25)	6887(2)	2988(2)	6135(2)	38(1)
C(26A)	6140(20)	2600(20)	6676(13)	69(8)
C(27A)	6250(20)	2630(30)	5477(9)	65(6)
C(26B)	5960(20)	2493(18)	6606(11)	53(5)

C(27B)	6376(17)	3091(19)	5459(9)	52(4)
S(1)	8396(1)	5172(1)	3956(1)	28(1)
F(1)	9288(2)	4467(1)	2868(1)	53(1)
F(2)	10716(2)	5085(2)	3488(1)	65(1)
F(3)	9451(2)	5984(2)	2942(1)	68(1)
O(1)	8574(2)	4239(1)	4237(1)	37(1)
O(2)	7189(2)	5316(2)	3639(1)	40(1)
O(3)	8827(2)	5949(1)	4361(1)	39(1)
C(28)	9521(3)	5181(2)	3282(2)	41(1)

Table 3. Bond lengths [Å] and angles [°] for 7.

N(1)-C(1)	1.332(4)
N(2)-C(1)	1.339(3)
N(2)-C(2)	1.395(4)
N(2)-C(4)	1.446(4)
N(3)-C(1)	1.337(3)
N(3)-C(3)	1.400(4)
N(3)-C(16)	1.445(3)
C(2)-C(3)	1.329(4)
C(4)-C(5)	1.390(4)
C(4)-C(9)	1.396(4)
C(5)-C(6)	1.393(4)
C(5)-C(10)	1.531(4)
C(6)-C(7)	1.389(4)
C(7)-C(8)	1.381(4)
C(8)-C(9)	1.385(4)
C(9)-C(13)	1.524(4)
C(10)-C(12)	1.472(5)
C(10)-C(11)	1.490(5)
C(13)-C(15)	1.517(4)
C(13)-C(14)	1.532(5)
C(16)-C(21)	1.398(4)
C(16)-C(17)	1.402(4)
C(17)-C(18)	1.393(4)
C(17)-C(22)	1.519(4)
C(18)-C(19)	1.383(4)
C(19)-C(20)	1.382(4)
C(20)-C(21)	1.397(4)
C(21)-C(25)	1.528(4)
C(22)-C(23)	1.523(4)
C(22)-C(24)	1.532(4)
C(25)-C(26A)	1.47(2)
C(25)-C(27B)	1.493(17)
C(25)-C(26B)	1.538(18)
C(25)-C(27A)	1.589(19)

S(1)-O(2)	1.438(2)
S(1)-O(1)	1.442(2)
S(1)-O(3)	1.445(2)
S(1)-C(28)	1.819(3)
F(1)-C(28)	1.335(4)
F(2)-C(28)	1.332(4)
F(3)-C(28)	1.328(4)

C(1)-N(2)-C(2)	108.5(2)
C(1)-N(2)-C(4)	126.0(2)
C(2)-N(2)-C(4)	125.5(2)
C(1)-N(3)-C(3)	108.4(2)
C(1)-N(3)-C(16)	125.4(2)
C(3)-N(3)-C(16)	126.1(2)
N(1)-C(1)-N(3)	125.7(3)
N(1)-C(1)-N(2)	126.1(3)
N(3)-C(1)-N(2)	108.1(2)
C(3)-C(2)-N(2)	107.5(3)
C(2)-C(3)-N(3)	107.4(3)
C(5)-C(4)-C(9)	124.3(2)
C(5)-C(4)-N(2)	117.8(2)
C(9)-C(4)-N(2)	117.8(2)
C(4)-C(5)-C(6)	116.7(3)
C(4)-C(5)-C(10)	121.4(3)
C(6)-C(5)-C(10)	122.0(3)
C(7)-C(6)-C(5)	120.4(3)
C(8)-C(7)-C(6)	121.0(3)
C(7)-C(8)-C(9)	120.7(3)
C(8)-C(9)-C(4)	116.8(3)
C(8)-C(9)-C(13)	121.4(2)
C(4)-C(9)-C(13)	121.8(2)
C(12)-C(10)-C(11)	115.8(3)
C(12)-C(10)-C(5)	112.7(3)
C(11)-C(10)-C(5)	111.8(3)
C(15)-C(13)-C(9)	112.4(3)
C(15)-C(13)-C(14)	110.7(3)

C(9)-C(13)-C(14)	110.2(3)
C(21)-C(16)-C(17)	124.0(3)
C(21)-C(16)-N(3)	118.2(2)
C(17)-C(16)-N(3)	117.8(2)
C(18)-C(17)-C(16)	116.7(3)
C(18)-C(17)-C(22)	120.8(2)
C(16)-C(17)-C(22)	122.6(2)
C(19)-C(18)-C(17)	120.9(3)
C(20)-C(19)-C(18)	120.8(3)
C(19)-C(20)-C(21)	121.1(3)
C(20)-C(21)-C(16)	116.5(3)
C(20)-C(21)-C(25)	121.3(3)
C(16)-C(21)-C(25)	122.2(3)
C(17)-C(22)-C(23)	111.7(2)
C(17)-C(22)-C(24)	110.7(3)
C(23)-C(22)-C(24)	110.5(2)
C(26A)-C(25)-C(21)	109.7(9)
C(27B)-C(25)-C(21)	114.1(8)
C(27B)-C(25)-C(26B)	113.5(12)
C(21)-C(25)-C(26B)	113.8(8)
C(26A)-C(25)-C(27A)	107.3(16)
C(21)-C(25)-C(27A)	108.3(7)
O(2)-S(1)-O(1)	114.98(13)
O(2)-S(1)-O(3)	115.52(14)
O(1)-S(1)-O(3)	114.47(12)
O(2)-S(1)-C(28)	103.15(14)
O(1)-S(1)-C(28)	103.03(14)
O(3)-S(1)-C(28)	103.23(14)
F(3)-C(28)-F(2)	107.7(3)
F(3)-C(28)-F(1)	107.0(3)
F(2)-C(28)-F(1)	107.4(3)
F(3)-C(28)-S(1)	111.7(2)
F(2)-C(28)-S(1)	111.8(2)
F(1)-C(28)-S(1)	111.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 7. 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}
N(1)	44(1)	32(1)	20(1)	2(1)	-1(1)	5(1)
N(2)	28(1)	31(1)	22(1)	1(1)	2(1)	7(1)
N(3)	26(1)	30(1)	19(1)	0(1)	1(1)	5(1)
C(1)	21(1)	34(1)	22(1)	0(1)	0(1)	4(1)
C(2)	32(2)	39(2)	20(2)	-2(1)	3(1)	7(1)
C(3)	32(2)	40(2)	18(2)	2(1)	3(1)	7(1)
C(4)	28(1)	29(1)	22(1)	-1(1)	1(1)	5(1)
C(5)	27(1)	45(2)	24(2)	3(1)	2(1)	-1(1)
C(6)	37(2)	46(2)	38(2)	1(2)	4(2)	-15(1)
C(7)	49(2)	31(2)	39(2)	5(1)	2(2)	-3(2)
C(8)	31(1)	36(2)	34(2)	3(1)	0(1)	7(1)
C(9)	26(1)	32(1)	24(2)	0(1)	2(1)	2(1)
C(10)	28(2)	74(2)	39(2)	5(2)	2(1)	4(2)
C(11)	35(2)	63(2)	52(2)	-14(2)	0(2)	6(2)
C(12)	44(2)	113(3)	53(2)	-38(2)	-12(2)	28(2)
C(13)	25(1)	39(2)	41(2)	6(1)	-4(1)	-1(1)
C(14)	42(2)	79(3)	54(2)	-23(2)	3(2)	-22(2)
C(15)	30(2)	59(2)	44(2)	4(2)	2(2)	-2(2)
C(16)	26(1)	31(2)	21(1)	4(1)	3(1)	2(1)
C(17)	28(1)	33(2)	22(2)	5(1)	3(1)	3(1)
C(18)	30(1)	35(2)	35(2)	4(1)	5(1)	6(1)
C(19)	44(2)	30(2)	40(2)	-2(2)	7(2)	2(1)
C(20)	37(2)	36(2)	41(2)	-1(1)	-1(2)	-8(1)
C(21)	28(1)	37(2)	29(2)	5(1)	2(1)	-2(1)
C(22)	24(1)	36(2)	39(2)	1(1)	-2(1)	2(1)
C(23)	37(2)	62(2)	44(2)	8(2)	-7(2)	-10(2)
C(24)	36(2)	69(2)	50(2)	14(2)	-1(2)	-14(2)
C(25)	24(1)	45(2)	45(2)	2(2)	-2(1)	-1(1)
C(26A)	21(6)	126(16)	62(11)	-11(9)	10(6)	25(8)
C(27A)	42(7)	119(15)	35(6)	-1(9)	-11(5)	30(10)
C(26B)	39(8)	85(10)	34(7)	35(7)	0(5)	-1(6)

C(27B)	38(5)	73(10)	45(5)	21(7)	0(4)	5(6)
S(1)	35(1)	26(1)	23(1)	0(1)	-4(1)	0(1)
F(1)	59(1)	60(1)	40(1)	-18(1)	4(1)	5(1)
F(2)	34(1)	78(2)	84(2)	-18(1)	4(1)	-6(1)
F(3)	96(2)	55(1)	55(1)	16(1)	28(1)	-8(1)
O(1)	51(1)	26(1)	33(1)	4(1)	-10(1)	-4(1)
O(2)	36(1)	49(1)	34(1)	3(1)	-6(1)	5(1)
O(3)	62(1)	26(1)	31(1)	-3(1)	-7(1)	0(1)
C(28)	42(2)	41(2)	40(2)	-4(2)	4(1)	-2(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 7.

	x	y	z	U(eq)
H(1A)	9170(30)	4330(20)	5305(17)	40(9)
H(1B)	9060(30)	5380(20)	5317(16)	37(9)
H(2)	8501	5787	7548	36
H(3)	8773	4052	7586	36
H(6)	10311	8519	6013	48
H(7)	8285	9134	5822	48
H(8)	6499	8167	5883	40
H(10)	10900	6045	6446	56
H(11A)	12048	7399	5627	75
H(11B)	11371	6437	5392	75
H(11C)	12639	6388	5823	75
H(12A)	12483	6757	7017	105
H(12B)	11122	7022	7318	105
H(12C)	11875	7784	6883	105
H(13)	6509	5731	6453	42
H(14A)	5544	6590	5286	88
H(14B)	5095	5580	5567	88
H(14C)	6516	5712	5300	88
H(15A)	5489	7012	7009	67
H(15B)	4494	6316	6659	67
H(15C)	4837	7322	6336	67
H(18)	11583	1637	6245	40
H(19)	9907	658	5937	46
H(20)	7850	1247	5866	46
H(22)	11270	4101	6743	39
H(23A)	11778	2953	7544	72
H(23B)	13034	3501	7311	72
H(23C)	12746	2449	7050	72
H(24A)	12907	3049	5887	78
H(24B)	13207	4092	6163	78

H(24C)	12050	3935	5666	78
H(25)	6892	3700	6152	46
H(26A)	6181	1900	6667	104
H(26B)	5248	2800	6632	104
H(26C)	6480	2831	7090	104
H(27A)	6163	1932	5490	98
H(27B)	6790	2808	5107	98
H(27C)	5409	2919	5428	98
H(26D)	5136	2820	6595	79
H(26E)	6306	2515	7049	79
H(26F)	5847	1827	6473	79
H(27D)	6935	3511	5207	78
H(27E)	5519	3365	5477	78
H(27F)	6340	2463	5251	78
