

Supporting Information

Synthesis of Potassium-Magnesium Ate Complexes with Bulky Diamido Ligand

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1. The crystallographic data of complexes **2-4**

1) The crystallographic data of **2**

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

Identification code	090604pi_Oma
Empirical formula	C ₅₂ H ₈₀ Mg ₂ N ₄ Si ₂
Formula weight	866.00
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 21.054(3) Å alpha = 90 deg. b = 18.704(2) Å beta = 90 deg. c = 13.4708(16) Å gamma = 90 deg.
Volume	5304.8(11) Å ³
Z, Calculated density	4, 1.084 Mg/m ³
Absorption coefficient	0.126 mm ⁻¹
F(000)	1888
Crystal size	0.25 x 0.10 x 0.08 mm
Theta range for data collection	1.86 to 26.01 deg.
Limiting indices	-25 ≤ h ≤ 24, -17 ≤ k ≤ 23, -16 ≤ l ≤ 16
Reflections collected / unique	27628 / 10245 [R(int) = 0.0413]
Completeness to theta = 26.01	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9900 and 0.9691
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10245 / 1 / 541

Goodness-of-fit on F^2	1.050
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0464, wR2 = 0.1158
R indices (all data)	R1 = 0.0616, wR2 = 0.1294
Absolute structure parameter	0.22(11)
Largest diff. peak and hole	0.423 and -0.422 e. $\text{\AA}^{-3}$

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

	x	y	z	U(eq)
Mg(1)	3095(1)	2971(1)	6747(1)	19(1)
Mg(2)	3062(1)	2692(1)	4671(1)	19(1)
N(1)	2735(1)	2246(1)	7639(2)	22(1)
N(2)	2418(1)	2499(1)	5790(2)	20(1)
N(3)	3678(1)	3288(1)	5605(2)	18(1)
N(4)	3885(1)	2374(1)	4137(2)	20(1)
Si(1)	2261(1)	1879(1)	6735(1)	21(1)
Si(2)	4314(1)	2837(1)	5016(1)	19(1)
C(1)	2792(1)	1943(2)	8598(2)	23(1)
C(2)	2340(2)	2098(2)	9345(2)	24(1)
C(3)	2387(2)	1775(2)	10278(2)	27(1)
C(4)	2883(2)	1313(2)	10497(2)	33(1)
C(5)	3342(2)	1182(2)	9786(2)	30(1)
C(6)	3309(2)	1483(2)	8849(2)	26(1)
C(7)	1811(2)	2644(2)	9196(2)	27(1)
C(8)	1154(2)	2371(2)	9507(3)	38(1)
C(9)	1962(2)	3328(2)	9758(3)	39(1)
C(10)	3856(2)	1341(2)	8137(3)	32(1)
C(11)	3994(2)	553(2)	8006(3)	49(1)
C(12)	4454(2)	1737(2)	8513(3)	43(1)
C(13)	1918(1)	2807(2)	5208(2)	20(1)
C(14)	1575(1)	3419(2)	5530(2)	22(1)
C(15)	1152(1)	3751(2)	4899(2)	28(1)
C(16)	1039(2)	3489(2)	3946(3)	34(1)
C(17)	1353(2)	2882(2)	3633(2)	35(1)
C(18)	1793(2)	2533(2)	4241(2)	29(1)
C(19)	2109(2)	1846(2)	3878(3)	46(1)
C(20)	1617(2)	1230(3)	3837(6)	98(3)
C(21)	2444(3)	1951(4)	2892(3)	107(3)
C(22)	1386(2)	1814(2)	6958(2)	28(1)
C(23)	2512(2)	946(2)	6425(3)	32(1)
C(24)	1670(1)	3722(2)	6578(2)	23(1)
C(25)	2086(2)	4396(2)	6552(3)	33(1)
C(26)	1045(2)	3869(2)	7094(3)	34(1)
C(27)	3753(1)	4037(2)	5784(2)	20(1)
C(28)	3939(1)	4284(2)	6737(3)	25(1)
C(29)	3972(2)	5017(2)	6915(3)	39(1)
C(30)	3822(2)	5507(2)	6203(3)	45(1)

C (31)	3643 (2)	5273 (2)	5267 (3)	38 (1)
C (32)	3614 (1)	4550 (2)	5041 (2)	24 (1)
C (33)	4095 (2)	3775 (2)	7584 (2)	27 (1)
C (34)	3595 (2)	3806 (2)	8409 (3)	39 (1)
C (35)	4758 (2)	3905 (2)	8025 (3)	41 (1)
C (36)	3425 (2)	4330 (2)	3989 (2)	26 (1)
C (37)	3743 (2)	4789 (2)	3183 (3)	39 (1)
C (38)	2706 (2)	4354 (2)	3858 (3)	37 (1)
C (39)	4155 (1)	1905 (2)	3429 (2)	22 (1)
C (40)	4368 (2)	2166 (2)	2495 (2)	27 (1)
C (41)	4638 (2)	1702 (2)	1812 (3)	36 (1)
C (42)	4711 (2)	984 (2)	2010 (2)	38 (1)
C (43)	4489 (2)	722 (2)	2904 (3)	31 (1)
C (44)	4205 (1)	1162 (2)	3603 (2)	25 (1)
C (45)	4282 (2)	2941 (2)	2191 (2)	30 (1)
C (46)	4905 (2)	3293 (2)	1851 (3)	44 (1)
C (47)	3776 (2)	3021 (2)	1376 (3)	43 (1)
C (48)	3929 (2)	815 (2)	4536 (2)	26 (1)
C (49)	4412 (2)	366 (2)	5101 (3)	38 (1)
C (50)	3356 (2)	344 (2)	4260 (3)	39 (1)
C (51)	4745 (2)	2247 (2)	5904 (2)	26 (1)
C (52)	4926 (1)	3485 (2)	4565 (2)	27 (1)

Table 3. Bond lengths [Å] and angles [deg] for **2**.

Mg(1)–N(1)	1.963(3)
Mg(1)–N(3)	2.057(3)
Mg(1)–N(2)	2.114(3)
Mg(1)–Mg(2)	2.8459(14)
Mg(2)–N(4)	1.969(3)
Mg(2)–N(2)	2.060(3)
Mg(2)–N(3)	2.124(2)
N(1)–C(1)	1.416(4)
N(1)–Si(1)	1.716(3)
N(2)–C(13)	1.433(4)
N(2)–Si(1)	1.754(3)
N(3)–C(27)	1.430(4)
N(3)–Si(2)	1.770(2)
N(4)–C(39)	1.415(4)
N(4)–Si(2)	1.722(2)
Si(1)–C(23)	1.870(3)
Si(1)–C(22)	1.871(3)
Si(2)–C(51)	1.864(3)
Si(2)–C(52)	1.871(3)
C(1)–C(2)	1.416(4)
C(1)–C(6)	1.427(4)
C(2)–C(3)	1.398(4)
C(2)–C(7)	1.525(4)
C(3)–C(4)	1.389(5)
C(3)–H(3A)	0.9500
C(4)–C(5)	1.382(5)
C(4)–H(4A)	0.9500
C(5)–C(6)	1.385(4)
C(5)–H(5A)	0.9500
C(6)–C(10)	1.523(4)
C(7)–C(9)	1.521(5)
C(7)–C(8)	1.533(5)
C(7)–H(7A)	1.0000
C(8)–H(8A)	0.9800
C(8)–H(8B)	0.9800
C(8)–H(8C)	0.9800
C(9)–H(9A)	0.9800
C(9)–H(9B)	0.9800
C(9)–H(9C)	0.9800
C(10)–C(11)	1.512(5)
C(10)–C(12)	1.545(5)
C(10)–H(10A)	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. 421 (4)
C (13) -C (18)	1. 424 (4)
C (14) -C (15)	1. 379 (4)
C (14) -C (24)	1. 534 (4)
C (15) -C (16)	1. 394 (5)
C (15) -H (15A)	0. 9500
C (16) -C (17)	1. 380 (5)
C (16) -H (16A)	0. 9500
C (17) -C (18)	1. 398 (5)
C (17) -H (17A)	0. 9500
C (18) -C (19)	1. 528 (5)
C (19) -C (21)	1. 517 (6)
C (19) -C (20)	1. 551 (6)
C (19) -H (19A)	1. 0000
C (20) -H (20A)	0. 9800
C (20) -H (20B)	0. 9800
C (20) -H (20C)	0. 9800
C (21) -H (21A)	0. 9800
C (21) -H (21B)	0. 9800
C (21) -H (21C)	0. 9800
C (22) -H (22A)	0. 9800
C (22) -H (22B)	0. 9800
C (22) -H (22C)	0. 9800
C (23) -H (23A)	0. 9800
C (23) -H (23B)	0. 9800
C (23) -H (23C)	0. 9800
C (24) -C (26)	1. 514 (4)
C (24) -C (25)	1. 536 (4)
C (24) -H (24A)	1. 0000
C (25) -H (25A)	0. 9800
C (25) -H (25B)	0. 9800
C (25) -H (25C)	0. 9800
C (26) -H (26A)	0. 9800
C (26) -H (26B)	0. 9800
C (26) -H (26C)	0. 9800
C (27) -C (32)	1. 416 (4)
C (27) -C (28)	1. 419 (4)
C (28) -C (29)	1. 393 (4)
C (28) -C (33)	1. 522 (5)
C (29) -C (30)	1. 364 (5)
C (29) -H (29A)	0. 9500
C (30) -C (31)	1. 386 (5)
C (30) -H (30A)	0. 9500
C (31) -C (32)	1. 388 (4)
C (31) -H (31A)	0. 9500
C (32) -C (36)	1. 529 (4)

C (33) –C (34)	1. 533 (5)
C (33) –C (35)	1. 535 (5)
C (33) –H (33A)	1. 0000
C (34) –H (34A)	0. 9800
C (34) –H (34B)	0. 9800
C (34) –H (34C)	0. 9800
C (35) –H (35A)	0. 9800
C (35) –H (35B)	0. 9800
C (35) –H (35C)	0. 9800
C (36) –C (38)	1. 523 (5)
C (36) –C (37)	1. 538 (4)
C (36) –H (36A)	1. 0000
C (37) –H (37A)	0. 9800
C (37) –H (37B)	0. 9800
C (37) –H (37C)	0. 9800
C (38) –H (38A)	0. 9800
C (38) –H (38B)	0. 9800
C (38) –H (38C)	0. 9800
C (39) –C (44)	1. 413 (4)
C (39) –C (40)	1. 423 (4)
C (40) –C (41)	1. 387 (4)
C (40) –C (45)	1. 517 (5)
C (41) –C (42)	1. 378 (5)
C (41) –H (41A)	0. 9500
C (42) –C (43)	1. 381 (5)
C (42) –H (42A)	0. 9500
C (43) –C (44)	1. 386 (4)
C (43) –H (43A)	0. 9500
C (44) –C (48)	1. 529 (4)
C (45) –C (47)	1. 537 (5)
C (45) –C (46)	1. 538 (5)
C (45) –H (45A)	1. 0000
C (46) –H (46A)	0. 9800
C (46) –H (46B)	0. 9800
C (46) –H (46C)	0. 9800
C (47) –H (47A)	0. 9800
C (47) –H (47B)	0. 9800
C (47) –H (47C)	0. 9800
C (48) –C (49)	1. 523 (5)
C (48) –C (50)	1. 539 (4)
C (48) –H (48A)	1. 0000
C (49) –H (49A)	0. 9800
C (49) –H (49B)	0. 9800
C (49) –H (49C)	0. 9800
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)–H(52A)	0.9800
C(52)–H(52B)	0.9800
C(52)–H(52C)	0.9800
N(1)–Mg(1)–N(3)	152.55(11)
N(1)–Mg(1)–N(2)	79.89(11)
N(3)–Mg(1)–N(2)	93.84(10)
N(1)–Mg(1)–Mg(2)	117.71(8)
N(3)–Mg(1)–Mg(2)	48.09(7)
N(2)–Mg(1)–Mg(2)	46.22(7)
N(4)–Mg(2)–N(2)	142.57(11)
N(4)–Mg(2)–N(3)	80.62(10)
N(2)–Mg(2)–N(3)	93.48(10)
N(4)–Mg(2)–Mg(1)	113.14(8)
N(2)–Mg(2)–Mg(1)	47.83(7)
N(3)–Mg(2)–Mg(1)	46.12(7)
C(1)–N(1)–Si(1)	122.5(2)
C(1)–N(1)–Mg(1)	143.2(2)
Si(1)–N(1)–Mg(1)	93.83(12)
C(13)–N(2)–Si(1)	121.70(19)
C(13)–N(2)–Mg(2)	90.69(17)
Si(1)–N(2)–Mg(2)	140.45(14)
C(13)–N(2)–Mg(1)	131.33(19)
Si(1)–N(2)–Mg(1)	87.72(11)
Mg(2)–N(2)–Mg(1)	85.96(10)
C(27)–N(3)–Si(2)	117.35(18)
C(27)–N(3)–Mg(1)	102.84(17)
Si(2)–N(3)–Mg(1)	130.50(13)
C(27)–N(3)–Mg(2)	132.99(19)
Si(2)–N(3)–Mg(2)	86.90(10)
Mg(1)–N(3)–Mg(2)	85.79(9)
C(39)–N(4)–Si(2)	124.4(2)
C(39)–N(4)–Mg(2)	141.9(2)
Si(2)–N(4)–Mg(2)	93.33(11)
N(1)–Si(1)–N(2)	98.10(12)
N(1)–Si(1)–C(23)	111.56(14)
N(2)–Si(1)–C(23)	113.70(14)
N(1)–Si(1)–C(22)	118.95(13)
N(2)–Si(1)–C(22)	110.13(13)
C(23)–Si(1)–C(22)	104.71(14)
N(4)–Si(2)–N(3)	98.76(11)
N(4)–Si(2)–C(51)	113.48(13)
N(3)–Si(2)–C(51)	111.29(13)
N(4)–Si(2)–C(52)	117.60(14)
N(3)–Si(2)–C(52)	110.99(13)
C(51)–Si(2)–C(52)	104.82(15)
N(1)–C(1)–C(2)	120.6(3)
N(1)–C(1)–C(6)	121.5(3)

C(2)–C(1)–C(6)	117.9(3)
C(3)–C(2)–C(1)	120.3(3)
C(3)–C(2)–C(7)	117.3(3)
C(1)–C(2)–C(7)	122.3(3)
C(4)–C(3)–C(2)	120.8(3)
C(4)–C(3)–H(3A)	119.6
C(2)–C(3)–H(3A)	119.6
C(5)–C(4)–C(3)	119.3(3)
C(5)–C(4)–H(4A)	120.3
C(3)–C(4)–H(4A)	120.3
C(4)–C(5)–C(6)	121.6(3)
C(4)–C(5)–H(5A)	119.2
C(6)–C(5)–H(5A)	119.2
C(5)–C(6)–C(1)	120.0(3)
C(5)–C(6)–C(10)	117.7(3)
C(1)–C(6)–C(10)	122.2(3)
C(9)–C(7)–C(2)	110.2(3)
C(9)–C(7)–C(8)	109.5(3)
C(2)–C(7)–C(8)	113.6(3)
C(9)–C(7)–H(7A)	107.8
C(2)–C(7)–H(7A)	107.8
C(8)–C(7)–H(7A)	107.8
C(7)–C(8)–H(8A)	109.5
C(7)–C(8)–H(8B)	109.5
H(8A)–C(8)–H(8B)	109.5
C(7)–C(8)–H(8C)	109.5
H(8A)–C(8)–H(8C)	109.5
H(8B)–C(8)–H(8C)	109.5
C(7)–C(9)–H(9A)	109.5
C(7)–C(9)–H(9B)	109.5
H(9A)–C(9)–H(9B)	109.5
C(7)–C(9)–H(9C)	109.5
H(9A)–C(9)–H(9C)	109.5
H(9B)–C(9)–H(9C)	109.5
C(11)–C(10)–C(6)	112.9(3)
C(11)–C(10)–C(12)	110.5(3)
C(6)–C(10)–C(12)	109.0(3)
C(11)–C(10)–H(10A)	108.1
C(6)–C(10)–H(10A)	108.1
C(12)–C(10)–H(10A)	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(14)–C(13)–C(18)	118.3(3)
C(14)–C(13)–N(2)	122.0(2)
C(18)–C(13)–N(2)	119.4(3)
C(15)–C(14)–C(13)	120.1(3)
C(15)–C(14)–C(24)	119.0(3)
C(13)–C(14)–C(24)	120.8(3)
C(14)–C(15)–C(16)	121.4(3)
C(14)–C(15)–H(15A)	119.3
C(16)–C(15)–H(15A)	119.3
C(17)–C(16)–C(15)	119.2(3)
C(17)–C(16)–H(16A)	120.4
C(15)–C(16)–H(16A)	120.4
C(16)–C(17)–C(18)	121.5(3)
C(16)–C(17)–H(17A)	119.2
C(18)–C(17)–H(17A)	119.2
C(17)–C(18)–C(13)	119.4(3)
C(17)–C(18)–C(19)	119.6(3)
C(13)–C(18)–C(19)	121.0(3)
C(21)–C(19)–C(18)	112.0(4)
C(21)–C(19)–C(20)	112.0(4)
C(18)–C(19)–C(20)	110.2(3)
C(21)–C(19)–H(19A)	107.4
C(18)–C(19)–H(19A)	107.4
C(20)–C(19)–H(19A)	107.4
C(19)–C(20)–H(20A)	109.5
C(19)–C(20)–H(20B)	109.5
H(20A)–C(20)–H(20B)	109.5
C(19)–C(20)–H(20C)	109.5
H(20A)–C(20)–H(20C)	109.5
H(20B)–C(20)–H(20C)	109.5
C(19)–C(21)–H(21A)	109.5
C(19)–C(21)–H(21B)	109.5
H(21A)–C(21)–H(21B)	109.5
C(19)–C(21)–H(21C)	109.5
H(21A)–C(21)–H(21C)	109.5
H(21B)–C(21)–H(21C)	109.5
Si(1)–C(22)–H(22A)	109.5
Si(1)–C(22)–H(22B)	109.5
H(22A)–C(22)–H(22B)	109.5
Si(1)–C(22)–H(22C)	109.5
H(22A)–C(22)–H(22C)	109.5
H(22B)–C(22)–H(22C)	109.5
Si(1)–C(23)–H(23A)	109.5
Si(1)–C(23)–H(23B)	109.5
H(23A)–C(23)–H(23B)	109.5
Si(1)–C(23)–H(23C)	109.5

H(23A)–C(23)–H(23C)	109.5
H(23B)–C(23)–H(23C)	109.5
C(26)–C(24)–C(14)	112.1(2)
C(26)–C(24)–C(25)	111.0(2)
C(14)–C(24)–C(25)	110.9(2)
C(26)–C(24)–H(24A)	107.6
C(14)–C(24)–H(24A)	107.6
C(25)–C(24)–H(24A)	107.6
C(24)–C(25)–H(25A)	109.5
C(24)–C(25)–H(25B)	109.5
H(25A)–C(25)–H(25B)	109.5
C(24)–C(25)–H(25C)	109.5
H(25A)–C(25)–H(25C)	109.5
H(25B)–C(25)–H(25C)	109.5
C(24)–C(26)–H(26A)	109.5
C(24)–C(26)–H(26B)	109.5
H(26A)–C(26)–H(26B)	109.5
C(24)–C(26)–H(26C)	109.5
H(26A)–C(26)–H(26C)	109.5
H(26B)–C(26)–H(26C)	109.5
C(32)–C(27)–C(28)	118.4(3)
C(32)–C(27)–N(3)	121.4(3)
C(28)–C(27)–N(3)	120.2(3)
C(29)–C(28)–C(27)	119.3(3)
C(29)–C(28)–C(33)	118.4(3)
C(27)–C(28)–C(33)	122.3(3)
C(30)–C(29)–C(28)	122.0(3)
C(30)–C(29)–H(29A)	119.0
C(28)–C(29)–H(29A)	119.0
C(29)–C(30)–C(31)	119.3(3)
C(29)–C(30)–H(30A)	120.4
C(31)–C(30)–H(30A)	120.4
C(30)–C(31)–C(32)	121.3(3)
C(30)–C(31)–H(31A)	119.3
C(32)–C(31)–H(31A)	119.3
C(31)–C(32)–C(27)	119.7(3)
C(31)–C(32)–C(36)	118.4(3)
C(27)–C(32)–C(36)	121.8(3)
C(28)–C(33)–C(34)	111.8(3)
C(28)–C(33)–C(35)	112.7(3)
C(34)–C(33)–C(35)	109.7(3)
C(28)–C(33)–H(33A)	107.4
C(34)–C(33)–H(33A)	107.4
C(35)–C(33)–H(33A)	107.4
C(33)–C(34)–H(34A)	109.5
C(33)–C(34)–H(34B)	109.5
H(34A)–C(34)–H(34B)	109.5
C(33)–C(34)–H(34C)	109.5
H(34A)–C(34)–H(34C)	109.5

H(34B)–C(34)–H(34C)	109.5
C(33)–C(35)–H(35A)	109.5
C(33)–C(35)–H(35B)	109.5
H(35A)–C(35)–H(35B)	109.5
C(33)–C(35)–H(35C)	109.5
H(35A)–C(35)–H(35C)	109.5
H(35B)–C(35)–H(35C)	109.5
C(38)–C(36)–C(32)	111.1(3)
C(38)–C(36)–C(37)	109.6(3)
C(32)–C(36)–C(37)	113.0(3)
C(38)–C(36)–H(36A)	107.7
C(32)–C(36)–H(36A)	107.7
C(37)–C(36)–H(36A)	107.7
C(36)–C(37)–H(37A)	109.5
C(36)–C(37)–H(37B)	109.5
H(37A)–C(37)–H(37B)	109.5
C(36)–C(37)–H(37C)	109.5
H(37A)–C(37)–H(37C)	109.5
H(37B)–C(37)–H(37C)	109.5
C(36)–C(38)–H(38A)	109.5
C(36)–C(38)–H(38B)	109.5
H(38A)–C(38)–H(38B)	109.5
C(36)–C(38)–H(38C)	109.5
H(38A)–C(38)–H(38C)	109.5
H(38B)–C(38)–H(38C)	109.5
C(44)–C(39)–N(4)	121.9(3)
C(44)–C(39)–C(40)	117.4(3)
N(4)–C(39)–C(40)	120.6(3)
C(41)–C(40)–C(39)	120.0(3)
C(41)–C(40)–C(45)	118.0(3)
C(39)–C(40)–C(45)	122.0(3)
C(42)–C(41)–C(40)	121.9(3)
C(42)–C(41)–H(41A)	119.1
C(40)–C(41)–H(41A)	119.1
C(41)–C(42)–C(43)	118.4(3)
C(41)–C(42)–H(42A)	120.8
C(43)–C(42)–H(42A)	120.8
C(42)–C(43)–C(44)	121.9(3)
C(42)–C(43)–H(43A)	119.1
C(44)–C(43)–H(43A)	119.1
C(43)–C(44)–C(39)	120.2(3)
C(43)–C(44)–C(48)	118.1(3)
C(39)–C(44)–C(48)	121.6(3)
C(40)–C(45)–C(47)	111.6(3)
C(40)–C(45)–C(46)	112.8(3)
C(47)–C(45)–C(46)	109.7(3)
C(40)–C(45)–H(45A)	107.5
C(47)–C(45)–H(45A)	107.5
C(46)–C(45)–H(45A)	107.5

C (45) -C (46) -H (46A)	109.5
C (45) -C (46) -H (46B)	109.5
H (46A) -C (46) -H (46B)	109.5
C (45) -C (46) -H (46C)	109.5
H (46A) -C (46) -H (46C)	109.5
H (46B) -C (46) -H (46C)	109.5
C (45) -C (47) -H (47A)	109.5
C (45) -C (47) -H (47B)	109.5
H (47A) -C (47) -H (47B)	109.5
C (45) -C (47) -H (47C)	109.5
H (47A) -C (47) -H (47C)	109.5
H (47B) -C (47) -H (47C)	109.5
C (49) -C (48) -C (44)	113.0 (3)
C (49) -C (48) -C (50)	109.2 (3)
C (44) -C (48) -C (50)	110.0 (3)
C (49) -C (48) -H (48A)	108.2
C (44) -C (48) -H (48A)	108.2
C (50) -C (48) -H (48A)	108.2
C (48) -C (49) -H (49A)	109.5
C (48) -C (49) -H (49B)	109.5
H (49A) -C (49) -H (49B)	109.5
C (48) -C (49) -H (49C)	109.5
H (49A) -C (49) -H (49C)	109.5
H (49B) -C (49) -H (49C)	109.5
C (48) -C (50) -H (50A)	109.5
C (48) -C (50) -H (50B)	109.5
H (50A) -C (50) -H (50B)	109.5
C (48) -C (50) -H (50C)	109.5
H (50A) -C (50) -H (50C)	109.5
H (50B) -C (50) -H (50C)	109.5
Si (2) -C (51) -H (51A)	109.5
Si (2) -C (51) -H (51B)	109.5
H (51A) -C (51) -H (51B)	109.5
Si (2) -C (51) -H (51C)	109.5
H (51A) -C (51) -H (51C)	109.5
H (51B) -C (51) -H (51C)	109.5
Si (2) -C (52) -H (52A)	109.5
Si (2) -C (52) -H (52B)	109.5
H (52A) -C (52) -H (52B)	109.5
Si (2) -C (52) -H (52C)	109.5
H (52A) -C (52) -H (52C)	109.5
H (52B) -C (52) -H (52C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
Mg(1)	19(1)	19(1)	20(1)	-2(1)	2(1)	-2(1)
Mg(2)	19(1)	18(1)	19(1)	-1(1)	0(1)	0(1)
N(1)	22(1)	19(1)	25(1)	1(1)	2(1)	1(1)
N(2)	17(1)	18(1)	25(1)	-5(1)	1(1)	0(1)
N(3)	20(1)	14(1)	21(1)	-2(1)	0(1)	0(1)
N(4)	20(1)	19(1)	20(1)	-2(1)	1(1)	2(1)
Si(1)	18(1)	17(1)	28(1)	-3(1)	3(1)	-1(1)
Si(2)	18(1)	16(1)	22(1)	-2(1)	1(1)	0(1)
C(1)	22(2)	21(2)	25(2)	-2(1)	1(1)	-3(1)
C(2)	26(2)	19(2)	26(2)	0(1)	2(1)	-1(1)
C(3)	35(2)	24(2)	22(2)	-2(1)	4(1)	2(1)
C(4)	50(2)	27(2)	22(2)	3(1)	-1(2)	4(2)
C(5)	34(2)	26(2)	31(2)	2(1)	-1(1)	5(1)
C(6)	28(2)	21(2)	28(2)	-1(1)	0(1)	1(1)
C(7)	31(2)	24(2)	26(2)	1(1)	4(1)	7(1)
C(8)	31(2)	44(2)	40(2)	7(2)	6(2)	7(2)
C(9)	47(2)	28(2)	41(2)	0(2)	10(2)	9(2)
C(10)	25(2)	39(2)	33(2)	10(2)	1(1)	9(1)
C(11)	51(2)	49(2)	48(2)	-1(2)	10(2)	22(2)
C(12)	28(2)	62(3)	39(2)	12(2)	2(2)	2(2)
C(13)	17(1)	24(1)	20(2)	-1(1)	3(1)	-4(1)
C(14)	19(2)	23(2)	23(2)	4(1)	3(1)	-4(1)
C(15)	22(2)	28(2)	35(2)	10(1)	-1(1)	-3(1)
C(16)	26(2)	46(2)	31(2)	15(2)	-5(1)	-6(2)
C(17)	31(2)	53(2)	22(2)	-1(2)	-5(1)	-13(2)
C(18)	21(2)	41(2)	24(2)	-3(1)	3(1)	-9(1)
C(19)	23(2)	71(3)	43(2)	-37(2)	0(2)	-1(2)
C(20)	31(2)	66(3)	195(7)	-90(4)	-15(3)	6(2)
C(21)	57(3)	240(8)	23(2)	-36(3)	-8(2)	61(4)
C(22)	22(2)	21(2)	41(2)	-1(1)	7(1)	0(1)
C(23)	26(2)	22(2)	49(2)	-4(1)	5(1)	1(1)
C(24)	21(1)	18(1)	30(2)	-1(1)	2(1)	2(1)
C(25)	28(2)	30(2)	41(2)	-6(2)	0(1)	-7(1)
C(26)	27(2)	33(2)	41(2)	-12(2)	7(1)	-4(1)
C(27)	17(1)	16(1)	28(2)	-2(1)	4(1)	2(1)
C(28)	19(1)	24(2)	32(2)	-7(1)	-1(1)	4(1)
C(29)	41(2)	27(2)	50(2)	-19(2)	-14(2)	3(2)
C(30)	48(2)	17(2)	71(3)	-14(2)	-19(2)	5(2)
C(31)	38(2)	22(2)	52(2)	4(2)	-4(2)	1(1)

C(32)	22(1)	18(1)	32(2)	0(1)	-1(1)	1(1)
C(33)	27(2)	27(2)	28(2)	-9(1)	0(1)	1(1)
C(34)	38(2)	44(2)	36(2)	-13(2)	4(2)	-4(2)
C(35)	35(2)	44(2)	44(2)	-5(2)	-13(2)	1(2)
C(36)	34(2)	17(2)	26(2)	4(1)	3(1)	2(1)
C(37)	39(2)	32(2)	46(2)	16(2)	4(2)	-5(2)
C(38)	35(2)	39(2)	36(2)	4(2)	1(2)	-6(2)
C(39)	21(1)	23(2)	21(1)	-5(1)	-3(1)	3(1)
C(40)	26(2)	31(2)	22(2)	-5(1)	-1(1)	3(1)
C(41)	40(2)	44(2)	23(2)	-5(2)	4(2)	9(2)
C(42)	42(2)	41(2)	31(2)	-16(2)	0(2)	14(2)
C(43)	34(2)	24(2)	35(2)	-10(1)	-4(1)	6(1)
C(44)	23(2)	24(2)	28(2)	-7(1)	-5(1)	2(1)
C(45)	30(2)	37(2)	22(2)	0(1)	6(1)	3(1)
C(46)	43(2)	48(2)	40(2)	8(2)	14(2)	2(2)
C(47)	54(2)	36(2)	39(2)	5(2)	-8(2)	4(2)
C(48)	28(2)	17(1)	33(2)	-4(1)	0(1)	2(1)
C(49)	40(2)	30(2)	44(2)	6(2)	5(2)	4(2)
C(50)	30(2)	32(2)	54(2)	-23(2)	10(2)	-2(2)
C(51)	26(2)	26(2)	28(2)	-5(1)	1(1)	8(1)
C(52)	19(2)	30(2)	33(2)	-5(1)	5(1)	-2(1)

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(3A)	2075	1874	10769	32
H(4A)	2907	1088	11129	40
H(5A)	3689	877	9945	36
H(7A)	1792	2763	8473	32
H(8A)	1055	1932	9141	58
H(8B)	833	2736	9358	58
H(8C)	1153	2271	10221	58
H(9A)	2382	3504	9558	58
H(9B)	1962	3231	10473	58
H(9C)	1641	3691	9606	58
H(10A)	3740	1543	7474	39
H(11A)	3610	310	7770	74
H(11B)	4125	348	8643	74
H(11C)	4335	492	7519	74
H(12A)	4357	2246	8595	65
H(12B)	4798	1680	8031	65
H(12C)	4584	1536	9153	65
H(15A)	933	4166	5117	34
H(16A)	749	3726	3516	41
H(17A)	1269	2697	2990	42
H(19A)	2439	1711	4378	55
H(20A)	1412	1180	4487	146
H(20B)	1833	782	3666	146
H(20C)	1295	1338	3333	146
H(21A)	2744	2349	2946	160
H(21B)	2130	2057	2376	160
H(21C)	2674	1513	2717	160
H(22A)	1250	1316	6887	42
H(22B)	1160	2111	6474	42
H(22C)	1289	1981	7631	42
H(23A)	2144	627	6461	48
H(23B)	2835	787	6900	48
H(23C)	2689	935	5753	48
H(24A)	1900	3353	6976	27
H(25A)	2142	4579	7229	49
H(25B)	1881	4761	6141	49
H(25C)	2502	4277	6271	49
H(26A)	789	3432	7106	50
H(26B)	814	4244	6735	50
H(26C)	1126	4028	7776	50

H(29A)	4102	5180	7551	47
H(30A)	3840	6004	6346	54
H(31A)	3537	5614	4771	45
H(33A)	4091	3279	7307	33
H(34A)	3173	3724	8124	59
H(34B)	3606	4277	8726	59
H(34C)	3686	3436	8905	59
H(35A)	5076	3886	7495	61
H(35B)	4851	3536	8520	61
H(35C)	4769	4377	8341	61
H(36A)	3564	3825	3888	31
H(37A)	3607	4624	2526	58
H(37B)	4206	4745	3238	58
H(37C)	3620	5291	3271	58
H(38A)	2597	4210	3179	55
H(38B)	2553	4841	3979	55
H(38C)	2506	4025	4331	55
H(41A)	4776	1884	1190	43
H(42A)	4909	676	1542	45
H(43A)	4533	227	3044	37
H(45A)	4128	3209	2787	35
H(46A)	5227	3239	2372	66
H(46B)	4832	3802	1724	66
H(46C)	5054	3061	1242	66
H(47A)	3379	2798	1596	65
H(47B)	3924	2786	768	65
H(47C)	3703	3529	1244	65
H(48A)	3776	1204	4986	31
H(49A)	4210	157	5689	57
H(49B)	4768	669	5308	57
H(49C)	4569	-17	4671	57
H(50A)	3183	123	4861	58
H(50B)	3492	-30	3797	58
H(50C)	3028	639	3945	58
H(51A)	5194	2384	5924	40
H(51B)	4708	1749	5687	40
H(51C)	4560	2298	6567	40
H(52A)	5339	3365	4857	41
H(52B)	4806	3970	4762	41
H(52C)	4955	3458	3840	41

Table 6. Torsion angles [deg] for **2**.

2) The crystallographic data of **3**

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

Identification code	090611pi_0m
Empirical formula	C ₅₅ H ₈₇ K ₂ Mg N ₄ Si ₂
Formula weight	962.98
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 13.0793(16) Å alpha = 93.883(2) deg. b = 18.673(2) Å beta = 100.717(2) deg. c = 23.230(3) Å gamma = 93.795(2) deg.
Volume	5543.6(12) Å ³
Z, Calculated density	4, 1.154 Mg/m ³
Absorption coefficient	0.263 mm ⁻¹
F(000)	2092
Crystal size	0.25 x 0.20 x 0.20 mm
Theta range for data collection	0.90 to 26.01 deg.
Limiting indices	-16<=h<=16, -19<=k<=23, -28<=l<=28
Reflections collected / unique	29911 / 21330 [R(int) = 0.0296]
Completeness to theta = 26.01	97.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9492 and 0.9371
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	21330 / 3 / 1202
Goodness-of-fit on F ²	1.032

Final R indices [I>2sigma(I)]	R1 = 0.0540, wR2 = 0.1463
R indices (all data)	R1 = 0.0773, wR2 = 0.1655
Largest diff. peak and hole	1.208 and -0.893 e.A ⁻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(eq)
Mg(1)	7853(1)	8135(1)	7877(1)	23(1)
Mg(2)	7010(1)	6792(1)	2604(1)	20(1)
K(1)	5853(1)	10138(1)	7852(1)	52(1)
K(2)	9823(1)	6120(1)	7842(1)	49(1)
K(3)	7075(1)	7058(1)	4633(1)	37(1)
K(4)	6997(1)	6916(1)	585(1)	38(1)
Si(1)	6948(1)	7764(1)	6693(1)	24(1)
Si(2)	8616(1)	8466(1)	9082(1)	28(1)
Si(3)	9185(1)	6700(1)	2805(1)	23(1)
Si(4)	4866(1)	6955(1)	2412(1)	29(1)
N(1)	6620(2)	8375(1)	7197(1)	24(1)
N(2)	8008(2)	7451(1)	7122(1)	24(1)
N(3)	8780(2)	7737(1)	8629(1)	26(1)
N(4)	7915(2)	8952(1)	8572(1)	25(1)
N(5)	8260(2)	6523(1)	2174(1)	22(1)
N(6)	8373(2)	6926(1)	3276(1)	23(1)
N(7)	5703(2)	6773(1)	3032(1)	22(1)
N(8)	5718(2)	6979(1)	1930(1)	23(1)
C(1)	5649(2)	8659(1)	7142(1)	26(1)
C(2)	4904(2)	8429(2)	7488(1)	32(1)
C(3)	3975(2)	8765(2)	7467(1)	39(1)
C(4)	3702(2)	9286(2)	7086(1)	42(1)
C(5)	4368(2)	9484(2)	6726(1)	38(1)
C(6)	5335(2)	9194(2)	6746(1)	31(1)
C(7)	6039(3)	9494(2)	6348(1)	39(1)
C(8)	5526(3)	9359(2)	5698(1)	57(1)
C(9)	6347(3)	10304(2)	6501(2)	60(1)
C(10)	5068(2)	7802(2)	7867(1)	35(1)
C(11)	5264(3)	8031(2)	8522(1)	46(1)
C(12)	4131(3)	7223(2)	7709(2)	48(1)
C(13)	8785(2)	7089(2)	6921(1)	26(1)
C(14)	8622(2)	6356(2)	6660(1)	29(1)
C(15)	9455(2)	6008(2)	6503(1)	34(1)
C(16)	10453(3)	6329(2)	6599(1)	43(1)
C(17)	10627(2)	7034(2)	6836(1)	41(1)
C(18)	9818(2)	7423(2)	6979(1)	34(1)
C(19)	10071(2)	8225(2)	7165(1)	37(1)
C(20)	10792(3)	8366(2)	7756(2)	53(1)

C (21)	10584 (3)	8622 (2)	6698 (2)	53 (1)
C (22)	7557 (2)	5928 (2)	6538 (1)	32 (1)
C (23)	7145 (3)	5783 (2)	5878 (1)	44 (1)
C (24)	7575 (3)	5202 (2)	6814 (2)	47 (1)
C (25)	5723 (2)	7165 (2)	6382 (1)	38 (1)
C (26)	7414 (3)	8070 (2)	6015 (1)	38 (1)
C (27)	9077 (2)	7073 (2)	8809 (1)	28 (1)
C (28)	8321 (2)	6465 (2)	8754 (1)	32 (1)
C (29)	8635 (3)	5782 (2)	8876 (1)	40 (1)
C (30)	9664 (3)	5668 (2)	9088 (1)	43 (1)
C (31)	10395 (2)	6253 (2)	9182 (1)	40 (1)
C (32)	10140 (2)	6945 (2)	9049 (1)	31 (1)
C (33)	11016 (2)	7539 (2)	9159 (1)	36 (1)
C (34)	11438 (3)	7720 (2)	9820 (1)	50 (1)
C (35)	11944 (3)	7360 (2)	8867 (2)	55 (1)
C (36)	7158 (2)	6552 (2)	8584 (1)	32 (1)
C (37)	6691 (3)	6214 (2)	7977 (1)	42 (1)
C (38)	6556 (3)	6247 (2)	9040 (2)	48 (1)
C (39)	7844 (2)	9692 (1)	8615 (1)	26 (1)
C (40)	7270 (2)	10050 (2)	9008 (1)	30 (1)
C (41)	7165 (2)	10792 (2)	9004 (1)	33 (1)
C (42)	7594 (2)	11207 (2)	8626 (1)	34 (1)
C (43)	8168 (2)	10877 (2)	8257 (1)	35 (1)
C (44)	8332 (2)	10149 (2)	8256 (1)	30 (1)
C (45)	9130 (2)	9872 (2)	7914 (1)	38 (1)
C (46)	8823 (3)	9928 (2)	7255 (2)	57 (1)
C (47)	10201 (3)	10280 (2)	8152 (2)	66 (1)
C (48)	6757 (3)	9653 (2)	9440 (1)	38 (1)
C (49)	5577 (3)	9734 (2)	9343 (2)	56 (1)
C (50)	7285 (4)	9910 (2)	10076 (1)	58 (1)
C (51)	7963 (3)	8086 (2)	9680 (1)	43 (1)
C (52)	9778 (3)	9064 (2)	9486 (2)	51 (1)
C (53)	8311 (2)	6175 (1)	1638 (1)	23 (1)
C (54)	7662 (2)	5530 (2)	1424 (1)	29 (1)
C (55)	7608 (2)	5227 (2)	851 (1)	38 (1)
C (56)	8219 (2)	5503 (2)	480 (1)	39 (1)
C (57)	8922 (2)	6089 (2)	696 (1)	33 (1)
C (58)	8988 (2)	6430 (2)	1256 (1)	26 (1)
C (59)	9803 (2)	7060 (2)	1451 (1)	32 (1)
C (60)	10899 (2)	6796 (2)	1567 (2)	47 (1)
C (61)	9751 (3)	7634 (2)	1001 (1)	44 (1)
C (62)	7124 (2)	5108 (2)	1840 (1)	37 (1)
C (63)	7766 (3)	4481 (2)	2037 (2)	57 (1)
C (64)	6007 (3)	4833 (3)	1616 (2)	76 (1)
C (65)	8676 (2)	7300 (2)	3826 (1)	26 (1)
C (66)	9220 (2)	6981 (2)	4331 (1)	32 (1)
C (67)	9448 (2)	7369 (2)	4882 (1)	40 (1)
C (68)	9158 (3)	8050 (2)	4969 (1)	45 (1)
C (69)	8658 (3)	8383 (2)	4488 (1)	42 (1)

C (70)	8432 (2)	8032 (2)	3924 (1)	31 (1)
C (71)	7977 (2)	8468 (2)	3421 (1)	35 (1)
C (72)	6895 (3)	8682 (2)	3468 (1)	44 (1)
C (73)	8713 (3)	9140 (2)	3390 (2)	53 (1)
C (74)	9556 (2)	6223 (2)	4294 (1)	42 (1)
C (75)	9109 (3)	5751 (2)	4718 (2)	60 (1)
C (76)	10750 (3)	6215 (3)	4419 (2)	67 (1)
C (77)	9930 (2)	5865 (2)	2887 (1)	40 (1)
C (78)	10243 (2)	7468 (2)	2907 (1)	38 (1)
C (79)	5449 (2)	6496 (1)	3534 (1)	22 (1)
C (80)	5762 (2)	5803 (1)	3698 (1)	27 (1)
C (81)	5611 (2)	5555 (2)	4233 (1)	32 (1)
C (82)	5087 (2)	5933 (2)	4607 (1)	33 (1)
C (83)	4721 (2)	6580 (2)	4440 (1)	31 (1)
C (84)	4897 (2)	6875 (1)	3924 (1)	26 (1)
C (85)	4488 (2)	7606 (2)	3812 (1)	32 (1)
C (86)	3292 (3)	7553 (2)	3675 (1)	45 (1)
C (87)	4906 (3)	8165 (2)	4333 (1)	44 (1)
C (88)	6182 (2)	5288 (2)	3279 (1)	31 (1)
C (89)	7264 (3)	5117 (3)	3501 (2)	72 (1)
C (90)	5467 (4)	4578 (2)	3153 (2)	72 (1)
C (91)	5499 (2)	7291 (2)	1395 (1)	25 (1)
C (92)	5967 (2)	7985 (2)	1324 (1)	29 (1)
C (93)	5779 (3)	8280 (2)	779 (1)	38 (1)
C (94)	5124 (3)	7928 (2)	295 (1)	40 (1)
C (95)	4640 (2)	7266 (2)	353 (1)	36 (1)
C (96)	4811 (2)	6937 (2)	885 (1)	27 (1)
C (97)	4271 (2)	6196 (2)	879 (1)	29 (1)
C (98)	4626 (3)	5658 (2)	444 (1)	40 (1)
C (99)	3076 (2)	6199 (2)	734 (1)	42 (1)
C (100)	6695 (3)	8418 (2)	1827 (1)	35 (1)
C (101)	7822 (3)	8304 (2)	1798 (1)	42 (1)
C (102)	6547 (4)	9227 (2)	1847 (2)	74 (1)
C (103)	4259 (3)	7855 (2)	2373 (1)	61 (1)
C (104)	3739 (2)	6255 (2)	2285 (1)	54 (1)
C (105)	1379 (5)	9910 (3)	4442 (3)	100 (2)
C (106)	1475 (6)	9526 (3)	4927 (3)	123 (2)
C (107)	2079 (5)	8897 (3)	4895 (3)	116 (3)
C (108)	2177 (4)	8468 (3)	5402 (2)	93 (2)
C (109)	2748 (5)	7831 (3)	5420 (3)	110 (2)
C (110)	2770 (4)	7282 (4)	5897 (2)	134 (3)

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

Mg(1)–N(1)	2.131(2)
Mg(1)–N(4)	2.131(2)
Mg(1)–N(3)	2.141(2)
Mg(1)–N(2)	2.147(2)
Mg(2)–N(6)	2.127(2)
Mg(2)–N(7)	2.131(2)
Mg(2)–N(5)	2.137(2)
Mg(2)–N(8)	2.145(2)
K(1)–C(6)	2.957(3)
K(1)–C(40)	2.986(3)
K(1)–C(41)	3.027(3)
K(1)–C(39)	3.064(3)
K(1)–C(5)	3.078(3)
K(1)–C(1)	3.089(3)
K(1)–C(42)	3.129(3)
K(1)–C(43)	3.189(3)
K(1)–C(44)	3.203(3)
K(1)–C(4)	3.282(3)
K(1)–C(2)	3.340(3)
K(1)–C(3)	3.383(3)
K(2)–C(14)	2.977(3)
K(2)–C(15)	3.048(3)
K(2)–C(32)	3.050(3)
K(2)–C(31)	3.053(3)
K(2)–C(13)	3.077(3)
K(2)–C(30)	3.108(3)
K(2)–C(27)	3.109(3)
K(2)–C(29)	3.169(3)
K(2)–C(16)	3.189(3)
K(2)–C(28)	3.208(3)
K(2)–C(18)	3.257(3)
K(2)–C(17)	3.271(3)
K(3)–C(84)	3.000(3)
K(3)–C(66)	3.026(3)
K(3)–C(67)	3.058(3)
K(3)–C(79)	3.076(3)
K(3)–C(83)	3.090(3)
K(3)–C(65)	3.090(2)
K(3)–C(68)	3.132(3)
K(3)–C(69)	3.196(3)
K(3)–C(70)	3.199(3)
K(3)–C(82)	3.222(3)
K(3)–C(80)	3.247(3)
K(3)–C(81)	3.267(3)
K(4)–C(58)	3.005(3)

K(4)-C(57)	3.021(3)
K(4)-C(91)	3.040(2)
K(4)-C(96)	3.069(3)
K(4)-C(92)	3.081(3)
K(4)-C(93)	3.142(3)
K(4)-C(95)	3.149(3)
K(4)-C(53)	3.171(2)
K(4)-C(94)	3.193(3)
K(4)-C(56)	3.193(3)
K(4)-C(55)	3.375(3)
K(4)-C(54)	3.407(3)
Si(1)-N(1)	1.711(2)
Si(1)-N(2)	1.712(2)
Si(1)-C(25)	1.887(3)
Si(1)-C(26)	1.900(3)
Si(2)-N(4)	1.710(2)
Si(2)-N(3)	1.713(2)
Si(2)-C(52)	1.883(3)
Si(2)-C(51)	1.911(3)
Si(3)-N(6)	1.712(2)
Si(3)-N(5)	1.715(2)
Si(3)-C(77)	1.895(3)
Si(3)-C(78)	1.897(3)
Si(4)-N(7)	1.709(2)
Si(4)-N(8)	1.7201(19)
Si(4)-C(104)	1.871(4)
Si(4)-C(103)	1.905(3)
N(1)-C(1)	1.396(3)
N(2)-C(13)	1.391(3)
N(3)-C(27)	1.390(3)
N(4)-C(39)	1.388(3)
N(5)-C(53)	1.382(3)
N(6)-C(65)	1.390(3)
N(7)-C(79)	1.393(3)
N(8)-C(91)	1.397(3)
C(1)-C(6)	1.433(4)
C(1)-C(2)	1.436(4)
C(2)-C(3)	1.398(4)
C(2)-C(10)	1.514(4)
C(3)-C(4)	1.380(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.367(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.402(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.528(4)
C(7)-C(8)	1.530(5)
C(7)-C(9)	1.539(5)
C(7)-H(7)	1.0000

C (8) -H (8A)	0. 9800
C (8) -H (8B)	0. 9800
C (8) -H (8C)	0. 9800
C (9) -H (9A)	0. 9800
C (9) -H (9B)	0. 9800
C (9) -H (9C)	0. 9800
C (10) -C (11)	1. 522 (4)
C (10) -C (12)	1. 553 (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 (18)	1. 429 (4)
C (13) -C (14)	1. 444 (4)
C (14) -C (15)	1. 397 (4)
C (14) -C (22)	1. 529 (4)
C (15) -C (16)	1. 372 (5)
C (15) -H (15)	0. 9500
C (16) -C (17)	1. 379 (5)
C (16) -H (16)	0. 9500
C (17) -C (18)	1. 400 (4)
C (17) -H (17)	0. 9500
C (18) -C (19)	1. 526 (4)
C (19) -C (20)	1. 510 (5)
C (19) -C (21)	1. 578 (4)
C (19) -H (19)	1. 0000
C (20) -H (20A)	0. 9800
C (20) -H (20B)	0. 9800
C (20) -H (20C)	0. 9800
C (21) -H (21A)	0. 9800
C (21) -H (21B)	0. 9800
C (21) -H (21C)	0. 9800
C (22) -C (23)	1. 527 (4)
C (22) -C (24)	1. 538 (4)
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) -H (25A)	0. 9800
C (25) -H (25B)	0. 9800
C (25) -H (25C)	0. 9800
C (26) -H (26A)	0. 9800
C (26) -H (26B)	0. 9800

C (26) -H (26C)	0. 9800
C (27) -C (28)	1. 438 (4)
C (27) -C (32)	1. 440 (4)
C (28) -C (29)	1. 396 (4)
C (28) -C (36)	1. 521 (4)
C (29) -C (30)	1. 380 (4)
C (29) -H (29)	0. 9500
C (30) -C (31)	1. 381 (5)
C (30) -H (30)	0. 9500
C (31) -C (32)	1. 397 (4)
C (31) -H (31)	0. 9500
C (32) -C (33)	1. 515 (4)
C (33) -C (34)	1. 539 (4)
C (33) -C (35)	1. 541 (4)
C (33) -H (33)	1. 0000
C (34) -H (34A)	0. 9800
C (34) -H (34B)	0. 9800
C (34) -H (34C)	0. 9800
C (35) -H (35A)	0. 9800
C (35) -H (35B)	0. 9800
C (35) -H (35C)	0. 9800
C (36) -C (37)	1. 507 (4)
C (36) -C (38)	1. 549 (4)
C (36) -H (36)	1. 0000
C (37) -H (37A)	0. 9800
C (37) -H (37B)	0. 9800
C (37) -H (37C)	0. 9800
C (38) -H (38A)	0. 9800
C (38) -H (38B)	0. 9800
C (38) -H (38C)	0. 9800
C (39) -C (44)	1. 433 (4)
C (39) -C (40)	1. 443 (4)
C (40) -C (41)	1. 401 (4)
C (40) -C (48)	1. 514 (4)
C (41) -C (42)	1. 381 (4)
C (41) -H (41)	0. 9500
C (42) -C (43)	1. 380 (4)
C (42) -H (42)	0. 9500
C (43) -C (44)	1. 391 (4)
C (43) -H (43)	0. 9500
C (44) -C (45)	1. 519 (4)
C (45) -C (46)	1. 522 (5)
C (45) -C (47)	1. 536 (5)
C (45) -H (45)	1. 0000
C (46) -H (46A)	0. 9800
C (46) -H (46B)	0. 9800
C (46) -H (46C)	0. 9800
C (47) -H (47A)	0. 9800
C (47) -H (47B)	0. 9800

C (47) -H (47C)	0. 9800
C (48) -C (49)	1. 536 (5)
C (48) -C (50)	1. 539 (5)
C (48) -H (48)	1. 0000
C (49) -H (49A)	0. 9800
C (49) -H (49B)	0. 9800
C (49) -H (49C)	0. 9800
C (50) -H (50A)	0. 9800
C (50) -H (50B)	0. 9800
C (50) -H (50C)	0. 9800
C (51) -K (4) #1	3. 469 (3)
C (51) -H (51A)	0. 9800
C (51) -H (51B)	0. 9800
C (51) -H (51C)	0. 9800
C (52) -H (52A)	0. 9800
C (52) -H (52B)	0. 9800
C (52) -H (52C)	0. 9800
C (53) -C (54)	1. 430 (4)
C (53) -C (58)	1. 446 (3)
C (54) -C (55)	1. 398 (4)
C (54) -C (62)	1. 528 (4)
C (55) -C (56)	1. 383 (4)
C (55) -H (55)	0. 9500
C (56) -C (57)	1. 383 (5)
C (56) -H (56)	0. 9500
C (57) -C (58)	1. 396 (4)
C (57) -H (57)	0. 9500
C (58) -C (59)	1. 519 (4)
C (59) -C (60)	1. 529 (4)
C (59) -C (61)	1. 541 (4)
C (59) -H (59)	1. 0000
C (60) -H (60A)	0. 9800
C (60) -H (60B)	0. 9800
C (60) -H (60C)	0. 9800
C (61) -H (61A)	0. 9800
C (61) -H (61B)	0. 9800
C (61) -H (61C)	0. 9800
C (62) -C (64)	1. 499 (5)
C (62) -C (63)	1. 531 (5)
C (62) -H (62)	1. 0000
C (63) -K (2) #2	3. 385 (4)
C (63) -H (63A)	0. 974 (10)
C (63) -H (63B)	0. 969 (10)
C (63) -H (63C)	0. 972 (10)
C (64) -H (64A)	0. 9800
C (64) -H (64B)	0. 9800
C (64) -H (64C)	0. 9800
C (65) -C (70)	1. 436 (4)
C (65) -C (66)	1. 442 (4)

C (66) –C (67)	1. 399 (4)
C (66) –C (74)	1. 510 (4)
C (67) –C (68)	1. 364 (5)
C (67) –H (67)	0. 9500
C (68) –C (69)	1. 391 (5)
C (68) –H (68)	0. 9500
C (69) –C (70)	1. 396 (4)
C (69) –H (69)	0. 9500
C (70) –C (71)	1. 522 (4)
C (71) –C (72)	1. 516 (4)
C (71) –C (73)	1. 545 (4)
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. 534 (4)
C (74) –C (76)	1. 535 (5)
C (74) –H (74)	1. 0000
C (75) –H (75A)	0. 9800
C (75) –H (75B)	0. 9800
C (75) –H (75C)	0. 9800
C (76) –H (76A)	0. 9800
C (76) –H (76B)	0. 9800
C (76) –H (76C)	0. 9800
C (77) –H (77A)	0. 9800
C (77) –H (77B)	0. 9800
C (77) –H (77C)	0. 9800
C (78) –H (78A)	0. 9800
C (78) –H (78B)	0. 9800
C (78) –H (78C)	0. 9800
C (79) –C (84)	1. 437 (3)
C (79) –C (80)	1. 437 (4)
C (80) –C (81)	1. 398 (3)
C (80) –C (88)	1. 522 (4)
C (81) –C (82)	1. 387 (4)
C (81) –H (81)	0. 9500
C (82) –C (83)	1. 382 (4)
C (82) –H (82)	0. 9500
C (83) –C (84)	1. 404 (3)
C (83) –H (83)	0. 9500
C (84) –C (85)	1. 520 (4)
C (85) –C (86)	1. 532 (4)
C (85) –C (87)	1. 537 (4)
C (85) –H (85)	1. 0000
C (86) –H (86A)	0. 9800
C (86) –H (86B)	0. 9800

C (86) –H (86C)	0. 9800
C (87) –H (87A)	0. 9800
C (87) –H (87B)	0. 9800
C (87) –H (87C)	0. 9800
C (88) –C (89)	1. 476 (5)
C (88) –C (90)	1. 550 (5)
C (88) –H (88)	1. 0000
C (89) –H (89A)	0. 9800
C (89) –H (89B)	0. 9800
C (89) –H (89C)	0. 9800
C (90) –H (90A)	0. 9800
C (90) –H (90B)	0. 9800
C (90) –H (90C)	0. 9800
C (91) –C (92)	1. 431 (4)
C (91) –C (96)	1. 438 (4)
C (92) –C (93)	1. 400 (4)
C (92) –C (100)	1. 511 (4)
C (93) –C (94)	1. 377 (5)
C (93) –H (93)	0. 9500
C (94) –C (95)	1. 378 (4)
C (94) –H (94)	0. 9500
C (95) –C (96)	1. 404 (4)
C (95) –H (95)	0. 9500
C (96) –C (97)	1. 510 (4)
C (97) –C (98)	1. 532 (4)
C (97) –C (99)	1. 537 (4)
C (97) –H (97)	1. 0000
C (98) –H (98A)	0. 9800
C (98) –H (98B)	0. 9800
C (98) –H (98C)	0. 9800
C (99) –H (99A)	0. 9800
C (99) –H (99B)	0. 9800
C (99) –H (99C)	0. 9800
C (100) –C (101)	1. 516 (4)
C (100) –C (102)	1. 534 (4)
C (100) –H (100)	1. 0000
C (101) –H (10A)	0. 9800
C (101) –H (10B)	0. 9800
C (101) –H (10C)	0. 9800
C (102) –H (10D)	0. 9800
C (102) –H (10E)	0. 9800
C (102) –H (10F)	0. 9800
C (103) –H (10G)	0. 9800
C (103) –H (10H)	0. 9800
C (103) –H (10I)	0. 9800
C (104) –H (10J)	0. 9800
C (104) –H (10K)	0. 9800
C (104) –H (10L)	0. 9800
C (105) –C (106)	1. 366 (8)

C(105)–H(10M)	0.9800
C(105)–H(10N)	0.9800
C(105)–H(10O)	0.9800
C(106)–C(107)	1.463(8)
C(106)–H(10P)	0.9900
C(106)–H(10Q)	0.9900
C(107)–C(108)	1.460(8)
C(107)–H(10R)	0.9900
C(107)–H(10S)	0.9900
C(108)–C(109)	1.446(7)
C(108)–H(10T)	0.9900
C(108)–H(10U)	0.9900
C(109)–C(110)	1.557(8)
C(109)–H(10V)	0.9900
C(109)–H(10W)	0.9900
C(110)–H(11D)	0.9800
C(110)–H(11E)	0.9800
C(110)–H(11F)	0.9800

N(1)–Mg(1)–N(4)	105.50(9)
N(1)–Mg(1)–N(3)	165.45(9)
N(4)–Mg(1)–N(3)	75.07(9)
N(1)–Mg(1)–N(2)	75.06(8)
N(4)–Mg(1)–N(2)	168.89(9)
N(3)–Mg(1)–N(2)	107.27(9)
N(6)–Mg(2)–N(7)	106.93(8)
N(6)–Mg(2)–N(5)	74.84(8)
N(7)–Mg(2)–N(5)	165.54(9)
N(6)–Mg(2)–N(8)	163.85(9)
N(7)–Mg(2)–N(8)	75.50(8)
N(5)–Mg(2)–N(8)	106.94(8)
C(6)–K(1)–C(40)	134.05(8)
C(6)–K(1)–C(41)	157.03(8)
C(40)–K(1)–C(41)	26.92(8)
C(6)–K(1)–C(39)	109.67(8)
C(40)–K(1)–C(39)	27.56(7)
C(41)–K(1)–C(39)	47.88(7)
C(6)–K(1)–C(5)	26.78(7)
C(40)–K(1)–C(5)	153.59(8)
C(41)–K(1)–C(5)	175.53(8)
C(39)–K(1)–C(5)	135.01(8)
C(6)–K(1)–C(1)	27.30(7)
C(40)–K(1)–C(1)	108.65(8)
C(41)–K(1)–C(1)	134.99(8)
C(39)–K(1)–C(1)	88.37(7)
C(5)–K(1)–C(1)	47.06(7)
C(6)–K(1)–C(42)	143.56(8)
C(40)–K(1)–C(42)	46.78(7)
C(41)–K(1)–C(42)	25.85(7)

C (39) -K (1) -C (42)	55. 17 (8)
C (5) -K (1) -C (42)	156. 94 (9)
C (1) -K (1) -C (42)	138. 92 (8)
C (6) -K (1) -C (43)	118. 96 (8)
C (40) -K (1) -C (43)	53. 24 (7)
C (41) -K (1) -C (43)	44. 70 (8)
C (39) -K (1) -C (43)	46. 17 (7)
C (5) -K (1) -C (43)	139. 55 (8)
C (1) -K (1) -C (43)	115. 79 (8)
C (42) -K (1) -C (43)	25. 21 (7)
C (6) -K (1) -C (44)	105. 18 (8)
C (40) -K (1) -C (44)	46. 16 (7)
C (41) -K (1) -C (44)	52. 94 (7)
C (39) -K (1) -C (44)	26. 31 (7)
C (5) -K (1) -C (44)	131. 38 (8)
C (1) -K (1) -C (44)	93. 80 (7)
C (42) -K (1) -C (44)	45. 12 (7)
C (43) -K (1) -C (44)	25. 14 (7)
C (6) -K (1) -C (4)	45. 34 (8)
C (40) -K (1) -C (4)	137. 95 (9)
C (41) -K (1) -C (4)	151. 34 (8)
C (39) -K (1) -C (4)	135. 37 (8)
C (5) -K (1) -C (4)	24. 55 (8)
C (1) -K (1) -C (4)	53. 20 (7)
C (42) -K (1) -C (4)	167. 85 (8)
C (43) -K (1) -C (4)	163. 77 (8)
C (44) -K (1) -C (4)	146. 97 (8)
C (6) -K (1) -C (2)	44. 95 (7)
C (40) -K (1) -C (2)	102. 67 (8)
C (41) -K (1) -C (2)	128. 46 (8)
C (39) -K (1) -C (2)	92. 44 (7)
C (5) -K (1) -C (2)	51. 06 (8)
C (1) -K (1) -C (2)	25. 44 (7)
C (42) -K (1) -C (2)	147. 30 (8)
C (43) -K (1) -C (2)	132. 73 (7)
C (44) -K (1) -C (2)	107. 76 (7)
C (4) -K (1) -C (2)	43. 01 (7)
C (6) -K (1) -C (3)	51. 43 (8)
C (40) -K (1) -C (3)	114. 91 (8)
C (41) -K (1) -C (3)	134. 69 (8)
C (39) -K (1) -C (3)	112. 94 (8)
C (5) -K (1) -C (3)	42. 60 (8)
C (1) -K (1) -C (3)	44. 41 (7)
C (42) -K (1) -C (3)	160. 46 (8)
C (43) -K (1) -C (3)	156. 56 (8)
C (44) -K (1) -C (3)	131. 44 (8)
C (4) -K (1) -C (3)	23. 83 (8)
C (2) -K (1) -C (3)	24. 00 (7)
C (14) -K (2) -C (15)	26. 79 (7)

C (14) -K (2) -C (32)	133. 83 (8)
C (15) -K (2) -C (32)	153. 64 (8)
C (14) -K (2) -C (31)	157. 06 (8)
C (15) -K (2) -C (31)	175. 00 (9)
C (32) -K (2) -C (31)	26. 47 (8)
C (14) -K (2) -C (13)	27. 53 (7)
C (15) -K (2) -C (13)	47. 43 (7)
C (32) -K (2) -C (13)	108. 19 (7)
C (31) -K (2) -C (13)	134. 28 (8)
C (14) -K (2) -C (30)	145. 02 (9)
C (15) -K (2) -C (30)	157. 48 (10)
C (32) -K (2) -C (30)	46. 60 (8)
C (31) -K (2) -C (30)	25. 88 (9)
C (13) -K (2) -C (30)	139. 91 (8)
C (14) -K (2) -C (27)	110. 30 (7)
C (15) -K (2) -C (27)	135. 83 (7)
C (32) -K (2) -C (27)	27. 02 (7)
C (31) -K (2) -C (27)	47. 03 (7)
C (13) -K (2) -C (27)	88. 91 (7)
C (30) -K (2) -C (27)	54. 88 (8)
C (14) -K (2) -C (29)	120. 12 (8)
C (15) -K (2) -C (29)	140. 12 (9)
C (32) -K (2) -C (29)	53. 21 (8)
C (31) -K (2) -C (29)	44. 73 (9)
C (13) -K (2) -C (29)	117. 06 (7)
C (30) -K (2) -C (29)	25. 38 (8)
C (27) -K (2) -C (29)	46. 19 (8)
C (14) -K (2) -C (16)	46. 24 (8)
C (15) -K (2) -C (16)	25. 29 (9)
C (32) -K (2) -C (16)	137. 99 (9)
C (31) -K (2) -C (16)	149. 89 (9)
C (13) -K (2) -C (16)	54. 36 (7)
C (30) -K (2) -C (16)	165. 72 (8)
C (27) -K (2) -C (16)	136. 92 (8)
C (29) -K (2) -C (16)	165. 36 (9)
C (14) -K (2) -C (28)	106. 10 (7)
C (15) -K (2) -C (28)	132. 16 (8)
C (32) -K (2) -C (28)	45. 83 (8)
C (31) -K (2) -C (28)	52. 54 (8)
C (13) -K (2) -C (28)	94. 74 (7)
C (30) -K (2) -C (28)	45. 20 (8)
C (27) -K (2) -C (28)	26. 25 (7)
C (29) -K (2) -C (28)	25. 29 (7)
C (16) -K (2) -C (28)	149. 08 (8)
C (14) -K (2) -C (18)	45. 68 (8)
C (15) -K (2) -C (18)	52. 01 (8)
C (32) -K (2) -C (18)	101. 81 (8)
C (31) -K (2) -C (18)	126. 84 (9)
C (13) -K (2) -C (18)	25. 88 (7)

C (30) -K (2) -C (18)	146. 98 (8)
C (27) -K (2) -C (18)	92. 78 (7)
C (29) -K (2) -C (18)	133. 82 (8)
C (16) -K (2) -C (18)	44. 25 (7)
C (28) -K (2) -C (18)	108. 62 (7)
C (14) -K (2) -C (17)	52. 60 (8)
C (15) -K (2) -C (17)	43. 75 (9)
C (32) -K (2) -C (17)	114. 20 (9)
C (31) -K (2) -C (17)	132. 72 (9)
C (13) -K (2) -C (17)	45. 50 (7)
C (30) -K (2) -C (17)	158. 60 (10)
C (27) -K (2) -C (17)	113. 71 (8)
C (29) -K (2) -C (17)	158. 21 (8)
C (16) -K (2) -C (17)	24. 60 (8)
C (28) -K (2) -C (17)	132. 93 (8)
C (18) -K (2) -C (17)	24. 76 (7)
C (84) -K (3) -C (66)	133. 91 (7)
C (84) -K (3) -C (67)	157. 54 (7)
C (66) -K (3) -C (67)	26. 59 (8)
C (84) -K (3) -C (79)	27. 32 (6)
C (66) -K (3) -C (79)	107. 95 (7)
C (67) -K (3) -C (79)	134. 09 (7)
C (84) -K (3) -C (83)	26. 61 (7)
C (66) -K (3) -C (83)	152. 24 (8)
C (67) -K (3) -C (83)	173. 58 (9)
C (79) -K (3) -C (83)	47. 16 (6)
C (84) -K (3) -C (65)	110. 46 (7)
C (66) -K (3) -C (65)	27. 24 (7)
C (67) -K (3) -C (65)	47. 25 (7)
C (79) -K (3) -C (65)	88. 39 (7)
C (83) -K (3) -C (65)	135. 34 (7)
C (84) -K (3) -C (68)	146. 07 (9)
C (66) -K (3) -C (68)	46. 25 (8)
C (67) -K (3) -C (68)	25. 42 (9)
C (79) -K (3) -C (68)	139. 26 (7)
C (83) -K (3) -C (68)	159. 68 (9)
C (65) -K (3) -C (68)	54. 67 (7)
C (84) -K (3) -C (69)	121. 10 (8)
C (66) -K (3) -C (69)	53. 09 (9)
C (67) -K (3) -C (69)	44. 51 (9)
C (79) -K (3) -C (69)	116. 54 (7)
C (83) -K (3) -C (69)	141. 90 (9)
C (65) -K (3) -C (69)	46. 05 (7)
C (68) -K (3) -C (69)	25. 36 (8)
C (84) -K (3) -C (70)	106. 62 (7)
C (66) -K (3) -C (70)	46. 09 (8)
C (67) -K (3) -C (70)	52. 73 (8)
C (79) -K (3) -C (70)	94. 13 (7)
C (83) -K (3) -C (70)	132. 78 (8)

C (65) -K (3) -C (70)	26. 33 (7)
C (68) -K (3) -C (70)	45. 18 (7)
C (69) -K (3) -C (70)	25. 22 (7)
C (84) -K (3) -C (82)	46. 05 (7)
C (66) -K (3) -C (82)	135. 85 (8)
C (67) -K (3) -C (82)	148. 46 (9)
C (79) -K (3) -C (82)	54. 29 (7)
C (83) -K (3) -C (82)	25. 18 (7)
C (65) -K (3) -C (82)	135. 16 (7)
C (68) -K (3) -C (82)	166. 22 (8)
C (69) -K (3) -C (82)	166. 78 (9)
C (70) -K (3) -C (82)	148. 41 (7)
C (84) -K (3) -C (80)	45. 69 (7)
C (66) -K (3) -C (80)	100. 33 (7)
C (67) -K (3) -C (80)	125. 64 (8)
C (79) -K (3) -C (80)	26. 10 (7)
C (83) -K (3) -C (80)	51. 94 (7)
C (65) -K (3) -C (80)	91. 10 (7)
C (68) -K (3) -C (80)	145. 05 (7)
C (69) -K (3) -C (80)	132. 27 (7)
C (70) -K (3) -C (80)	107. 10 (7)
C (82) -K (3) -C (80)	44. 29 (6)
C (84) -K (3) -C (81)	52. 55 (7)
C (66) -K (3) -C (81)	112. 11 (8)
C (67) -K (3) -C (81)	131. 14 (9)
C (79) -K (3) -C (81)	45. 61 (7)
C (83) -K (3) -C (81)	43. 70 (7)
C (65) -K (3) -C (81)	111. 64 (7)
C (68) -K (3) -C (81)	156. 54 (9)
C (69) -K (3) -C (81)	156. 36 (7)
C (70) -K (3) -C (81)	131. 23 (7)
C (82) -K (3) -C (81)	24. 68 (7)
C (80) -K (3) -C (81)	24. 78 (6)
C (58) -K (4) -C (57)	26. 79 (7)
C (58) -K (4) -C (91)	111. 49 (7)
C (57) -K (4) -C (91)	134. 65 (7)
C (58) -K (4) -C (96)	130. 98 (7)
C (57) -K (4) -C (96)	144. 00 (8)
C (91) -K (4) -C (96)	27. 23 (7)
C (58) -K (4) -C (92)	113. 01 (8)
C (57) -K (4) -C (92)	139. 76 (8)
C (91) -K (4) -C (92)	27. 03 (7)
C (96) -K (4) -C (92)	46. 62 (8)
C (58) -K (4) -C (93)	131. 78 (8)
C (57) -K (4) -C (93)	154. 29 (9)
C (91) -K (4) -C (93)	46. 90 (7)
C (96) -K (4) -C (93)	53. 19 (8)
C (92) -K (4) -C (93)	25. 99 (7)
C (58) -K (4) -C (95)	156. 94 (7)

C (57) -K (4) -C (95)	161. 15 (9)
C (91) -K (4) -C (95)	46. 94 (7)
C (96) -K (4) -C (95)	26. 05 (6)
C (92) -K (4) -C (95)	52. 97 (8)
C (93) -K (4) -C (95)	44. 23 (9)
C (58) -K (4) -C (53)	26. 90 (6)
C (57) -K (4) -C (53)	46. 83 (6)
C (91) -K (4) -C (53)	87. 90 (6)
C (96) -K (4) -C (53)	104. 26 (7)
C (92) -K (4) -C (53)	97. 90 (7)
C (93) -K (4) -C (53)	122. 81 (7)
C (95) -K (4) -C (53)	130. 32 (7)
C (58) -K (4) -C (94)	156. 85 (8)
C (57) -K (4) -C (94)	169. 97 (8)
C (91) -K (4) -C (94)	54. 66 (7)
C (96) -K (4) -C (94)	45. 69 (7)
C (92) -K (4) -C (94)	45. 53 (8)
C (93) -K (4) -C (94)	25. 09 (8)
C (95) -K (4) -C (94)	25. 09 (8)
C (53) -K (4) -C (94)	141. 82 (7)
C (58) -K (4) -C (56)	46. 16 (8)
C (57) -K (4) -C (56)	25. 53 (8)
C (91) -K (4) -C (56)	129. 35 (8)
C (96) -K (4) -C (56)	124. 57 (8)
C (92) -K (4) -C (56)	150. 00 (7)
C (93) -K (4) -C (56)	175. 96 (7)
C (95) -K (4) -C (56)	135. 65 (9)
C (53) -K (4) -C (56)	53. 57 (7)
C (94) -K (4) -C (56)	156. 70 (9)
C (58) -K (4) -C (55)	51. 31 (8)
C (57) -K (4) -C (55)	43. 08 (8)
C (91) -K (4) -C (55)	105. 46 (7)
C (96) -K (4) -C (55)	102. 28 (7)
C (92) -K (4) -C (55)	128. 82 (7)
C (93) -K (4) -C (55)	152. 33 (7)
C (95) -K (4) -C (55)	119. 55 (8)
C (53) -K (4) -C (55)	43. 96 (7)
C (94) -K (4) -C (55)	144. 63 (8)
C (56) -K (4) -C (55)	24. 11 (7)
C (58) -K (4) -C (54)	44. 15 (7)
C (57) -K (4) -C (54)	50. 80 (7)
C (91) -K (4) -C (54)	87. 67 (6)
C (96) -K (4) -C (54)	93. 73 (7)
C (92) -K (4) -C (54)	107. 14 (7)
C (93) -K (4) -C (54)	132. 80 (7)
C (95) -K (4) -C (54)	117. 54 (7)
C (53) -K (4) -C (54)	24. 78 (7)
C (94) -K (4) -C (54)	139. 18 (7)
C (56) -K (4) -C (54)	43. 17 (7)

C(55)-K(4)-C(54)	23.79(7)
N(1)-Si(1)-N(2)	99.17(10)
N(1)-Si(1)-C(25)	106.42(12)
N(2)-Si(1)-C(25)	122.12(13)
N(1)-Si(1)-C(26)	120.78(12)
N(2)-Si(1)-C(26)	105.95(12)
C(25)-Si(1)-C(26)	103.75(15)
N(4)-Si(2)-N(3)	98.99(10)
N(4)-Si(2)-C(52)	107.85(14)
N(3)-Si(2)-C(52)	120.48(14)
N(4)-Si(2)-C(51)	119.17(13)
N(3)-Si(2)-C(51)	105.82(13)
C(52)-Si(2)-C(51)	105.40(16)
N(6)-Si(3)-N(5)	98.27(10)
N(6)-Si(3)-C(77)	120.98(12)
N(5)-Si(3)-C(77)	105.91(13)
N(6)-Si(3)-C(78)	105.96(12)
N(5)-Si(3)-C(78)	122.99(12)
C(77)-Si(3)-C(78)	104.14(15)
N(7)-Si(4)-N(8)	99.52(10)
N(7)-Si(4)-C(104)	107.35(13)
N(8)-Si(4)-C(104)	120.11(13)
N(7)-Si(4)-C(103)	120.35(15)
N(8)-Si(4)-C(103)	105.05(12)
C(104)-Si(4)-C(103)	105.43(19)
C(1)-N(1)-Si(1)	124.25(18)
C(1)-N(1)-Mg(1)	138.56(16)
Si(1)-N(1)-Mg(1)	93.19(9)
C(13)-N(2)-Si(1)	126.00(17)
C(13)-N(2)-Mg(1)	137.84(18)
Si(1)-N(2)-Mg(1)	92.57(9)
C(27)-N(3)-Si(2)	125.80(17)
C(27)-N(3)-Mg(1)	137.28(19)
Si(2)-N(3)-Mg(1)	92.68(10)
C(39)-N(4)-Si(2)	126.48(18)
C(39)-N(4)-Mg(1)	136.03(16)
Si(2)-N(4)-Mg(1)	93.10(10)
C(53)-N(5)-Si(3)	130.97(17)
C(53)-N(5)-Mg(2)	134.22(17)
Si(3)-N(5)-Mg(2)	93.22(9)
C(65)-N(6)-Si(3)	125.83(18)
C(65)-N(6)-Mg(2)	136.67(17)
Si(3)-N(6)-Mg(2)	93.64(9)
C(79)-N(7)-Si(4)	127.60(18)
C(79)-N(7)-Mg(2)	136.55(16)
Si(4)-N(7)-Mg(2)	92.86(9)
C(91)-N(8)-Si(4)	122.75(16)
C(91)-N(8)-Mg(2)	140.81(17)
Si(4)-N(8)-Mg(2)	92.06(9)

N(1)-C(1)-C(6)	122.7(2)
N(1)-C(1)-C(2)	121.3(2)
C(6)-C(1)-C(2)	116.0(2)
N(1)-C(1)-K(1)	110.33(17)
C(6)-C(1)-K(1)	71.20(15)
C(2)-C(1)-K(1)	87.08(15)
C(3)-C(2)-C(1)	120.5(3)
C(3)-C(2)-C(10)	117.6(3)
C(1)-C(2)-C(10)	121.9(2)
C(3)-C(2)-K(1)	79.74(18)
C(1)-C(2)-K(1)	67.49(15)
C(10)-C(2)-K(1)	126.87(19)
C(4)-C(3)-C(2)	121.8(3)
C(4)-C(3)-K(1)	73.97(19)
C(2)-C(3)-K(1)	76.26(18)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-H(3)	119.1
K(1)-C(3)-H(3)	121.9
C(5)-C(4)-C(3)	118.8(3)
C(5)-C(4)-K(1)	69.33(18)
C(3)-C(4)-K(1)	82.20(19)
C(5)-C(4)-H(4)	120.6
C(3)-C(4)-H(4)	120.6
K(1)-C(4)-H(4)	118.7
C(4)-C(5)-C(6)	122.1(3)
C(4)-C(5)-K(1)	86.12(19)
C(6)-C(5)-K(1)	71.80(17)
C(4)-C(5)-H(5)	118.9
C(6)-C(5)-H(5)	118.9
K(1)-C(5)-H(5)	113.1
C(5)-C(6)-C(1)	120.5(3)
C(5)-C(6)-C(7)	117.1(3)
C(1)-C(6)-C(7)	122.3(2)
C(5)-C(6)-K(1)	81.42(17)
C(1)-C(6)-K(1)	81.50(15)
C(7)-C(6)-K(1)	105.53(18)
C(6)-C(7)-C(8)	111.6(3)
C(6)-C(7)-C(9)	111.8(2)
C(8)-C(7)-C(9)	109.7(3)
C(6)-C(7)-H(7)	107.9
C(8)-C(7)-H(7)	107.9
C(9)-C(7)-H(7)	107.9
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5

C (7) -C (9) -H (9B)	109. 5
H (9A) -C (9) -H (9B)	109. 5
C (7) -C (9) -H (9C)	109. 5
H (9A) -C (9) -H (9C)	109. 5
H (9B) -C (9) -H (9C)	109. 5
C (2) -C (10) -C (11)	113. 0 (3)
C (2) -C (10) -C (12)	111. 3 (3)
C (11) -C (10) -C (12)	109. 6 (2)
C (2) -C (10) -H (10)	107. 6
C (11) -C (10) -H (10)	107. 6
C (12) -C (10) -H (10)	107. 6
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
N (2) -C (13) -C (18)	121. 0 (3)
N (2) -C (13) -C (14)	123. 2 (2)
C (18) -C (13) -C (14)	115. 8 (2)
N (2) -C (13) -K (2)	111. 11 (14)
C (18) -C (13) -K (2)	84. 09 (16)
C (14) -C (13) -K (2)	72. 36 (14)
C (15) -C (14) -C (13)	120. 2 (3)
C (15) -C (14) -C (22)	116. 9 (3)
C (13) -C (14) -C (22)	122. 9 (2)
C (15) -C (14) -K (2)	79. 45 (16)
C (13) -C (14) -K (2)	80. 11 (15)
C (22) -C (14) -K (2)	111. 07 (16)
C (16) -C (15) -C (14)	122. 5 (3)
C (16) -C (15) -K (2)	83. 10 (19)
C (14) -C (15) -K (2)	73. 76 (15)
C (16) -C (15) -H (15)	118. 7
C (14) -C (15) -H (15)	118. 7
K (2) -C (15) -H (15)	114. 6
C (15) -C (16) -C (17)	118. 4 (3)
C (15) -C (16) -K (2)	71. 61 (17)
C (17) -C (16) -K (2)	81. 03 (18)
C (15) -C (16) -H (16)	120. 8
C (17) -C (16) -H (16)	120. 8
K (2) -C (16) -H (16)	117. 4
C (16) -C (17) -C (18)	121. 9 (3)
C (16) -C (17) -K (2)	74. 37 (18)

C(18)–C(17)–K(2)	77.05(17)
C(16)–C(17)–H(17)	119.1
C(18)–C(17)–H(17)	119.1
K(2)–C(17)–H(17)	120.5
C(17)–C(18)–C(13)	121.0(3)
C(17)–C(18)–C(19)	117.4(3)
C(13)–C(18)–C(19)	121.6(2)
C(17)–C(18)–K(2)	78.19(17)
C(13)–C(18)–K(2)	70.03(15)
C(19)–C(18)–K(2)	126.81(18)
C(20)–C(19)–C(18)	112.8(3)
C(20)–C(19)–C(21)	108.3(3)
C(18)–C(19)–C(21)	111.5(2)
C(20)–C(19)–H(19)	108.0
C(18)–C(19)–H(19)	108.0
C(21)–C(19)–H(19)	108.0
C(19)–C(20)–H(20A)	109.5
C(19)–C(20)–H(20B)	109.5
H(20A)–C(20)–H(20B)	109.5
C(19)–C(20)–H(20C)	109.5
H(20A)–C(20)–H(20C)	109.5
H(20B)–C(20)–H(20C)	109.5
C(19)–C(21)–H(21A)	109.5
C(19)–C(21)–H(21B)	109.5
H(21A)–C(21)–H(21B)	109.5
C(19)–C(21)–H(21C)	109.5
H(21A)–C(21)–H(21C)	109.5
H(21B)–C(21)–H(21C)	109.5
C(23)–C(22)–C(14)	110.9(2)
C(23)–C(22)–C(24)	108.3(3)
C(14)–C(22)–C(24)	113.1(2)
C(23)–C(22)–H(22)	108.1
C(14)–C(22)–H(22)	108.1
C(24)–C(22)–H(22)	108.1
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
Si(1)–C(25)–H(25A)	109.5
Si(1)–C(25)–H(25B)	109.5
H(25A)–C(25)–H(25B)	109.5

Si (1)–C (25)–H (25C)	109.5
H (25A)–C (25)–H (25C)	109.5
H (25B)–C (25)–H (25C)	109.5
Si (1)–C (26)–H (26A)	109.5
Si (1)–C (26)–H (26B)	109.5
H (26A)–C (26)–H (26B)	109.5
Si (1)–C (26)–H (26C)	109.5
H (26A)–C (26)–H (26C)	109.5
H (26B)–C (26)–H (26C)	109.5
N (3)–C (27)–C (28)	120.8 (2)
N (3)–C (27)–C (32)	123.2 (3)
C (28)–C (27)–C (32)	116.0 (2)
N (3)–C (27)–K (2)	113.51 (15)
C (28)–C (27)–K (2)	80.69 (16)
C (32)–C (27)–K (2)	74.20 (15)
C (29)–C (28)–C (27)	120.7 (3)
C (29)–C (28)–C (36)	118.2 (3)
C (27)–C (28)–C (36)	121.1 (2)
C (29)–C (28)–K (2)	75.80 (17)
C (27)–C (28)–K (2)	73.06 (15)
C (36)–C (28)–K (2)	124.96 (18)
C (30)–C (29)–C (28)	122.0 (3)
C (30)–C (29)–K (2)	74.84 (18)
C (28)–C (29)–K (2)	78.91 (17)
C (30)–C (29)–H (29)	119.0
C (28)–C (29)–H (29)	119.0
K (2)–C (29)–H (29)	117.9
C (29)–C (30)–C (31)	118.3 (3)
C (29)–C (30)–K (2)	79.78 (18)
C (31)–C (30)–K (2)	74.82 (17)
C (29)–C (30)–H (30)	120.9
C (31)–C (30)–H (30)	120.9
K (2)–C (30)–H (30)	115.3
C (30)–C (31)–C (32)	122.6 (3)
C (30)–C (31)–K (2)	79.30 (19)
C (32)–C (31)–K (2)	76.68 (17)
C (30)–C (31)–H (31)	118.7
C (32)–C (31)–H (31)	118.7
K (2)–C (31)–H (31)	115.7
C (31)–C (32)–C (27)	120.1 (3)
C (31)–C (32)–C (33)	117.6 (3)
C (27)–C (32)–C (33)	122.2 (2)
C (31)–C (32)–K (2)	76.85 (18)
C (27)–C (32)–K (2)	78.77 (16)
C (33)–C (32)–K (2)	114.26 (16)
C (32)–C (33)–C (34)	111.6 (2)
C (32)–C (33)–C (35)	113.4 (3)
C (34)–C (33)–C (35)	107.9 (3)
C (32)–C (33)–H (33)	107.9

C (34) -C (33) -H (33)	107.9
C (35) -C (33) -H (33)	107.9
C (33) -C (34) -H (34A)	109.5
C (33) -C (34) -H (34B)	109.5
H (34A) -C (34) -H (34B)	109.5
C (33) -C (34) -H (34C)	109.5
H (34A) -C (34) -H (34C)	109.5
H (34B) -C (34) -H (34C)	109.5
C (33) -C (35) -H (35A)	109.5
C (33) -C (35) -H (35B)	109.5
H (35A) -C (35) -H (35B)	109.5
C (33) -C (35) -H (35C)	109.5
H (35A) -C (35) -H (35C)	109.5
H (35B) -C (35) -H (35C)	109.5
C (37) -C (36) -C (28)	112.6 (2)
C (37) -C (36) -C (38)	110.2 (3)
C (28) -C (36) -C (38)	111.2 (2)
C (37) -C (36) -H (36)	107.5
C (28) -C (36) -H (36)	107.5
C (38) -C (36) -H (36)	107.5
C (36) -C (37) -H (37A)	109.5
C (36) -C (37) -H (37B)	109.5
H (37A) -C (37) -H (37B)	109.5
C (36) -C (37) -H (37C)	109.5
H (37A) -C (37) -H (37C)	109.5
H (37B) -C (37) -H (37C)	109.5
C (36) -C (38) -H (38A)	109.5
C (36) -C (38) -H (38B)	109.5
H (38A) -C (38) -H (38B)	109.5
C (36) -C (38) -H (38C)	109.5
H (38A) -C (38) -H (38C)	109.5
H (38B) -C (38) -H (38C)	109.5
N (4) -C (39) -C (44)	121.1 (2)
N (4) -C (39) -C (40)	123.2 (2)
C (44) -C (39) -C (40)	115.7 (2)
N (4) -C (39) -K (1)	112.59 (16)
C (44) -C (39) -K (1)	82.25 (16)
C (40) -C (39) -K (1)	73.22 (15)
C (41) -C (40) -C (39)	120.7 (2)
C (41) -C (40) -C (48)	116.9 (2)
C (39) -C (40) -C (48)	122.4 (2)
C (41) -C (40) -K (1)	78.18 (16)
C (39) -C (40) -K (1)	79.22 (15)
C (48) -C (40) -K (1)	113.34 (19)
C (42) -C (41) -C (40)	121.9 (3)
C (42) -C (41) -K (1)	81.19 (17)
C (40) -C (41) -K (1)	74.90 (16)
C (42) -C (41) -H (41)	119.0
C (40) -C (41) -H (41)	119.0

K (1) -C (41) -H (41)	115. 2
C (43) -C (42) -C (41)	118. 2 (3)
C (43) -C (42) -K (1)	79. 81 (18)
C (41) -C (42) -K (1)	72. 95 (17)
C (43) -C (42) -H (42)	120. 9
C (41) -C (42) -H (42)	120. 9
K (1) -C (42) -H (42)	117. 2
C (42) -C (43) -C (44)	122. 6 (3)
C (42) -C (43) -K (1)	74. 98 (18)
C (44) -C (43) -K (1)	77. 99 (17)
C (42) -C (43) -H (43)	118. 7
C (44) -C (43) -H (43)	118. 7
K (1) -C (43) -H (43)	119. 1
C (43) -C (44) -C (39)	120. 7 (2)
C (43) -C (44) -C (45)	117. 9 (2)
C (39) -C (44) -C (45)	121. 1 (2)
C (43) -C (44) -K (1)	76. 87 (17)
C (39) -C (44) -K (1)	71. 43 (15)
C (45) -C (44) -K (1)	129. 06 (19)
C (44) -C (45) -C (46)	113. 3 (3)
C (44) -C (45) -C (47)	109. 6 (3)
C (46) -C (45) -C (47)	110. 0 (3)
C (44) -C (45) -H (45)	107. 9
C (46) -C (45) -H (45)	107. 9
C (47) -C (45) -H (45)	107. 9
C (45) -C (46) -H (46A)	109. 5
C (45) -C (46) -H (46B)	109. 5
H (46A) -C (46) -H (46B)	109. 5
C (45) -C (46) -H (46C)	109. 5
H (46A) -C (46) -H (46C)	109. 5
H (46B) -C (46) -H (46C)	109. 5
C (45) -C (47) -H (47A)	109. 5
C (45) -C (47) -H (47B)	109. 5
H (47A) -C (47) -H (47B)	109. 5
C (45) -C (47) -H (47C)	109. 5
H (47A) -C (47) -H (47C)	109. 5
H (47B) -C (47) -H (47C)	109. 5
C (40) -C (48) -C (49)	111. 9 (3)
C (40) -C (48) -C (50)	110. 5 (3)
C (49) -C (48) -C (50)	110. 8 (3)
C (40) -C (48) -H (48)	107. 8
C (49) -C (48) -H (48)	107. 8
C (50) -C (48) -H (48)	107. 8
C (48) -C (49) -H (49A)	109. 5
C (48) -C (49) -H (49B)	109. 5
H (49A) -C (49) -H (49B)	109. 5
C (48) -C (49) -H (49C)	109. 5
H (49A) -C (49) -H (49C)	109. 5
H (49B) -C (49) -H (49C)	109. 5

C (48) –C (50) –H (50A)	109. 5
C (48) –C (50) –H (50B)	109. 5
H (50A) –C (50) –H (50B)	109. 5
C (48) –C (50) –H (50C)	109. 5
H (50A) –C (50) –H (50C)	109. 5
H (50B) –C (50) –H (50C)	109. 5
Si (2) –C (51) –K (4) #1	162. 68 (15)
Si (2) –C (51) –H (51A)	109. 5
K (4) #1 –C (51) –H (51A)	85. 8
Si (2) –C (51) –H (51B)	109. 5
K (4) #1 –C (51) –H (51B)	56. 0
H (51A) –C (51) –H (51B)	109. 5
Si (2) –C (51) –H (51C)	109. 5
K (4) #1 –C (51) –H (51C)	71. 2
H (51A) –C (51) –H (51C)	109. 5
H (51B) –C (51) –H (51C)	109. 5
Si (2) –C (52) –H (52A)	109. 5
Si (2) –C (52) –H (52B)	109. 5
H (52A) –C (52) –H (52B)	109. 5
Si (2) –C (52) –H (52C)	109. 5
H (52A) –C (52) –H (52C)	109. 5
H (52B) –C (52) –H (52C)	109. 5
N (5) –C (53) –C (54)	120. 3 (2)
N (5) –C (53) –C (58)	123. 7 (2)
C (54) –C (53) –C (58)	115. 9 (2)
N (5) –C (53) –K (4)	111. 31 (15)
C (54) –C (53) –K (4)	86. 86 (16)
C (58) –C (53) –K (4)	70. 12 (14)
C (55) –C (54) –C (53)	120. 7 (2)
C (55) –C (54) –C (62)	118. 4 (3)
C (53) –C (54) –C (62)	120. 5 (2)
C (55) –C (54) –K (4)	76. 82 (17)
C (53) –C (54) –K (4)	68. 36 (14)
C (62) –C (54) –K (4)	133. 92 (17)
C (56) –C (55) –C (54)	122. 3 (3)
C (56) –C (55) –K (4)	70. 58 (17)
C (54) –C (55) –K (4)	79. 39 (17)
C (56) –C (55) –H (55)	118. 9
C (54) –C (55) –H (55)	118. 9
K (4) –C (55) –H (55)	122. 4
C (55) –C (56) –C (57)	117. 9 (3)
C (55) –C (56) –K (4)	85. 31 (17)
C (57) –C (56) –K (4)	70. 24 (16)
C (55) –C (56) –H (56)	121. 0
C (57) –C (56) –H (56)	121. 0
K (4) –C (56) –H (56)	114. 0
C (56) –C (57) –C (58)	122. 4 (3)
C (56) –C (57) –K (4)	84. 23 (18)
C (58) –C (57) –K (4)	75. 97 (15)

C (56) –C (57) –H (57)	118. 8
C (58) –C (57) –H (57)	118. 8
K (4) –C (57) –H (57)	110. 9
C (57) –C (58) –C (53)	120. 3 (3)
C (57) –C (58) –C (59)	117. 9 (2)
C (53) –C (58) –C (59)	121. 8 (2)
C (57) –C (58) –K (4)	77. 24 (16)
C (53) –C (58) –K (4)	82. 98 (14)
C (59) –C (58) –K (4)	111. 19 (17)
C (58) –C (59) –C (60)	110. 5 (2)
C (58) –C (59) –C (61)	112. 8 (2)
C (60) –C (59) –C (61)	109. 4 (2)
C (58) –C (59) –H (59)	108. 0
C (60) –C (59) –H (59)	108. 0
C (61) –C (59) –H (59)	108. 0
C (59) –C (60) –H (60A)	109. 5
C (59) –C (60) –H (60B)	109. 5
H (60A) –C (60) –H (60B)	109. 5
C (59) –C (60) –H (60C)	109. 5
H (60A) –C (60) –H (60C)	109. 5
H (60B) –C (60) –H (60C)	109. 5
C (59) –C (61) –H (61A)	109. 5
C (59) –C (61) –H (61B)	109. 5
H (61A) –C (61) –H (61B)	109. 5
C (59) –C (61) –H (61C)	109. 5
H (61A) –C (61) –H (61C)	109. 5
H (61B) –C (61) –H (61C)	109. 5
C (64) –C (62) –C (54)	116. 7 (3)
C (64) –C (62) –C (63)	109. 5 (3)
C (54) –C (62) –C (63)	109. 3 (2)
C (64) –C (62) –H (62)	107. 0
C (54) –C (62) –H (62)	107. 0
C (63) –C (62) –H (62)	107. 0
C (62) –C (63) –K (2) #2	143. 0 (2)
C (62) –C (63) –H (63A)	112 (3)
K (2) #2 –C (63) –H (63A)	104 (3)
C (62) –C (63) –H (63B)	109 (3)
K (2) #2 –C (63) –H (63B)	73 (3)
H (63A) –C (63) –H (63B)	101 (4)
C (62) –C (63) –H (63C)	112 (3)
K (2) #2 –C (63) –H (63C)	41 (3)
H (63A) –C (63) –H (63C)	114 (4)
H (63B) –C (63) –H (63C)	109 (4)
C (62) –C (64) –H (64A)	109. 5
C (62) –C (64) –H (64B)	109. 5
H (64A) –C (64) –H (64B)	109. 5
C (62) –C (64) –H (64C)	109. 5
H (64A) –C (64) –H (64C)	109. 5
H (64B) –C (64) –H (64C)	109. 5

N(6)–C(65)–C(70)	121.0(2)
N(6)–C(65)–C(66)	122.9(2)
C(70)–C(65)–C(66)	116.1(2)
N(6)–C(65)–K(3)	112.87(16)
C(70)–C(65)–K(3)	81.06(14)
C(66)–C(65)–K(3)	73.91(14)
C(67)–C(66)–C(65)	120.3(3)
C(67)–C(66)–C(74)	117.3(3)
C(65)–C(66)–C(74)	122.4(2)
C(67)–C(66)–K(3)	77.97(16)
C(65)–C(66)–K(3)	78.86(15)
C(74)–C(66)–K(3)	113.15(18)
C(68)–C(67)–C(66)	122.3(3)
C(68)–C(67)–K(3)	80.33(19)
C(66)–C(67)–K(3)	75.44(16)
C(68)–C(67)–H(67)	118.8
C(66)–C(67)–H(67)	118.8
K(3)–C(67)–H(67)	115.8
C(67)–C(68)–C(69)	118.9(3)
C(67)–C(68)–K(3)	74.25(19)
C(69)–C(68)–K(3)	79.89(19)
C(67)–C(68)–H(68)	120.6
C(69)–C(68)–H(68)	120.6
K(3)–C(68)–H(68)	116.1
C(68)–C(69)–C(70)	121.6(3)
C(68)–C(69)–K(3)	74.75(18)
C(70)–C(69)–K(3)	77.51(17)
C(68)–C(69)–H(69)	119.2
C(70)–C(69)–H(69)	119.2
K(3)–C(69)–H(69)	119.4
C(69)–C(70)–C(65)	120.6(3)
C(69)–C(70)–C(71)	117.3(3)
C(65)–C(70)–C(71)	122.0(2)
C(69)–C(70)–K(3)	77.27(16)
C(65)–C(70)–K(3)	72.61(14)
C(71)–C(70)–K(3)	124.56(19)
C(72)–C(71)–C(70)	112.0(2)
C(72)–C(71)–C(73)	110.5(3)
C(70)–C(71)–C(73)	110.8(3)
C(72)–C(71)–H(71)	107.8
C(70)–C(71)–H(71)	107.8
C(73)–C(71)–H(71)	107.8
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 (66) –C (74) –C (75)	112. 2 (3)
C (66) –C (74) –C (76)	111. 7 (3)
C (75) –C (74) –C (76)	108. 9 (3)
C (66) –C (74) –H (74)	108. 0
C (75) –C (74) –H (74)	108. 0
C (76) –C (74) –H (74)	108. 0
C (74) –C (75) –H (75A)	109. 5
C (74) –C (75) –H (75B)	109. 5
H (75A) –C (75) –H (75B)	109. 5
C (74) –C (75) –H (75C)	109. 5
H (75A) –C (75) –H (75C)	109. 5
H (75B) –C (75) –H (75C)	109. 5
C (74) –C (76) –H (76A)	109. 5
C (74) –C (76) –H (76B)	109. 5
H (76A) –C (76) –H (76B)	109. 5
C (74) –C (76) –H (76C)	109. 5
H (76A) –C (76) –H (76C)	109. 5
H (76B) –C (76) –H (76C)	109. 5
Si (3) –C (77) –H (77A)	109. 5
Si (3) –C (77) –H (77B)	109. 5
H (77A) –C (77) –H (77B)	109. 5
Si (3) –C (77) –H (77C)	109. 5
H (77A) –C (77) –H (77C)	109. 5
H (77B) –C (77) –H (77C)	109. 5
Si (3) –C (78) –H (78A)	109. 5
Si (3) –C (78) –H (78B)	109. 5
H (78A) –C (78) –H (78B)	109. 5
Si (3) –C (78) –H (78C)	109. 5
H (78A) –C (78) –H (78C)	109. 5
H (78B) –C (78) –H (78C)	109. 5
N (7) –C (79) –C (84)	123. 7 (2)
N (7) –C (79) –C (80)	120. 4 (2)
C (84) –C (79) –C (80)	115. 9 (2)
N (7) –C (79) –K (3)	110. 91 (16)
C (84) –C (79) –K (3)	73. 40 (15)
C (80) –C (79) –K (3)	83. 61 (16)
C (81) –C (80) –C (79)	120. 8 (2)
C (81) –C (80) –C (88)	117. 4 (2)
C (79) –C (80) –C (88)	121. 6 (2)
C (81) –C (80) –K (3)	78. 43 (17)
C (79) –C (80) –K (3)	70. 29 (15)
C (88) –C (80) –K (3)	127. 56 (18)
C (82) –C (81) –C (80)	122. 3 (3)
C (82) –C (81) –K (3)	75. 84 (17)

C (80) –C (81) –K (3)	76.80 (17)
C (82) –C (81) –H (81)	118.9
C (80) –C (81) –H (81)	118.9
K (3) –C (81) –H (81)	119.3
C (83) –C (82) –C (81)	117.8 (2)
C (83) –C (82) –K (3)	72.06 (17)
C (81) –C (82) –K (3)	79.49 (17)
C (83) –C (82) –H (82)	121.1
C (81) –C (82) –H (82)	121.1
K (3) –C (82) –H (82)	118.4
C (82) –C (83) –C (84)	122.5 (2)
C (82) –C (83) –K (3)	82.76 (18)
C (84) –C (83) –K (3)	73.12 (16)
C (82) –C (83) –H (83)	118.8
C (84) –C (83) –H (83)	118.8
K (3) –C (83) –H (83)	115.6
C (83) –C (84) –C (79)	120.5 (2)
C (83) –C (84) –C (85)	116.5 (2)
C (79) –C (84) –C (85)	123.0 (2)
C (83) –C (84) –K (3)	80.27 (17)
C (79) –C (84) –K (3)	79.29 (15)
C (85) –C (84) –K (3)	110.21 (18)
C (84) –C (85) –C (86)	111.2 (2)
C (84) –C (85) –C (87)	111.6 (2)
C (86) –C (85) –C (87)	110.3 (2)
C (84) –C (85) –H (85)	107.9
C (86) –C (85) –H (85)	107.9
C (87) –C (85) –H (85)	107.9
C (85) –C (86) –H (86A)	109.5
C (85) –C (86) –H (86B)	109.5
H (86A) –C (86) –H (86B)	109.5
C (85) –C (86) –H (86C)	109.5
H (86A) –C (86) –H (86C)	109.5
H (86B) –C (86) –H (86C)	109.5
C (85) –C (87) –H (87A)	109.5
C (85) –C (87) –H (87B)	109.5
H (87A) –C (87) –H (87B)	109.5
C (85) –C (87) –H (87C)	109.5
H (87A) –C (87) –H (87C)	109.5
H (87B) –C (87) –H (87C)	109.5
C (89) –C (88) –C (80)	113.7 (3)
C (89) –C (88) –C (90)	108.8 (3)
C (80) –C (88) –C (90)	109.6 (2)
C (89) –C (88) –H (88)	108.2
C (80) –C (88) –H (88)	108.2
C (90) –C (88) –H (88)	108.2
C (88) –C (89) –H (89A)	109.5
C (88) –C (89) –H (89B)	109.5
H (89A) –C (89) –H (89B)	109.5

C (88) –C (89) –H (89C)	109. 5
H (89A) –C (89) –H (89C)	109. 5
H (89B) –C (89) –H (89C)	109. 5
C (88) –C (90) –H (90A)	109. 5
C (88) –C (90) –H (90B)	109. 5
H (90A) –C (90) –H (90B)	109. 5
C (88) –C (90) –H (90C)	109. 5
H (90A) –C (90) –H (90C)	109. 5
H (90B) –C (90) –H (90C)	109. 5
N (8) –C (91) –C (92)	121. 2 (2)
N (8) –C (91) –C (96)	122. 8 (2)
C (92) –C (91) –C (96)	116. 0 (2)
N (8) –C (91) –K (4)	112. 84 (15)
C (92) –C (91) –K (4)	78. 10 (13)
C (96) –C (91) –K (4)	77. 50 (13)
C (93) –C (92) –C (91)	120. 8 (3)
C (93) –C (92) –C (100)	117. 8 (3)
C (91) –C (92) –C (100)	121. 4 (2)
C (93) –C (92) –K (4)	79. 42 (16)
C (91) –C (92) –K (4)	74. 87 (14)
C (100) –C (92) –K (4)	115. 64 (17)
C (94) –C (93) –C (92)	122. 0 (3)
C (94) –C (93) –K (4)	79. 52 (18)
C (92) –C (93) –K (4)	74. 59 (16)
C (94) –C (93) –H (93)	119. 0
C (92) –C (93) –H (93)	119. 0
K (4) –C (93) –H (93)	117. 5
C (93) –C (94) –C (95)	118. 6 (3)
C (93) –C (94) –K (4)	75. 39 (18)
C (95) –C (94) –K (4)	75. 67 (17)
C (93) –C (94) –H (94)	120. 7
C (95) –C (94) –H (94)	120. 7
K (4) –C (94) –H (94)	119. 3
C (94) –C (95) –C (96)	122. 0 (3)
C (94) –C (95) –K (4)	79. 24 (18)
C (96) –C (95) –K (4)	73. 78 (16)
C (94) –C (95) –H (95)	119. 0
C (96) –C (95) –H (95)	119. 0
K (4) –C (95) –H (95)	118. 7
C (95) –C (96) –C (91)	120. 5 (3)
C (95) –C (96) –C (97)	116. 5 (3)
C (91) –C (96) –C (97)	123. 0 (2)
C (95) –C (96) –K (4)	80. 17 (16)
C (91) –C (96) –K (4)	75. 28 (14)
C (97) –C (96) –K (4)	113. 49 (15)
C (96) –C (97) –C (98)	111. 4 (2)
C (96) –C (97) –C (99)	112. 2 (2)
C (98) –C (97) –C (99)	109. 4 (3)
C (96) –C (97) –H (97)	107. 9

C (98) –C (97) –H (97)	107. 9
C (99) –C (97) –H (97)	107. 9
C (97) –C (98) –H (98A)	109. 5
C (97) –C (98) –H (98B)	109. 5
H (98A) –C (98) –H (98B)	109. 5
C (97) –C (98) –H (98C)	109. 5
H (98A) –C (98) –H (98C)	109. 5
H (98B) –C (98) –H (98C)	109. 5
C (97) –C (99) –H (99A)	109. 5
C (97) –C (99) –H (99B)	109. 5
H (99A) –C (99) –H (99B)	109. 5
C (97) –C (99) –H (99C)	109. 5
H (99A) –C (99) –H (99C)	109. 5
H (99B) –C (99) –H (99C)	109. 5
C (92) –C (100) –C (101)	110. 5 (2)
C (92) –C (100) –C (102)	113. 3 (3)
C (101) –C (100) –C (102)	109. 3 (3)
C (92) –C (100) –H (100)	107. 9
C (101) –C (100) –H (100)	107. 9
C (102) –C (100) –H (100)	107. 9
C (100) –C (101) –H (10A)	109. 5
C (100) –C (101) –H (10B)	109. 5
H (10A) –C (101) –H (10B)	109. 5
C (100) –C (101) –H (10C)	109. 5
H (10A) –C (101) –H (10C)	109. 5
H (10B) –C (101) –H (10C)	109. 5
C (100) –C (102) –H (10D)	109. 5
C (100) –C (102) –H (10E)	109. 5
H (10D) –C (102) –H (10E)	109. 5
C (100) –C (102) –H (10F)	109. 5
H (10D) –C (102) –H (10F)	109. 5
H (10E) –C (102) –H (10F)	109. 5
Si (4) –C (103) –H (10G)	109. 5
Si (4) –C (103) –H (10H)	109. 5
H (10G) –C (103) –H (10H)	109. 5
Si (4) –C (103) –H (10I)	109. 5
H (10G) –C (103) –H (10I)	109. 5
H (10H) –C (103) –H (10I)	109. 5
Si (4) –C (104) –H (10J)	109. 5
Si (4) –C (104) –H (10K)	109. 5
H (10J) –C (104) –H (10K)	109. 5
Si (4) –C (104) –H (10L)	109. 5
H (10J) –C (104) –H (10L)	109. 5
H (10K) –C (104) –H (10L)	109. 5
C (106) –C (105) –H (10M)	109. 5
C (106) –C (105) –H (10N)	109. 5
H (10M) –C (105) –H (10N)	109. 5
C (106) –C (105) –H (100)	109. 5
H (10M) –C (105) –H (100)	109. 5

H(10N)-C(105)-H(100)	109.5
C(105)-C(106)-C(107)	114.5(6)
C(105)-C(106)-H(10P)	108.6
C(107)-C(106)-H(10P)	108.6
C(105)-C(106)-H(10Q)	108.6
C(107)-C(106)-H(10Q)	108.6
H(10P)-C(106)-H(10Q)	107.6
C(108)-C(107)-C(106)	115.6(5)
C(108)-C(107)-H(10R)	108.4
C(106)-C(107)-H(10R)	108.4
C(108)-C(107)-H(10S)	108.4
C(106)-C(107)-H(10S)	108.4
H(10R)-C(107)-H(10S)	107.4
C(109)-C(108)-C(107)	120.8(4)
C(109)-C(108)-H(10T)	107.1
C(107)-C(108)-H(10T)	107.1
C(109)-C(108)-H(10U)	107.1
C(107)-C(108)-H(10U)	107.1
H(10T)-C(108)-H(10U)	106.8
C(108)-C(109)-C(110)	124.7(5)
C(108)-C(109)-H(10V)	106.2
C(110)-C(109)-H(10V)	106.2
C(108)-C(109)-H(10W)	106.2
C(110)-C(109)-H(10W)	106.2
H(10V)-C(109)-H(10W)	106.4
C(109)-C(110)-H(11D)	109.5
C(109)-C(110)-H(11E)	109.5
H(11D)-C(110)-H(11E)	109.5
C(109)-C(110)-H(11F)	109.5
H(11D)-C(110)-H(11F)	109.5
H(11E)-C(110)-H(11F)	109.5

Symmetry transformations used to generate equivalent atoms:

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

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

	U11	U22	U33	U23	U13	U12
Mg(1)	21(1)	30(1)	18(1)	4(1)	5(1)	4(1)
Mg(2)	18(1)	24(1)	19(1)	3(1)	4(1)	4(1)
K(1)	34(1)	75(1)	42(1)	-19(1)	1(1)	5(1)
K(2)	41(1)	71(1)	38(1)	10(1)	6(1)	21(1)
K(3)	30(1)	48(1)	32(1)	3(1)	8(1)	-3(1)
K(4)	32(1)	50(1)	33(1)	0(1)	10(1)	13(1)
Si(1)	25(1)	31(1)	18(1)	2(1)	4(1)	11(1)
Si(2)	29(1)	35(1)	20(1)	1(1)	1(1)	6(1)
Si(3)	17(1)	30(1)	22(1)	2(1)	3(1)	2(1)
Si(4)	22(1)	48(1)	21(1)	12(1)	8(1)	15(1)
N(1)	23(1)	30(1)	19(1)	1(1)	5(1)	10(1)
N(2)	24(1)	31(1)	20(1)	4(1)	7(1)	10(1)
N(3)	24(1)	32(1)	22(1)	4(1)	4(1)	4(1)
N(4)	27(1)	27(1)	20(1)	1(1)	4(1)	2(1)
N(5)	17(1)	29(1)	21(1)	1(1)	5(1)	1(1)
N(6)	20(1)	29(1)	19(1)	2(1)	3(1)	1(1)
N(7)	21(1)	31(1)	18(1)	6(1)	7(1)	7(1)
N(8)	19(1)	35(1)	19(1)	8(1)	6(1)	11(1)
C(1)	28(2)	28(1)	21(1)	-7(1)	2(1)	8(1)
C(2)	27(2)	37(2)	32(2)	-4(1)	7(1)	11(1)
C(3)	29(2)	44(2)	44(2)	-6(1)	9(1)	10(1)
C(4)	27(2)	41(2)	52(2)	-15(2)	-4(1)	16(1)
C(5)	39(2)	33(2)	37(2)	-4(1)	-3(1)	15(1)
C(6)	36(2)	27(2)	28(1)	-5(1)	-2(1)	12(1)
C(7)	55(2)	32(2)	34(2)	7(1)	11(1)	15(1)
C(8)	75(3)	68(3)	34(2)	13(2)	9(2)	33(2)
C(9)	82(3)	33(2)	77(3)	15(2)	37(2)	15(2)
C(10)	28(2)	41(2)	38(2)	4(1)	14(1)	9(1)
C(11)	51(2)	52(2)	39(2)	3(2)	13(2)	10(2)
C(12)	40(2)	47(2)	59(2)	2(2)	15(2)	1(2)
C(13)	26(1)	36(2)	19(1)	4(1)	5(1)	9(1)
C(14)	31(2)	35(2)	26(1)	9(1)	10(1)	13(1)
C(15)	36(2)	35(2)	35(2)	3(1)	14(1)	14(1)
C(16)	35(2)	46(2)	53(2)	5(2)	21(2)	18(2)
C(17)	24(2)	50(2)	53(2)	5(2)	13(1)	8(1)
C(18)	28(2)	43(2)	32(2)	5(1)	8(1)	9(1)
C(19)	27(2)	46(2)	37(2)	1(1)	7(1)	5(1)
C(20)	47(2)	67(2)	45(2)	3(2)	9(2)	8(2)
C(21)	56(2)	56(2)	48(2)	7(2)	13(2)	-2(2)

C(22)	31(2)	30(2)	38(2)	5(1)	12(1)	12(1)
C(23)	43(2)	47(2)	42(2)	-9(1)	10(2)	8(2)
C(24)	44(2)	36(2)	68(2)	14(2)	23(2)	15(2)
C(25)	29(2)	40(2)	42(2)	-8(1)	-1(1)	10(1)
C(26)	49(2)	44(2)	25(1)	7(1)	12(1)	20(2)
C(27)	26(2)	38(2)	20(1)	7(1)	4(1)	5(1)
C(28)	31(2)	33(2)	32(2)	5(1)	5(1)	4(1)
C(29)	36(2)	36(2)	51(2)	13(1)	9(1)	3(1)
C(30)	43(2)	39(2)	51(2)	18(2)	8(2)	12(2)
C(31)	31(2)	50(2)	40(2)	15(1)	3(1)	13(1)
C(32)	29(2)	38(2)	26(1)	6(1)	5(1)	6(1)
C(33)	25(2)	44(2)	39(2)	5(1)	8(1)	4(1)
C(34)	42(2)	59(2)	43(2)	6(2)	-5(2)	1(2)
C(35)	36(2)	59(2)	75(3)	4(2)	24(2)	3(2)
C(36)	26(2)	35(2)	35(2)	3(1)	6(1)	2(1)
C(37)	42(2)	42(2)	42(2)	3(1)	3(1)	1(1)
C(38)	41(2)	61(2)	45(2)	12(2)	13(2)	-2(2)
C(39)	23(1)	31(2)	22(1)	0(1)	-1(1)	1(1)
C(40)	30(2)	31(2)	26(1)	-2(1)	3(1)	-2(1)
C(41)	34(2)	32(2)	30(1)	-4(1)	5(1)	3(1)
C(42)	35(2)	28(2)	37(2)	3(1)	-1(1)	1(1)
C(43)	37(2)	33(2)	36(2)	8(1)	4(1)	-1(1)
C(44)	27(2)	32(2)	30(1)	4(1)	4(1)	1(1)
C(45)	37(2)	35(2)	45(2)	4(1)	18(1)	-1(1)
C(46)	84(3)	48(2)	52(2)	11(2)	37(2)	15(2)
C(47)	41(2)	51(2)	111(3)	-7(2)	33(2)	-6(2)
C(48)	49(2)	30(2)	37(2)	-3(1)	20(2)	2(1)
C(49)	53(2)	38(2)	88(3)	1(2)	44(2)	5(2)
C(50)	100(3)	42(2)	32(2)	-2(1)	22(2)	-9(2)
C(51)	60(2)	51(2)	22(1)	10(1)	12(1)	21(2)
C(52)	40(2)	48(2)	53(2)	-17(2)	-14(2)	6(2)
C(53)	18(1)	30(1)	22(1)	3(1)	3(1)	9(1)
C(54)	22(1)	32(2)	34(2)	-4(1)	7(1)	7(1)
C(55)	28(2)	40(2)	43(2)	-12(1)	4(1)	6(1)
C(56)	40(2)	48(2)	29(2)	-10(1)	6(1)	17(2)
C(57)	31(2)	46(2)	28(1)	3(1)	13(1)	14(1)
C(58)	20(1)	34(2)	26(1)	3(1)	7(1)	9(1)
C(59)	26(2)	43(2)	30(1)	4(1)	11(1)	0(1)
C(60)	23(2)	67(2)	53(2)	3(2)	14(2)	1(2)
C(61)	48(2)	50(2)	37(2)	9(1)	15(2)	-6(2)
C(62)	34(2)	30(2)	47(2)	-3(1)	14(1)	0(1)
C(63)	53(2)	68(3)	54(2)	22(2)	11(2)	22(2)
C(64)	41(2)	86(3)	99(3)	56(3)	-5(2)	-9(2)
C(65)	18(1)	38(2)	23(1)	2(1)	6(1)	-5(1)
C(66)	22(2)	52(2)	22(1)	3(1)	4(1)	0(1)
C(67)	29(2)	63(2)	24(1)	4(1)	2(1)	-8(1)
C(68)	47(2)	61(2)	22(2)	-8(1)	6(1)	-13(2)
C(69)	53(2)	41(2)	31(2)	-8(1)	12(1)	-10(2)
C(70)	35(2)	35(2)	24(1)	-3(1)	10(1)	-5(1)

C(71)	49(2)	26(2)	30(2)	-1(1)	13(1)	-1(1)
C(72)	54(2)	40(2)	41(2)	1(1)	15(2)	9(2)
C(73)	76(3)	40(2)	43(2)	2(2)	18(2)	-16(2)
C(74)	38(2)	60(2)	27(2)	10(1)	0(1)	13(2)
C(75)	86(3)	60(2)	33(2)	17(2)	3(2)	10(2)
C(76)	43(2)	104(3)	51(2)	8(2)	-4(2)	31(2)
C(77)	36(2)	48(2)	37(2)	6(1)	7(1)	16(1)
C(78)	27(2)	51(2)	32(2)	-4(1)	7(1)	-11(1)
C(79)	18(1)	30(1)	19(1)	2(1)	4(1)	1(1)
C(80)	27(2)	31(2)	24(1)	5(1)	7(1)	3(1)
C(81)	39(2)	27(2)	31(1)	9(1)	9(1)	2(1)
C(82)	39(2)	39(2)	24(1)	9(1)	11(1)	-2(1)
C(83)	31(2)	39(2)	27(1)	4(1)	13(1)	3(1)
C(84)	24(1)	31(1)	23(1)	5(1)	7(1)	4(1)
C(85)	36(2)	36(2)	29(1)	7(1)	17(1)	12(1)
C(86)	41(2)	57(2)	43(2)	12(2)	19(2)	23(2)
C(87)	62(2)	35(2)	40(2)	4(1)	23(2)	11(2)
C(88)	38(2)	26(1)	32(2)	5(1)	12(1)	8(1)
C(89)	56(3)	103(3)	57(2)	-7(2)	7(2)	38(2)
C(90)	73(3)	65(3)	76(3)	-26(2)	24(2)	-8(2)
C(91)	21(1)	36(2)	23(1)	8(1)	9(1)	13(1)
C(92)	33(2)	31(2)	29(1)	6(1)	14(1)	11(1)
C(93)	50(2)	35(2)	33(2)	13(1)	17(1)	7(1)
C(94)	47(2)	49(2)	29(2)	19(1)	10(1)	12(2)
C(95)	35(2)	51(2)	24(1)	10(1)	4(1)	12(1)
C(96)	23(1)	38(2)	23(1)	9(1)	7(1)	12(1)
C(97)	23(1)	42(2)	23(1)	6(1)	3(1)	8(1)
C(98)	40(2)	45(2)	35(2)	0(1)	8(1)	4(1)
C(99)	28(2)	58(2)	41(2)	11(2)	4(1)	3(1)
C(100)	51(2)	27(2)	29(1)	3(1)	15(1)	8(1)
C(101)	47(2)	44(2)	37(2)	5(1)	13(1)	-13(2)
C(102)	125(4)	41(2)	59(2)	-3(2)	20(3)	27(2)
C(103)	68(3)	96(3)	37(2)	34(2)	30(2)	63(2)
C(104)	26(2)	107(3)	29(2)	13(2)	8(1)	-8(2)
C(105)	100(4)	94(4)	109(4)	-17(3)	44(4)	-14(3)
C(106)	126(6)	83(4)	166(7)	-16(4)	58(5)	-6(4)
C(107)	108(4)	56(3)	209(7)	-26(4)	117(5)	-19(3)
C(108)	49(3)	117(5)	108(4)	-37(3)	29(3)	-30(3)
C(109)	131(5)	78(4)	142(5)	-6(3)	98(5)	-23(3)
C(110)	45(3)	294(9)	57(3)	33(4)	10(2)	-45(4)

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(3)	3519	8630	7722	47
H(4)	3063	9503	7075	50
H(5)	4169	9829	6452	45
H(7)	6693	9237	6411	47
H(8A)	5298	8847	5608	86
H(8B)	6030	9500	5455	86
H(8C)	4920	9645	5617	86
H(9A)	5717	10567	6450	90
H(9B)	6802	10476	6240	90
H(9C)	6718	10384	6910	90
H(10)	5701	7574	7783	42
H(11A)	5913	8344	8631	69
H(11B)	5323	7603	8745	69
H(11C)	4681	8294	8613	69
H(12A)	3506	7423	7809	73
H(12B)	4289	6803	7932	73
H(12C)	4007	7076	7287	73
H(15)	9326	5530	6324	41
H(16)	11011	6072	6504	51
H(17)	11315	7261	6904	49
H(19)	9401	8442	7192	44
H(20A)	10453	8167	8059	79
H(20B)	10949	8886	7847	79
H(20C)	11441	8136	7745	79
H(21A)	10680	9141	6812	80
H(21B)	10128	8535	6311	80
H(21C)	11263	8438	6681	80
H(22)	7056	6222	6707	38
H(23A)	7126	6240	5693	66
H(23B)	6439	5542	5810	66
H(23C)	7605	5473	5706	66
H(24A)	8060	4904	6653	70
H(24B)	6873	4954	6724	70
H(24C)	7803	5286	7241	70
H(25A)	5520	6889	6692	57
H(25B)	5855	6833	6063	57
H(25C)	5160	7462	6228	57
H(26A)	6811	8169	5720	57
H(26B)	7787	7691	5853	57
H(26C)	7883	8509	6123	57

H(29)	8124	5384	8811	48
H(30)	9864	5199	9166	52
H(31)	11099	6181	9344	47
H(33)	10730	7981	8993	43
H(34A)	10870	7867	10012	75
H(34B)	11989	8114	9876	75
H(34C)	11723	7295	9994	75
H(35A)	12281	6957	9050	82
H(35B)	12449	7782	8918	82
H(35C)	11692	7227	8446	82
H(36)	7067	7080	8585	39
H(37A)	7058	6426	7690	64
H(37B)	5950	6302	7882	64
H(37C)	6761	5694	7963	64
H(38A)	5853	6414	8978	72
H(38B)	6928	6413	9438	72
H(38C)	6507	5719	8993	72
H(41)	6788	11015	9269	39
H(42)	7497	11706	8619	41
H(43)	8461	11158	7994	42
H(45)	9192	9352	7982	45
H(46A)	8180	9621	7100	86
H(46B)	9384	9770	7062	86
H(46C)	8708	10429	7179	86
H(47A)	10159	10792	8092	100
H(47B)	10720	10085	7943	100
H(47C)	10407	10222	8573	100
H(48)	6859	9130	9376	45
H(49A)	5456	10242	9412	84
H(49B)	5268	9450	9616	84
H(49C)	5255	9560	8938	84
H(50A)	8032	9841	10132	86
H(50B)	6968	9630	10349	86
H(50C)	7190	10422	10152	86
H(51A)	8029	8452	10011	64
H(51B)	8303	7660	9816	64
H(51C)	7222	7952	9520	64
H(52A)	10283	9134	9228	76
H(52B)	10107	8839	9835	76
H(52C)	9550	9532	9606	76
H(55)	7135	4817	712	45
H(56)	8158	5297	88	47
H(57)	9377	6265	453	40
H(59)	9674	7294	1828	39
H(60A)	10930	6426	1847	71
H(60B)	11409	7201	1730	71
H(60C)	11061	6593	1197	71
H(61A)	9853	7413	624	66
H(61B)	10299	8022	1145	66

H(61C)	9066	7831	951	66
H(62)	7137	5439	2199	44
H(63A)	7420(30)	4177(19)	2281(17)	85
H(63B)	7750(40)	4145(18)	1698(12)	85
H(63C)	8486(14)	4640(20)	2211(17)	85
H(64A)	5585	5240	1525	114
H(64B)	5747	4569	1917	114
H(64C)	5960	4511	1260	114
H(67)	9817	7151	5207	47
H(68)	9295	8294	5351	54
H(69)	8466	8860	4545	50
H(71)	7915	8158	3046	42
H(72A)	6428	8248	3463	66
H(72B)	6627	8956	3134	66
H(72C)	6932	8980	3836	66
H(73A)	8717	9483	3730	79
H(73B)	8468	9368	3027	79
H(73C)	9422	8997	3394	79
H(74)	9288	6003	3885	50
H(75A)	9386	5945	5124	90
H(75B)	9309	5259	4663	90
H(75C)	8346	5749	4639	90
H(76A)	11047	6546	4172	100
H(76B)	10940	5727	4330	100
H(76C)	11024	6368	4834	100
H(77A)	10559	5969	3193	59
H(77B)	10130	5718	2513	59
H(77C)	9486	5474	2999	59
H(78A)	9946	7895	2741	56
H(78B)	10803	7328	2705	56
H(78C)	10526	7578	3327	56
H(81)	5876	5113	4344	38
H(82)	4982	5752	4966	40
H(83)	4336	6835	4684	38
H(85)	4740	7776	3460	38
H(86A)	3036	7188	3347	67
H(86B)	3051	8021	3568	67
H(86C)	3025	7416	4023	67
H(87A)	4685	8003	4687	65
H(87B)	4629	8629	4246	65
H(87C)	5670	8219	4398	65
H(88)	6165	5516	2901	37
H(89A)	7711	5565	3616	107
H(89B)	7518	4838	3190	107
H(89C)	7280	4834	3842	107
H(90A)	5663	4282	2832	108
H(90B)	4738	4689	3039	108
H(90C)	5546	4314	3507	108
H(93)	6114	8737	742	45

H(94)	5009	8137	-71	48
H(95)	4177	7024	23	43
H(97)	4467	6026	1281	35
H(98A)	4462	5820	48	60
H(98B)	4263	5183	451	60
H(98C)	5381	5626	556	60
H(99A)	2854	6578	986	63
H(99B)	2757	5731	803	63
H(99C)	2855	6291	321	63
H(100)	6551	8238	2202	41
H(10A)	7925	7789	1799	64
H(10B)	8282	8565	2140	64
H(10C)	7988	8485	1437	64
H(10D)	6786	9431	1513	111
H(10E)	6954	9466	2215	111
H(10F)	5806	9299	1826	111
H(10G)	3648	7835	2562	91
H(10H)	4044	7953	1961	91
H(10I)	4772	8238	2577	91
H(10J)	3981	5784	2189	81
H(10K)	3205	6375	1959	81
H(10L)	3442	6239	2642	81
H(10M)	2041	10189	4443	150
H(10N)	826	10239	4450	150
H(10O)	1200	9579	4086	150
H(10P)	768	9363	4985	147
H(10Q)	1813	9849	5275	147
H(10R)	1749	8582	4540	139
H(10S)	2788	9063	4843	139
H(10T)	2501	8794	5752	112
H(10U)	1460	8319	5452	112
H(10V)	3485	7999	5429	132
H(10W)	2498	7550	5037	132
H(11D)	3199	7495	6268	201
H(11E)	3068	6844	5769	201
H(11F)	2057	7160	5955	201

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

3) The crystallographic data of **4**

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

Identification code	090603pi_0m
Empirical formula	C ₆₄ H ₁₀₄ K ₂ Mg N ₄ O ₃ Si ₂
Formula weight	1136.20
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 15.294(3) Å alpha = 90 deg. b = 24.825(6) Å beta = 112.095(2) deg. c = 18.800(4) Å gamma = 90 deg.
Volume	6614(3) Å ³
Z, Calculated density	4, 1.141 Mg/m ³
Absorption coefficient	0.234 mm ⁻¹
F(000)	2472
Crystal size	0.30 x 0.25 x 0.20 mm
Theta range for data collection	1.64 to 25.01 deg.
Limiting indices	-18<=h<=18, -26<=k<=29, -22<=l<=22
Reflections collected / unique	43645 / 11639 [R(int) = 0.0575]
Completeness to theta = 25.01	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9548 and 0.9332
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11639 / 0 / 685

Goodness-of-fit on F^2	1.044
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0550, wR2 = 0.1446
R indices (all data)	R1 = 0.0671, wR2 = 0.1541
Largest diff. peak and hole	0.709 and -0.538 e. $\text{\AA}^{-3}$

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(eq)
Mg(1)	1852(1)	6271(1)	2979(1)	17(1)
K(1)	5025(1)	7024(1)	3909(1)	27(1)
K(2)	-1187(1)	5538(1)	2175(1)	38(1)
N(1)	3030(1)	5894(1)	2839(1)	18(1)
N(2)	1454(1)	5447(1)	2742(1)	21(1)
N(3)	575(1)	6692(1)	2797(1)	19(1)
N(4)	2300(1)	7038(1)	3496(1)	19(1)
O(1)	6669(1)	6910(1)	5178(1)	40(1)
O(2)	6031(2)	7774(1)	3484(1)	40(1)
O(3)	-2962(2)	5208(1)	1503(2)	61(1)
Si(1)	2493(1)	5278(1)	2648(1)	19(1)
Si(2)	1161(1)	7263(1)	3232(1)	21(1)
C(1)	3812(2)	6070(1)	2706(1)	20(1)
C(2)	4761(2)	5884(1)	3141(2)	23(1)
C(3)	5530(2)	6117(1)	3035(2)	28(1)
C(4)	5428(2)	6527(1)	2509(2)	32(1)
C(5)	4524(2)	6684(1)	2050(2)	28(1)
C(6)	3729(2)	6461(1)	2126(2)	23(1)
C(7)	4945(2)	5421(1)	3698(2)	29(1)
C(8)	5711(2)	5541(1)	4485(2)	40(1)
C(9)	5222(2)	4918(1)	3353(2)	39(1)
C(10)	2770(2)	6610(1)	1529(2)	27(1)
C(11)	2541(2)	7202(1)	1554(2)	40(1)
C(12)	2708(2)	6449(1)	719(2)	39(1)
C(13)	828(2)	5094(1)	2872(2)	23(1)
C(14)	268(2)	4710(1)	2317(2)	28(1)
C(15)	-400(2)	4395(1)	2466(2)	37(1)
C(16)	-570(2)	4436(1)	3130(2)	41(1)
C(17)	-19(2)	4791(1)	3685(2)	37(1)
C(18)	685(2)	5102(1)	3586(2)	28(1)
C(19)	354(2)	4632(1)	1544(2)	31(1)
C(20)	741(2)	4073(1)	1485(2)	44(1)
C(21)	-589(2)	4718(2)	867(2)	43(1)
C(22)	1342(2)	5409(1)	4280(2)	32(1)
C(23)	1810(2)	5013(1)	4957(2)	43(1)
C(24)	853(2)	5852(1)	4536(2)	40(1)
C(25)	2957(2)	4680(1)	3307(2)	29(1)
C(26)	2530(2)	5056(1)	1698(2)	29(1)

C (27)	3075 (2)	7271 (1)	4069 (1)	19 (1)
C (28)	3551 (2)	6997 (1)	4784 (1)	22 (1)
C (29)	4368 (2)	7210 (1)	5337 (2)	26 (1)
C (30)	4740 (2)	7699 (1)	5242 (2)	27 (1)
C (31)	4269 (2)	7984 (1)	4575 (2)	25 (1)
C (32)	3457 (2)	7786 (1)	3997 (2)	22 (1)
C (33)	3182 (2)	6469 (1)	4961 (2)	25 (1)
C (34)	3162 (2)	6449 (1)	5775 (2)	37 (1)
C (35)	3761 (2)	6000 (1)	4848 (2)	34 (1)
C (36)	3007 (2)	8147 (1)	3303 (2)	28 (1)
C (37)	3672 (2)	8277 (2)	2893 (2)	41 (1)
C (38)	2652 (2)	8669 (1)	3531 (2)	41 (1)
C (39)	-361 (2)	6680 (1)	2291 (1)	20 (1)
C (40)	-1143 (2)	6721 (1)	2537 (2)	24 (1)
C (41)	-2071 (2)	6675 (1)	2007 (2)	31 (1)
C (42)	-2282 (2)	6588 (1)	1238 (2)	34 (1)
C (43)	-1539 (2)	6555 (1)	986 (2)	31 (1)
C (44)	-603 (2)	6615 (1)	1483 (2)	23 (1)
C (45)	-1010 (2)	6799 (1)	3369 (2)	30 (1)
C (46)	-1448 (2)	7327 (2)	3487 (2)	46 (1)
C (47)	-1422 (2)	6327 (2)	3671 (2)	46 (1)
C (48)	145 (2)	6625 (1)	1136 (1)	26 (1)
C (49)	-96 (2)	7031 (2)	479 (2)	42 (1)
C (50)	303 (2)	6069 (1)	869 (2)	36 (1)
C (51)	686 (2)	7822 (1)	2502 (2)	35 (1)
C (52)	1038 (2)	7524 (1)	4129 (2)	38 (1)
C (53)	6877 (2)	6867 (2)	5988 (2)	42 (1)
C (54)	7938 (2)	6837 (2)	6374 (2)	46 (1)
C (55)	8220 (3)	6581 (2)	5783 (3)	70 (1)
C (56)	7498 (2)	6777 (2)	5038 (2)	58 (1)
C (57)	5976 (2)	7996 (2)	2766 (2)	44 (1)
C (58)	6329 (4)	8560 (2)	2930 (3)	90 (2)
C (59)	6696 (7)	8609 (3)	3763 (3)	172 (4)
C (60)	6580 (3)	8134 (2)	4075 (2)	56 (1)
C (61)	-3514 (3)	5315 (2)	722 (2)	70 (1)
C (62)	-4403 (3)	5574 (2)	746 (3)	73 (1)
C (63)	-4567 (3)	5256 (2)	1375 (3)	70 (1)
C (64)	-3564 (3)	5139 (2)	1918 (3)	69 (1)

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

Mg(1)–N(3)	2.127(2)
Mg(1)–N(2)	2.131(2)
Mg(1)–N(4)	2.131(2)
Mg(1)–N(1)	2.133(2)
K(1)–O(2)	2.719(2)
K(1)–O(1)	2.753(2)
K(1)–C(3)	3.052(3)
K(1)–C(32)	3.108(3)
K(1)–C(31)	3.112(3)
K(1)–C(2)	3.132(3)
K(1)–C(27)	3.168(3)
K(1)–C(4)	3.169(3)
K(1)–C(30)	3.179(3)
K(1)–C(29)	3.236(3)
K(1)–C(28)	3.254(3)
K(1)–C(1)	3.318(3)
K(2)–O(3)	2.656(3)
K(2)–C(14)	2.968(3)
K(2)–C(40)	3.008(3)
K(2)–C(15)	3.051(3)
K(2)–C(13)	3.066(3)
K(2)–C(39)	3.077(3)
K(2)–C(41)	3.093(3)
K(2)–C(16)	3.213(3)
K(2)–C(42)	3.235(3)
K(2)–C(44)	3.242(3)
K(2)–C(18)	3.270(3)
K(2)–C(43)	3.279(3)
N(1)–C(1)	1.382(3)
N(1)–Si(1)	1.708(2)
N(2)–C(13)	1.386(3)
N(2)–Si(1)	1.715(2)
N(3)–C(39)	1.389(3)
N(3)–Si(2)	1.711(2)
N(4)–C(27)	1.393(3)
N(4)–Si(2)	1.715(2)
O(1)–C(56)	1.428(4)
O(1)–C(53)	1.437(4)
O(2)–C(60)	1.428(4)
O(2)–C(57)	1.432(4)
O(3)–C(61)	1.417(5)
O(3)–C(64)	1.423(5)
Si(1)–C(26)	1.891(3)
Si(1)–C(25)	1.894(3)
Si(2)–C(52)	1.880(3)

Si (2)–C (51)	1. 894 (3)
C (1)–C (6)	1. 429 (4)
C (1)–C (2)	1. 446 (3)
C (2)–C (3)	1. 391 (4)
C (2)–C (7)	1. 509 (4)
C (3)–C (4)	1. 385 (4)
C (3)–H (3A)	1. 0000
C (4)–C (5)	1. 383 (4)
C (4)–H (4A)	1. 0000
C (5)–C (6)	1. 392 (4)
C (5)–H (5A)	1. 0000
C (6)–C (10)	1. 520 (4)
C (7)–C (8)	1. 533 (4)
C (7)–C (9)	1. 538 (4)
C (7)–H (7A)	1. 0000
C (8)–H (8A)	0. 9800
C (8)–H (8B)	0. 9800
C (8)–H (8C)	0. 9800
C (9)–H (9A)	0. 9800
C (9)–H (9B)	0. 9800
C (9)–H (9C)	0. 9800
C (10)–C (11)	1. 515 (4)
C (10)–C (12)	1. 542 (4)
C (10)–H (10A)	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. 436 (4)
C (13)–C (18)	1. 438 (4)
C (14)–C (15)	1. 396 (4)
C (14)–C (19)	1. 519 (4)
C (15)–C (16)	1. 372 (5)
C (15)–H (15A)	1. 0000
C (16)–C (17)	1. 382 (4)
C (16)–H (16A)	1. 0000
C (17)–C (18)	1. 393 (4)
C (17)–H (17A)	1. 0000
C (18)–C (22)	1. 518 (4)
C (19)–C (20)	1. 530 (4)
C (19)–C (21)	1. 539 (4)
C (19)–H (19A)	1. 0000
C (20)–H (20A)	0. 9800
C (20)–H (20B)	0. 9800
C (20)–H (20C)	0. 9800
C (21)–H (21A)	0. 9800
C (21)–H (21B)	0. 9800

C (21) -H (21C)	0. 9800
C (22) -C (24)	1. 508 (4)
C (22) -C (23)	1. 554 (4)
C (22) -H (22A)	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) -H (25A)	0. 9800
C (25) -H (25B)	0. 9800
C (25) -H (25C)	0. 9800
C (26) -H (26A)	0. 9800
C (26) -H (26B)	0. 9800
C (26) -H (26C)	0. 9800
C (27) -C (32)	1. 432 (4)
C (27) -C (28)	1. 436 (4)
C (28) -C (29)	1. 395 (4)
C (28) -C (33)	1. 515 (4)
C (29) -C (30)	1. 379 (4)
C (29) -H (29A)	1. 0000
C (30) -C (31)	1. 383 (4)
C (30) -H (30A)	1. 0000
C (31) -C (32)	1. 397 (4)
C (31) -H (31A)	1. 0000
C (32) -C (36)	1. 517 (4)
C (33) -C (35)	1. 525 (4)
C (33) -C (34)	1. 543 (4)
C (33) -H (33A)	1. 0000
C (34) -H (34A)	0. 9800
C (34) -H (34B)	0. 9800
C (34) -H (34C)	0. 9800
C (35) -H (35A)	0. 9800
C (35) -H (35B)	0. 9800
C (35) -H (35C)	0. 9800
C (36) -C (37)	1. 524 (4)
C (36) -C (38)	1. 528 (4)
C (36) -H (36A)	1. 0000
C (37) -H (37A)	0. 9800
C (37) -H (37B)	0. 9800
C (37) -H (37C)	0. 9800
C (38) -H (38A)	0. 9800
C (38) -H (38B)	0. 9800
C (38) -H (38C)	0. 9800
C (39) -C (44)	1. 430 (4)
C (39) -C (40)	1. 439 (4)
C (40) -C (41)	1. 399 (4)
C (40) -C (45)	1. 512 (4)

C (41) -C (42)	1. 375 (4)
C (41) -H (41A)	1. 0000
C (42) -C (43)	1. 388 (4)
C (42) -H (42A)	1. 0000
C (43) -C (44)	1. 393 (4)
C (43) -H (43A)	1. 0000
C (44) -C (48)	1. 515 (4)
C (45) -C (46)	1. 527 (4)
C (45) -C (47)	1. 538 (5)
C (45) -H (45A)	1. 0000
C (46) -H (46A)	0. 9800
C (46) -H (46B)	0. 9800
C (46) -H (46C)	0. 9800
C (47) -H (47A)	0. 9800
C (47) -H (47B)	0. 9800
C (47) -H (47C)	0. 9800
C (48) -C (50)	1. 520 (4)
C (48) -C (49)	1. 527 (4)
C (48) -H (48A)	1. 0000
C (49) -H (49A)	0. 9800
C (49) -H (49B)	0. 9800
C (49) -H (49C)	0. 9800
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) -H (52A)	0. 9800
C (52) -H (52B)	0. 9800
C (52) -H (52C)	0. 9800
C (53) -C (54)	1. 510 (4)
C (53) -H (53A)	0. 9900
C (53) -H (53B)	0. 9900
C (54) -C (55)	1. 479 (6)
C (54) -H (54A)	0. 9900
C (54) -H (54B)	0. 9900
C (55) -C (56)	1. 502 (6)
C (55) -H (55A)	0. 9900
C (55) -H (55B)	0. 9900
C (56) -H (56A)	0. 9900
C (56) -H (56B)	0. 9900
C (57) -C (58)	1. 491 (6)
C (57) -H (57A)	0. 9900
C (57) -H (57B)	0. 9900
C (58) -C (59)	1. 455 (7)
C (58) -H (58A)	0. 9900
C (58) -H (58B)	0. 9900
C (59) -C (60)	1. 357 (6)

C (59) –H (59A)	0. 9900
C (59) –H (59B)	0. 9900
C (60) –H (60A)	0. 9900
C (60) –H (60B)	0. 9900
C (61) –C (62)	1. 520 (6)
C (61) –H (61A)	0. 9900
C (61) –H (61B)	0. 9900
C (62) –C (63)	1. 519 (7)
C (62) –H (62A)	0. 9900
C (62) –H (62B)	0. 9900
C (63) –C (64)	1. 518 (6)
C (63) –H (63A)	0. 9900
C (63) –H (63B)	0. 9900
C (64) –H (64A)	0. 9900
C (64) –H (64B)	0. 9900

N (3) –Mg (1) –N (2)	105. 37 (9)
N (3) –Mg (1) –N (4)	75. 64 (8)
N (2) –Mg (1) –N (4)	165. 95 (9)
N (3) –Mg (1) –N (1)	164. 40 (9)
N (2) –Mg (1) –N (1)	75. 03 (8)
N (4) –Mg (1) –N (1)	107. 88 (8)
O (2) –K (1) –O (1)	83. 80 (7)
O (2) –K (1) –C (3)	93. 54 (8)
O (1) –K (1) –C (3)	93. 32 (7)
O (2) –K (1) –C (32)	97. 57 (7)
O (1) –K (1) –C (32)	119. 17 (7)
C (3) –K (1) –C (32)	146. 52 (7)
O (2) –K (1) –C (31)	86. 01 (8)
O (1) –K (1) –C (31)	94. 92 (7)
C (3) –K (1) –C (31)	171. 65 (7)
C (32) –K (1) –C (31)	25. 97 (7)
O (2) –K (1) –C (2)	118. 21 (7)
O (1) –K (1) –C (2)	102. 99 (7)
C (3) –K (1) –C (2)	25. 96 (7)
C (32) –K (1) –C (2)	127. 27 (7)
C (31) –K (1) –C (2)	150. 97 (7)
O (2) –K (1) –C (27)	123. 47 (7)
O (1) –K (1) –C (27)	121. 50 (7)
C (3) –K (1) –C (27)	129. 19 (7)
C (32) –K (1) –C (27)	26. 35 (7)
C (31) –K (1) –C (27)	46. 16 (7)
C (2) –K (1) –C (27)	104. 82 (7)
O (2) –K (1) –C (4)	73. 45 (7)
O (1) –K (1) –C (4)	106. 30 (7)
C (3) –K (1) –C (4)	25. 64 (8)
C (32) –K (1) –C (4)	132. 54 (7)
C (31) –K (1) –C (4)	148. 27 (8)
C (2) –K (1) –C (4)	45. 37 (7)

C (27) -K (1) -C (4)	129. 66 (7)
O (2) -K (1) -C (30)	97. 53 (7)
O (1) -K (1) -C (30)	73. 84 (7)
C (3) -K (1) -C (30)	161. 94 (8)
C (32) -K (1) -C (30)	45. 53 (7)
C (31) -K (1) -C (30)	25. 37 (7)
C (2) -K (1) -C (30)	143. 82 (8)
C (27) -K (1) -C (30)	53. 80 (6)
C (4) -K (1) -C (30)	170. 80 (8)
O (2) -K (1) -C (29)	122. 16 (7)
O (1) -K (1) -C (29)	76. 25 (7)
C (3) -K (1) -C (29)	140. 60 (8)
C (32) -K (1) -C (29)	51. 82 (7)
C (31) -K (1) -C (29)	43. 74 (7)
C (2) -K (1) -C (29)	119. 02 (7)
C (27) -K (1) -C (29)	45. 25 (6)
C (4) -K (1) -C (29)	164. 34 (8)
C (30) -K (1) -C (29)	24. 82 (7)
O (2) -K (1) -C (28)	137. 58 (7)
O (1) -K (1) -C (28)	98. 05 (7)
C (3) -K (1) -C (28)	128. 39 (7)
C (32) -K (1) -C (28)	44. 74 (7)
C (31) -K (1) -C (28)	51. 57 (7)
C (2) -K (1) -C (28)	102. 76 (7)
C (27) -K (1) -C (28)	25. 79 (6)
C (4) -K (1) -C (28)	143. 13 (7)
C (30) -K (1) -C (28)	44. 36 (7)
C (29) -K (1) -C (28)	24. 83 (6)
O (2) -K (1) -C (1)	121. 45 (7)
O (1) -K (1) -C (1)	127. 73 (7)
C (3) -K (1) -C (1)	45. 30 (7)
C (32) -K (1) -C (1)	103. 04 (7)
C (31) -K (1) -C (1)	128. 61 (7)
C (2) -K (1) -C (1)	25. 71 (6)
C (27) -K (1) -C (1)	84. 15 (6)
C (4) -K (1) -C (1)	52. 38 (7)
C (30) -K (1) -C (1)	134. 93 (7)
C (29) -K (1) -C (1)	113. 53 (7)
C (28) -K (1) -C (1)	90. 81 (7)
O (3) -K (2) -C (14)	115. 25 (9)
O (3) -K (2) -C (40)	109. 94 (8)
C (14) -K (2) -C (40)	134. 69 (8)
O (3) -K (2) -C (15)	93. 55 (9)
C (14) -K (2) -C (15)	26. 78 (8)
C (40) -K (2) -C (15)	153. 28 (8)
O (3) -K (2) -C (13)	140. 86 (8)
C (14) -K (2) -C (13)	27. 47 (7)
C (40) -K (2) -C (13)	108. 69 (7)
C (15) -K (2) -C (13)	47. 40 (7)

O(3)-K(2)-C(39)	129.57(8)
C(14)-K(2)-C(39)	110.95(7)
C(40)-K(2)-C(39)	27.32(7)
C(15)-K(2)-C(39)	136.06(8)
C(13)-K(2)-C(39)	88.90(7)
O(3)-K(2)-C(41)	84.50(8)
C(14)-K(2)-C(41)	157.73(8)
C(40)-K(2)-C(41)	26.46(7)
C(15)-K(2)-C(41)	174.11(9)
C(13)-K(2)-C(41)	134.60(7)
C(39)-K(2)-C(41)	47.08(7)
O(3)-K(2)-C(16)	92.04(9)
C(14)-K(2)-C(16)	46.14(8)
C(40)-K(2)-C(16)	136.66(8)
C(15)-K(2)-C(16)	25.12(9)
C(13)-K(2)-C(16)	54.40(8)
C(39)-K(2)-C(16)	135.89(8)
C(41)-K(2)-C(16)	149.20(9)
O(3)-K(2)-C(42)	76.29(8)
C(14)-K(2)-C(42)	145.46(8)
C(40)-K(2)-C(42)	45.64(7)
C(15)-K(2)-C(42)	159.22(8)
C(13)-K(2)-C(42)	138.90(7)
C(39)-K(2)-C(42)	53.97(7)
C(41)-K(2)-C(42)	24.96(8)
C(16)-K(2)-C(42)	166.55(8)
O(3)-K(2)-C(44)	116.79(8)
C(14)-K(2)-C(44)	107.25(8)
C(40)-K(2)-C(44)	45.58(7)
C(15)-K(2)-C(44)	133.55(8)
C(13)-K(2)-C(44)	94.78(7)
C(39)-K(2)-C(44)	26.00(6)
C(41)-K(2)-C(44)	51.89(7)
C(16)-K(2)-C(44)	149.17(8)
C(42)-K(2)-C(44)	44.14(7)
O(3)-K(2)-C(18)	135.20(8)
C(14)-K(2)-C(18)	45.51(7)
C(40)-K(2)-C(18)	101.61(7)
C(15)-K(2)-C(18)	51.70(8)
C(13)-K(2)-C(18)	25.98(7)
C(39)-K(2)-C(18)	92.10(7)
C(41)-K(2)-C(18)	126.91(8)
C(16)-K(2)-C(18)	44.03(7)
C(42)-K(2)-C(18)	145.49(7)
C(44)-K(2)-C(18)	108.00(7)
O(3)-K(2)-C(43)	92.15(8)
C(14)-K(2)-C(43)	121.33(8)
C(40)-K(2)-C(43)	52.19(7)
C(15)-K(2)-C(43)	142.28(9)

C (13) -K (2) -C (43)	116. 70 (7)
C (39) -K (2) -C (43)	45. 33 (7)
C (41) -K (2) -C (43)	43. 51 (8)
C (16) -K (2) -C (43)	167. 11 (9)
C (42) -K (2) -C (43)	24. 59 (7)
C (44) -K (2) -C (43)	24. 66 (6)
C (18) -K (2) -C (43)	132. 61 (7)
C (1) -N (1) -Si (1)	128. 79 (17)
C (1) -N (1) -Mg (1)	135. 44 (17)
Si (1) -N (1) -Mg (1)	93. 20 (9)
C (13) -N (2) -Si (1)	126. 25 (18)
C (13) -N (2) -Mg (1)	137. 03 (18)
Si (1) -N (2) -Mg (1)	93. 07 (10)
C (39) -N (3) -Si (2)	124. 39 (17)
C (39) -N (3) -Mg (1)	138. 32 (17)
Si (2) -N (3) -Mg (1)	92. 62 (9)
C (27) -N (4) -Si (2)	124. 45 (17)
C (27) -N (4) -Mg (1)	139. 30 (16)
Si (2) -N (4) -Mg (1)	92. 37 (9)
C (56) -O (1) -C (53)	108. 7 (2)
C (56) -O (1) -K (1)	116. 62 (19)
C (53) -O (1) -K (1)	133. 81 (17)
C (60) -O (2) -C (57)	107. 6 (3)
C (60) -O (2) -K (1)	115. 61 (19)
C (57) -O (2) -K (1)	134. 58 (18)
C (61) -O (3) -C (64)	109. 6 (3)
C (61) -O (3) -K (2)	122. 6 (2)
C (64) -O (3) -K (2)	122. 2 (2)
N (1) -Si (1) -N (2)	98. 68 (10)
N (1) -Si (1) -C (26)	106. 06 (12)
N (2) -Si (1) -C (26)	121. 83 (12)
N (1) -Si (1) -C (25)	122. 14 (11)
N (2) -Si (1) -C (25)	105. 00 (12)
C (26) -Si (1) -C (25)	104. 54 (13)
N (3) -Si (2) -N (4)	99. 31 (10)
N (3) -Si (2) -C (52)	120. 21 (13)
N (4) -Si (2) -C (52)	106. 61 (12)
N (3) -Si (2) -C (51)	105. 71 (12)
N (4) -Si (2) -C (51)	121. 22 (13)
C (52) -Si (2) -C (51)	104. 90 (15)
N (1) -C (1) -C (6)	121. 2 (2)
N (1) -C (1) -C (2)	123. 3 (2)
C (6) -C (1) -C (2)	115. 5 (2)
N (1) -C (1) -K (1)	113. 74 (15)
C (6) -C (1) -K (1)	84. 36 (15)
C (2) -C (1) -K (1)	69. 97 (14)
C (3) -C (2) -C (1)	120. 6 (2)
C (3) -C (2) -C (7)	118. 0 (2)
C (1) -C (2) -C (7)	121. 4 (2)

C(3)-C(2)-K(1)	73.80(16)
C(1)-C(2)-K(1)	84.32(15)
C(7)-C(2)-K(1)	114.25(16)
C(4)-C(3)-C(2)	122.2(3)
C(4)-C(3)-K(1)	81.91(17)
C(2)-C(3)-K(1)	80.24(16)
C(4)-C(3)-H(3A)	118.5
C(2)-C(3)-H(3A)	118.5
K(1)-C(3)-H(3A)	118.5
C(5)-C(4)-C(3)	118.1(3)
C(5)-C(4)-K(1)	86.98(17)
C(3)-C(4)-K(1)	72.46(16)
C(5)-C(4)-H(4A)	120.4
C(3)-C(4)-H(4A)	120.4
K(1)-C(4)-H(4A)	120.4
C(4)-C(5)-C(6)	122.1(3)
C(4)-C(5)-K(1)	68.98(16)
C(6)-C(5)-K(1)	81.99(16)
C(4)-C(5)-H(5A)	119.0
C(6)-C(5)-H(5A)	119.0
K(1)-C(5)-H(5A)	119.0
C(5)-C(6)-C(1)	121.2(2)
C(5)-C(6)-C(10)	117.7(2)
C(1)-C(6)-C(10)	120.9(2)
C(5)-C(6)-K(1)	74.68(16)
C(1)-C(6)-K(1)	71.53(14)
C(10)-C(6)-K(1)	130.98(17)
C(2)-C(7)-C(8)	113.4(2)
C(2)-C(7)-C(9)	109.6(2)
C(8)-C(7)-C(9)	109.5(2)
C(2)-C(7)-H(7A)	108.1
C(8)-C(7)-H(7A)	108.1
C(9)-C(7)-H(7A)	108.1
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(11)-C(10)-C(6)	112.5(2)
C(11)-C(10)-C(12)	110.7(2)
C(6)-C(10)-C(12)	110.5(2)
C(11)-C(10)-H(10A)	107.7

C(6)–C(10)–H(10A)	107.7
C(12)–C(10)–H(10A)	107.7
C(10)–C(11)–H(11A)	109.5
C(10)–C(11)–H(11B)	109.5
H(11A)–C(11)–H(11B)	109.5
C(10)–C(11)–H(11C)	109.5
H(11A)–C(11)–H(11C)	109.5
H(11B)–C(11)–H(11C)	109.5
C(10)–C(12)–H(12A)	109.5
C(10)–C(12)–H(12B)	109.5
H(12A)–C(12)–H(12B)	109.5
C(10)–C(12)–H(12C)	109.5
H(12A)–C(12)–H(12C)	109.5
H(12B)–C(12)–H(12C)	109.5
N(2)–C(13)–C(14)	123.7(2)
N(2)–C(13)–C(18)	120.9(2)
C(14)–C(13)–C(18)	115.4(2)
N(2)–C(13)–K(2)	110.32(16)
C(14)–C(13)–K(2)	72.48(15)
C(18)–C(13)–K(2)	84.98(16)
C(15)–C(14)–C(13)	120.5(3)
C(15)–C(14)–C(19)	117.0(3)
C(13)–C(14)–C(19)	122.5(2)
C(15)–C(14)–K(2)	79.92(18)
C(13)–C(14)–K(2)	80.05(16)
C(19)–C(14)–K(2)	109.52(17)
C(16)–C(15)–C(14)	123.0(3)
C(16)–C(15)–K(2)	84.1(2)
C(14)–C(15)–K(2)	73.30(17)
C(16)–C(15)–H(15A)	118.4
C(14)–C(15)–H(15A)	118.4
K(2)–C(15)–H(15A)	118.4
C(15)–C(16)–C(17)	117.6(3)
C(15)–C(16)–K(2)	70.81(19)
C(17)–C(16)–K(2)	81.23(19)
C(15)–C(16)–H(16A)	121.1
C(17)–C(16)–H(16A)	121.1
K(2)–C(16)–H(16A)	121.1
C(16)–C(17)–C(18)	122.3(3)
C(16)–C(17)–K(2)	74.30(19)
C(18)–C(17)–K(2)	76.62(17)
C(16)–C(17)–H(17A)	118.8
C(18)–C(17)–H(17A)	118.8
K(2)–C(17)–H(17A)	118.8
C(17)–C(18)–C(13)	120.9(3)
C(17)–C(18)–C(22)	117.3(3)
C(13)–C(18)–C(22)	121.6(2)
C(17)–C(18)–K(2)	78.90(17)
C(13)–C(18)–K(2)	69.04(14)

C (22) –C (18) –K (2)	128. 70 (19)
C (14) –C (19) –C (20)	111. 1 (3)
C (14) –C (19) –C (21)	112. 5 (3)
C (20) –C (19) –C (21)	109. 5 (2)
C (14) –C (19) –H (19A)	107. 9
C (20) –C (19) –H (19A)	107. 9
C (21) –C (19) –H (19A)	107. 9
C (19) –C (20) –H (20A)	109. 5
C (19) –C (20) –H (20B)	109. 5
H (20A) –C (20) –H (20B)	109. 5
C (19) –C (20) –H (20C)	109. 5
H (20A) –C (20) –H (20C)	109. 5
H (20B) –C (20) –H (20C)	109. 5
C (19) –C (21) –H (21A)	109. 5
C (19) –C (21) –H (21B)	109. 5
H (21A) –C (21) –H (21B)	109. 5
C (19) –C (21) –H (21C)	109. 5
H (21A) –C (21) –H (21C)	109. 5
H (21B) –C (21) –H (21C)	109. 5
C (24) –C (22) –C (18)	113. 2 (2)
C (24) –C (22) –C (23)	109. 4 (3)
C (18) –C (22) –C (23)	109. 8 (3)
C (24) –C (22) –H (22A)	108. 1
C (18) –C (22) –H (22A)	108. 1
C (23) –C (22) –H (22A)	108. 1
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
Si (1) –C (25) –H (25A)	109. 5
Si (1) –C (25) –H (25B)	109. 5
H (25A) –C (25) –H (25B)	109. 5
Si (1) –C (25) –H (25C)	109. 5
H (25A) –C (25) –H (25C)	109. 5
H (25B) –C (25) –H (25C)	109. 5
Si (1) –C (26) –H (26A)	109. 5
Si (1) –C (26) –H (26B)	109. 5
H (26A) –C (26) –H (26B)	109. 5
Si (1) –C (26) –H (26C)	109. 5
H (26A) –C (26) –H (26C)	109. 5
H (26B) –C (26) –H (26C)	109. 5

N(4)–C(27)–C(32)	123.8(2)
N(4)–C(27)–C(28)	120.7(2)
C(32)–C(27)–C(28)	115.5(2)
N(4)–C(27)–K(1)	113.86(15)
C(32)–C(27)–K(1)	74.47(14)
C(28)–C(27)–K(1)	80.44(14)
C(29)–C(28)–C(27)	121.0(2)
C(29)–C(28)–C(33)	117.9(2)
C(27)–C(28)–C(33)	121.1(2)
C(29)–C(28)–K(1)	76.85(15)
C(27)–C(28)–K(1)	73.76(14)
C(33)–C(28)–K(1)	121.03(16)
C(30)–C(29)–C(28)	122.2(2)
C(30)–C(29)–K(1)	75.32(16)
C(28)–C(29)–K(1)	78.32(15)
C(30)–C(29)–H(29A)	118.9
C(28)–C(29)–H(29A)	118.9
K(1)–C(29)–H(29A)	118.9
C(29)–C(30)–C(31)	117.9(2)
C(29)–C(30)–K(1)	79.87(16)
C(31)–C(30)–K(1)	74.60(16)
C(29)–C(30)–H(30A)	120.9
C(31)–C(30)–H(30A)	120.9
K(1)–C(30)–H(30A)	120.9
C(30)–C(31)–C(32)	122.2(3)
C(30)–C(31)–K(1)	80.03(16)
C(32)–C(31)–K(1)	76.84(15)
C(30)–C(31)–H(31A)	118.8
C(32)–C(31)–H(31A)	118.8
K(1)–C(31)–H(31A)	118.8
C(31)–C(32)–C(27)	121.0(2)
C(31)–C(32)–C(36)	116.4(2)
C(27)–C(32)–C(36)	122.6(2)
C(31)–C(32)–K(1)	77.20(15)
C(27)–C(32)–K(1)	79.17(14)
C(36)–C(32)–K(1)	115.01(17)
C(28)–C(33)–C(35)	110.2(2)
C(28)–C(33)–C(34)	113.2(2)
C(35)–C(33)–C(34)	110.1(2)
C(28)–C(33)–H(33A)	107.7
C(35)–C(33)–H(33A)	107.7
C(34)–C(33)–H(33A)	107.7
C(33)–C(34)–H(34A)	109.5
C(33)–C(34)–H(34B)	109.5
H(34A)–C(34)–H(34B)	109.5
C(33)–C(34)–H(34C)	109.5
H(34A)–C(34)–H(34C)	109.5
H(34B)–C(34)–H(34C)	109.5
C(33)–C(35)–H(35A)	109.5

C (33) –C (35) –H (35B)	109. 5
H (35A) –C (35) –H (35B)	109. 5
C (33) –C (35) –H (35C)	109. 5
H (35A) –C (35) –H (35C)	109. 5
H (35B) –C (35) –H (35C)	109. 5
C (32) –C (36) –C (37)	112. 7 (2)
C (32) –C (36) –C (38)	110. 7 (2)
C (37) –C (36) –C (38)	109. 7 (3)
C (32) –C (36) –H (36A)	107. 8
C (37) –C (36) –H (36A)	107. 8
C (38) –C (36) –H (36A)	107. 8
C (36) –C (37) –H (37A)	109. 5
C (36) –C (37) –H (37B)	109. 5
H (37A) –C (37) –H (37B)	109. 5
C (36) –C (37) –H (37C)	109. 5
H (37A) –C (37) –H (37C)	109. 5
H (37B) –C (37) –H (37C)	109. 5
C (36) –C (38) –H (38A)	109. 5
C (36) –C (38) –H (38B)	109. 5
H (38A) –C (38) –H (38B)	109. 5
C (36) –C (38) –H (38C)	109. 5
H (38A) –C (38) –H (38C)	109. 5
H (38B) –C (38) –H (38C)	109. 5
N (3) –C (39) –C (44)	121. 2 (2)
N (3) –C (39) –C (40)	123. 0 (2)
C (44) –C (39) –C (40)	115. 8 (2)
N (3) –C (39) –K (2)	110. 98 (15)
C (44) –C (39) –K (2)	83. 45 (15)
C (40) –C (39) –K (2)	73. 67 (14)
C (41) –C (40) –C (39)	120. 6 (2)
C (41) –C (40) –C (45)	116. 9 (2)
C (39) –C (40) –C (45)	122. 5 (2)
C (41) –C (40) –K (2)	80. 15 (16)
C (39) –C (40) –K (2)	79. 02 (15)
C (45) –C (40) –K (2)	110. 01 (18)
C (42) –C (41) –C (40)	122. 4 (3)
C (42) –C (41) –K (2)	83. 34 (18)
C (40) –C (41) –K (2)	73. 38 (16)
C (42) –C (41) –H (41A)	118. 7
C (40) –C (41) –H (41A)	118. 7
K (2) –C (41) –H (41A)	118. 7
C (41) –C (42) –C (43)	118. 0 (2)
C (41) –C (42) –K (2)	71. 70 (17)
C (43) –C (42) –K (2)	79. 45 (18)
C (41) –C (42) –H (42A)	121. 0
C (43) –C (42) –H (42A)	121. 0
K (2) –C (42) –H (42A)	121. 0
C (42) –C (43) –C (44)	122. 2 (3)
C (42) –C (43) –K (2)	75. 96 (18)

C (44) -C (43) -K (2)	76.20 (16)
C (42) -C (43) -H (43A)	118.9
C (44) -C (43) -H (43A)	118.9
K (2) -C (43) -H (43A)	118.9
C (43) -C (44) -C (39)	120.9 (2)
C (43) -C (44) -C (48)	117.7 (2)
C (39) -C (44) -C (48)	121.3 (2)
C (43) -C (44) -K (2)	79.14 (17)
C (39) -C (44) -K (2)	70.55 (14)
C (48) -C (44) -K (2)	123.59 (17)
C (40) -C (45) -C (46)	111.4 (3)
C (40) -C (45) -C (47)	111.7 (2)
C (46) -C (45) -C (47)	109.7 (3)
C (40) -C (45) -H (45A)	107.9
C (46) -C (45) -H (45A)	107.9
C (47) -C (45) -H (45A)	107.9
C (45) -C (46) -H (46A)	109.5
C (45) -C (46) -H (46B)	109.5
H (46A) -C (46) -H (46B)	109.5
C (45) -C (46) -H (46C)	109.5
H (46A) -C (46) -H (46C)	109.5
H (46B) -C (46) -H (46C)	109.5
C (45) -C (47) -H (47A)	109.5
C (45) -C (47) -H (47B)	109.5
H (47A) -C (47) -H (47B)	109.5
C (45) -C (47) -H (47C)	109.5
H (47A) -C (47) -H (47C)	109.5
H (47B) -C (47) -H (47C)	109.5
C (44) -C (48) -C (50)	111.5 (2)
C (44) -C (48) -C (49)	111.5 (2)
C (50) -C (48) -C (49)	110.6 (2)
C (44) -C (48) -H (48A)	107.7
C (50) -C (48) -H (48A)	107.7
C (49) -C (48) -H (48A)	107.7
C (48) -C (49) -H (49A)	109.5
C (48) -C (49) -H (49B)	109.5
H (49A) -C (49) -H (49B)	109.5
C (48) -C (49) -H (49C)	109.5
H (49A) -C (49) -H (49C)	109.5
H (49B) -C (49) -H (49C)	109.5
C (48) -C (50) -H (50A)	109.5
C (48) -C (50) -H (50B)	109.5
H (50A) -C (50) -H (50B)	109.5
C (48) -C (50) -H (50C)	109.5
H (50A) -C (50) -H (50C)	109.5
H (50B) -C (50) -H (50C)	109.5
Si (2) -C (51) -H (51A)	109.5
Si (2) -C (51) -H (51B)	109.5
H (51A) -C (51) -H (51B)	109.5

Si (2) -C (51) -H (51C)	109. 5
H (51A) -C (51) -H (51C)	109. 5
H (51B) -C (51) -H (51C)	109. 5
Si (2) -C (52) -H (52A)	109. 5
Si (2) -C (52) -H (52B)	109. 5
H (52A) -C (52) -H (52B)	109. 5
Si (2) -C (52) -H (52C)	109. 5
H (52A) -C (52) -H (52C)	109. 5
H (52B) -C (52) -H (52C)	109. 5
O (1) -C (53) -C (54)	106. 5 (3)
O (1) -C (53) -H (53A)	110. 4
C (54) -C (53) -H (53A)	110. 4
O (1) -C (53) -H (53B)	110. 4
C (54) -C (53) -H (53B)	110. 4
H (53A) -C (53) -H (53B)	108. 6
C (55) -C (54) -C (53)	103. 0 (3)
C (55) -C (54) -H (54A)	111. 2
C (53) -C (54) -H (54A)	111. 2
C (55) -C (54) -H (54B)	111. 2
C (53) -C (54) -H (54B)	111. 2
H (54A) -C (54) -H (54B)	109. 1
C (54) -C (55) -C (56)	104. 0 (3)
C (54) -C (55) -H (55A)	111. 0
C (56) -C (55) -H (55A)	111. 0
C (54) -C (55) -H (55B)	111. 0
C (56) -C (55) -H (55B)	111. 0
H (55A) -C (55) -H (55B)	109. 0
O (1) -C (56) -C (55)	107. 2 (3)
O (1) -C (56) -H (56A)	110. 3
C (55) -C (56) -H (56A)	110. 3
O (1) -C (56) -H (56B)	110. 3
C (55) -C (56) -H (56B)	110. 3
H (56A) -C (56) -H (56B)	108. 5
O (2) -C (57) -C (58)	106. 1 (3)
O (2) -C (57) -H (57A)	110. 5
C (58) -C (57) -H (57A)	110. 5
O (2) -C (57) -H (57B)	110. 5
C (58) -C (57) -H (57B)	110. 5
H (57A) -C (57) -H (57B)	108. 7
C (59) -C (58) -C (57)	105. 3 (3)
C (59) -C (58) -H (58A)	110. 7
C (57) -C (58) -H (58A)	110. 7
C (59) -C (58) -H (58B)	110. 7
C (57) -C (58) -H (58B)	110. 7
H (58A) -C (58) -H (58B)	108. 8
C (60) -C (59) -C (58)	109. 5 (4)
C (60) -C (59) -H (59A)	109. 8
C (58) -C (59) -H (59A)	109. 8
C (60) -C (59) -H (59B)	109. 8

C (58)–C (59)–H (59B)	109.8
H (59A)–C (59)–H (59B)	108.2
C (59)–C (60)–O (2)	109.9 (3)
C (59)–C (60)–H (60A)	109.7
O (2)–C (60)–H (60A)	109.7
C (59)–C (60)–H (60B)	109.7
O (2)–C (60)–H (60B)	109.7
H (60A)–C (60)–H (60B)	108.2
O (3)–C (61)–C (62)	103.8 (4)
O (3)–C (61)–H (61A)	111.0
C (62)–C (61)–H (61A)	111.0
O (3)–C (61)–H (61B)	111.0
C (62)–C (61)–H (61B)	111.0
H (61A)–C (61)–H (61B)	109.0
C (63)–C (62)–C (61)	102.4 (4)
C (63)–C (62)–H (62A)	111.3
C (61)–C (62)–H (62A)	111.3
C (63)–C (62)–H (62B)	111.3
C (61)–C (62)–H (62B)	111.3
H (62A)–C (62)–H (62B)	109.2
C (64)–C (63)–C (62)	101.6 (4)
C (64)–C (63)–H (63A)	111.4
C (62)–C (63)–H (63A)	111.4
C (64)–C (63)–H (63B)	111.4
C (62)–C (63)–H (63B)	111.4
H (63A)–C (63)–H (63B)	109.3
O (3)–C (64)–C (63)	107.9 (4)
O (3)–C (64)–H (64A)	110.1
C (63)–C (64)–H (64A)	110.1
O (3)–C (64)–H (64B)	110.1
C (63)–C (64)–H (64B)	110.1
H (64A)–C (64)–H (64B)	108.4

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

	U11	U22	U33	U23	U13	U12
Mg(1)	17(1)	19(1)	14(1)	-1(1)	5(1)	0(1)
K(1)	26(1)	30(1)	25(1)	-1(1)	11(1)	2(1)
K(2)	36(1)	36(1)	41(1)	-3(1)	13(1)	0(1)
N(1)	18(1)	20(1)	16(1)	1(1)	6(1)	1(1)
N(2)	20(1)	21(1)	20(1)	-1(1)	7(1)	-2(1)
N(3)	16(1)	25(1)	17(1)	-2(1)	6(1)	1(1)
N(4)	14(1)	23(1)	18(1)	-2(1)	4(1)	1(1)
O(1)	29(1)	64(2)	28(1)	5(1)	11(1)	7(1)
O(2)	45(1)	45(1)	26(1)	3(1)	9(1)	-14(1)
O(3)	54(2)	70(2)	60(2)	-14(1)	21(1)	-18(1)
Si(1)	22(1)	19(1)	17(1)	-1(1)	7(1)	0(1)
Si(2)	16(1)	24(1)	22(1)	-6(1)	4(1)	2(1)
C(1)	21(1)	20(1)	18(1)	-4(1)	8(1)	1(1)
C(2)	22(1)	25(1)	22(1)	-4(1)	7(1)	1(1)
C(3)	19(1)	34(2)	30(1)	-5(1)	9(1)	3(1)
C(4)	26(1)	40(2)	35(2)	-5(1)	19(1)	-5(1)
C(5)	29(2)	33(2)	27(1)	4(1)	16(1)	-2(1)
C(6)	24(1)	24(1)	23(1)	0(1)	11(1)	0(1)
C(7)	24(1)	30(2)	27(1)	2(1)	5(1)	6(1)
C(8)	28(2)	50(2)	32(2)	6(1)	1(1)	6(1)
C(9)	41(2)	33(2)	41(2)	5(1)	14(2)	11(1)
C(10)	25(1)	31(2)	25(1)	9(1)	10(1)	-1(1)
C(11)	34(2)	36(2)	47(2)	10(2)	13(1)	3(1)
C(12)	35(2)	55(2)	24(2)	7(1)	7(1)	-1(1)
C(13)	22(1)	21(1)	24(1)	1(1)	7(1)	0(1)
C(14)	27(1)	25(1)	29(2)	0(1)	7(1)	-2(1)
C(15)	37(2)	30(2)	37(2)	-3(1)	8(1)	-13(1)
C(16)	39(2)	43(2)	43(2)	2(2)	16(2)	-18(1)
C(17)	37(2)	45(2)	32(2)	4(1)	16(1)	-9(1)
C(18)	24(1)	33(2)	26(1)	0(1)	9(1)	-4(1)
C(19)	32(2)	30(2)	26(2)	-8(1)	6(1)	-7(1)
C(20)	51(2)	35(2)	45(2)	-13(2)	18(2)	-4(2)
C(21)	38(2)	53(2)	30(2)	-9(2)	4(1)	-10(2)
C(22)	29(2)	41(2)	26(2)	-4(1)	11(1)	-7(1)
C(23)	38(2)	46(2)	38(2)	8(2)	6(1)	2(1)
C(24)	39(2)	44(2)	35(2)	-2(1)	13(1)	1(1)
C(25)	32(2)	24(1)	28(2)	3(1)	9(1)	1(1)
C(26)	31(2)	33(2)	25(1)	-5(1)	12(1)	1(1)
C(27)	15(1)	21(1)	21(1)	-4(1)	7(1)	3(1)

C(28)	19(1)	26(1)	19(1)	-3(1)	6(1)	3(1)
C(29)	20(1)	36(2)	18(1)	-2(1)	4(1)	3(1)
C(30)	19(1)	36(2)	24(1)	-6(1)	4(1)	-2(1)
C(31)	20(1)	27(1)	27(1)	-6(1)	7(1)	-1(1)
C(32)	18(1)	26(1)	22(1)	0(1)	8(1)	2(1)
C(33)	25(1)	26(1)	21(1)	1(1)	4(1)	1(1)
C(34)	46(2)	39(2)	26(2)	-5(1)	16(1)	-8(1)
C(35)	39(2)	32(2)	27(2)	1(1)	8(1)	5(1)
C(36)	22(1)	27(2)	30(2)	3(1)	3(1)	-1(1)
C(37)	32(2)	56(2)	31(2)	14(2)	7(1)	-6(1)
C(38)	34(2)	29(2)	48(2)	3(1)	3(1)	4(1)
C(39)	19(1)	20(1)	19(1)	-1(1)	5(1)	-2(1)
C(40)	19(1)	27(1)	25(1)	-3(1)	8(1)	-1(1)
C(41)	17(1)	37(2)	38(2)	-4(1)	11(1)	-1(1)
C(42)	19(1)	45(2)	30(2)	-1(1)	0(1)	-3(1)
C(43)	25(1)	42(2)	20(1)	-1(1)	2(1)	-3(1)
C(44)	22(1)	26(1)	19(1)	2(1)	6(1)	-1(1)
C(45)	21(1)	45(2)	28(2)	-8(1)	12(1)	-2(1)
C(46)	30(2)	64(2)	44(2)	-22(2)	14(1)	4(2)
C(47)	34(2)	76(3)	33(2)	-3(2)	19(1)	-10(2)
C(48)	24(1)	35(2)	15(1)	1(1)	5(1)	-2(1)
C(49)	36(2)	62(2)	28(2)	16(2)	11(1)	-1(2)
C(50)	34(2)	46(2)	29(2)	-6(1)	11(1)	1(1)
C(51)	22(1)	26(2)	47(2)	2(1)	-1(1)	4(1)
C(52)	25(1)	48(2)	41(2)	-25(2)	13(1)	-4(1)
C(53)	34(2)	63(2)	25(2)	9(2)	8(1)	5(2)
C(54)	33(2)	56(2)	40(2)	9(2)	3(2)	3(2)
C(55)	37(2)	92(3)	73(3)	-19(2)	11(2)	9(2)
C(56)	40(2)	90(3)	52(2)	2(2)	27(2)	6(2)
C(57)	40(2)	60(2)	33(2)	13(2)	16(2)	1(2)
C(58)	133(5)	69(3)	64(3)	19(2)	32(3)	-39(3)
C(59)	306(11)	95(5)	62(3)	3(3)	8(5)	-131(6)
C(60)	63(2)	59(2)	38(2)	-7(2)	11(2)	-27(2)
C(61)	70(3)	77(3)	55(2)	-18(2)	17(2)	-29(2)
C(62)	55(3)	77(3)	73(3)	-13(2)	9(2)	-19(2)
C(63)	58(3)	83(3)	69(3)	-27(2)	24(2)	-24(2)
C(64)	70(3)	85(3)	58(3)	-17(2)	31(2)	-2(2)

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

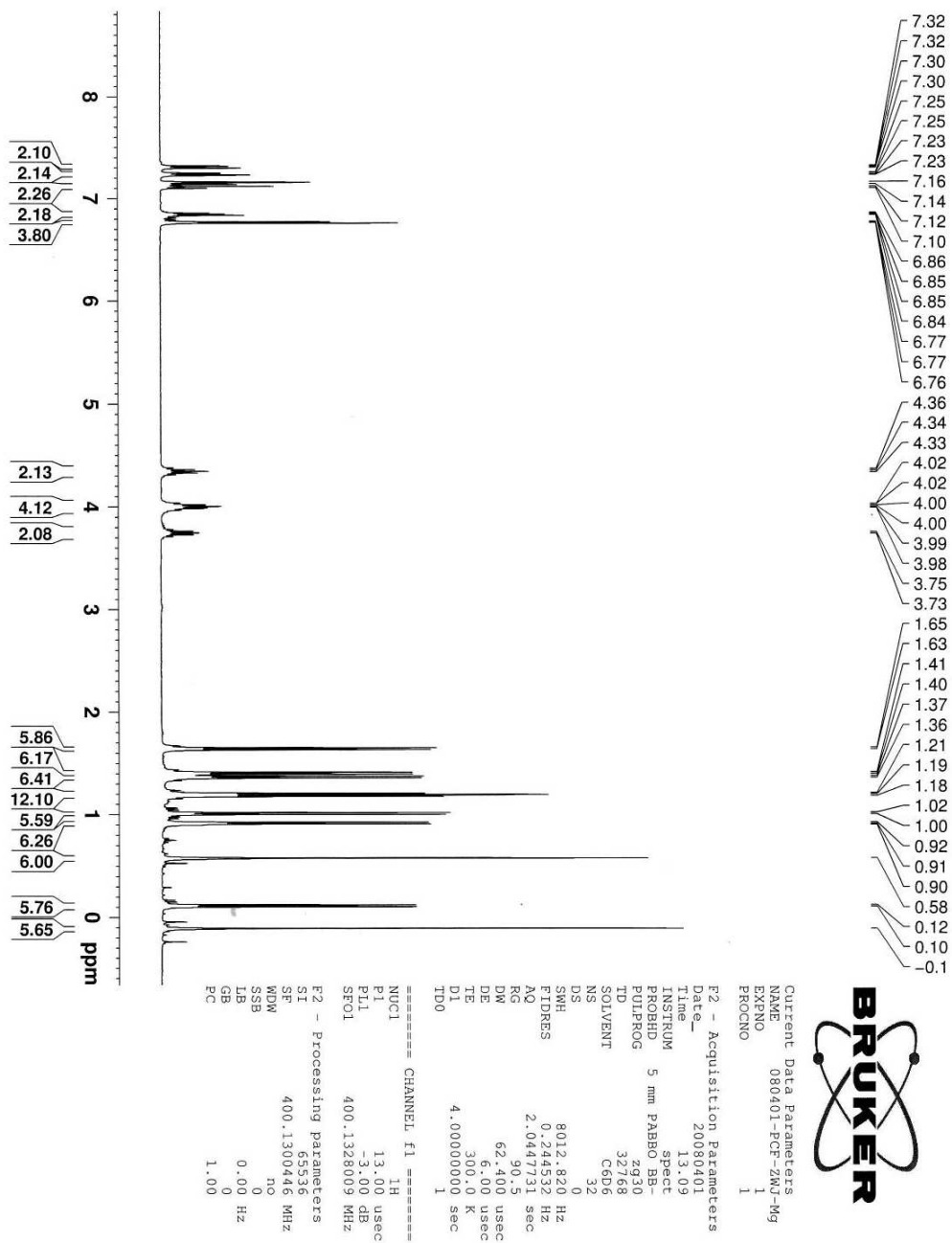
	x	y	z	U(eq)
H(3A)	6161	5940	3276	33
H(4A)	5982	6651	2393	38
H(5A)	4440	6977	1664	34
H(7A)	4345	5340	3773	34
H(8A)	5535	5862	4705	59
H(8B)	6313	5604	4428	59
H(8C)	5774	5233	4828	59
H(9A)	4732	4841	2849	58
H(9B)	5287	4610	3695	58
H(9C)	5824	4982	3294	58
H(10A)	2282	6398	1643	32
H(11A)	2585	7296	2072	59
H(11B)	1900	7273	1187	59
H(11C)	2991	7419	1419	59
H(12A)	2086	6547	341	58
H(12B)	2801	6060	701	58
H(12C)	3198	6639	600	58
H(15A)	-734	4107	2090	44
H(16A)	-1046	4201	3224	50
H(17A)	-150	4838	4164	44
H(19A)	813	4905	1501	37
H(20A)	1345	4020	1914	65
H(20B)	835	4043	999	65
H(20C)	291	3798	1505	65
H(21A)	-834	5078	901	64
H(21B)	-1044	4445	884	64
H(21C)	-491	4685	383	64
H(22A)	1851	5575	4140	38
H(23A)	2131	4725	4792	64
H(23B)	1325	4856	5117	64
H(23C)	2271	5208	5389	64
H(24A)	558	6103	4109	60
H(24B)	1315	6046	4968	60
H(24C)	367	5696	4695	60
H(25A)	3127	4391	3027	43
H(25B)	2469	4550	3485	43
H(25C)	3516	4788	3750	43
H(26A)	2787	4690	1748	43
H(26B)	2932	5302	1549	43
H(26C)	1890	5060	1304	43

H(29A)	4691	7004	5823	31
H(30A)	5291	7860	5666	33
H(31A)	4487	8357	4524	30
H(33A)	2519	6424	4585	30
H(34A)	2789	6752	5842	55
H(34B)	3808	6474	6156	55
H(34C)	2877	6109	5844	55
H(35A)	3769	6016	4329	51
H(35B)	3478	5659	4914	51
H(35C)	4408	6024	5226	51
H(36A)	2449	7952	2931	34
H(37A)	3897	7941	2747	62
H(37B)	4212	8483	3237	62
H(37C)	3336	8490	2432	62
H(38A)	2225	8584	3794	61
H(38B)	2315	8882	3070	61
H(38C)	3190	8876	3876	61
H(41A)	-2600	6735	2187	37
H(42A)	-2951	6563	868	40
H(43A)	-1680	6480	431	38
H(45A)	-317	6815	3679	37
H(46A)	-1183	7627	3294	69
H(46B)	-1310	7379	4035	69
H(46C)	-2133	7315	3207	69
H(47A)	-1140	5988	3594	69
H(47B)	-2107	6313	3392	69
H(47C)	-1283	6378	4220	69
H(48A)	751	6743	1546	31
H(49A)	-197	7386	661	63
H(49B)	-673	6916	57	63
H(49C)	425	7050	297	63
H(50A)	459	5814	1297	55
H(50B)	825	6083	686	55
H(50C)	-272	5949	450	55
H(51A)	490	8126	2739	53
H(51B)	144	7688	2065	53
H(51C)	1180	7940	2323	53
H(52A)	771	7888	4036	57
H(52B)	1660	7534	4547	57
H(52C)	619	7286	4271	57
H(53A)	6583	6539	6100	50
H(53B)	6633	7185	6172	50
H(54A)	8218	7201	6507	55
H(54B)	8130	6615	6846	55
H(55A)	8205	6184	5818	84
H(55B)	8863	6695	5838	84
H(56A)	7737	7098	4855	69
H(56B)	7357	6493	4641	69
H(57A)	5316	7992	2390	53

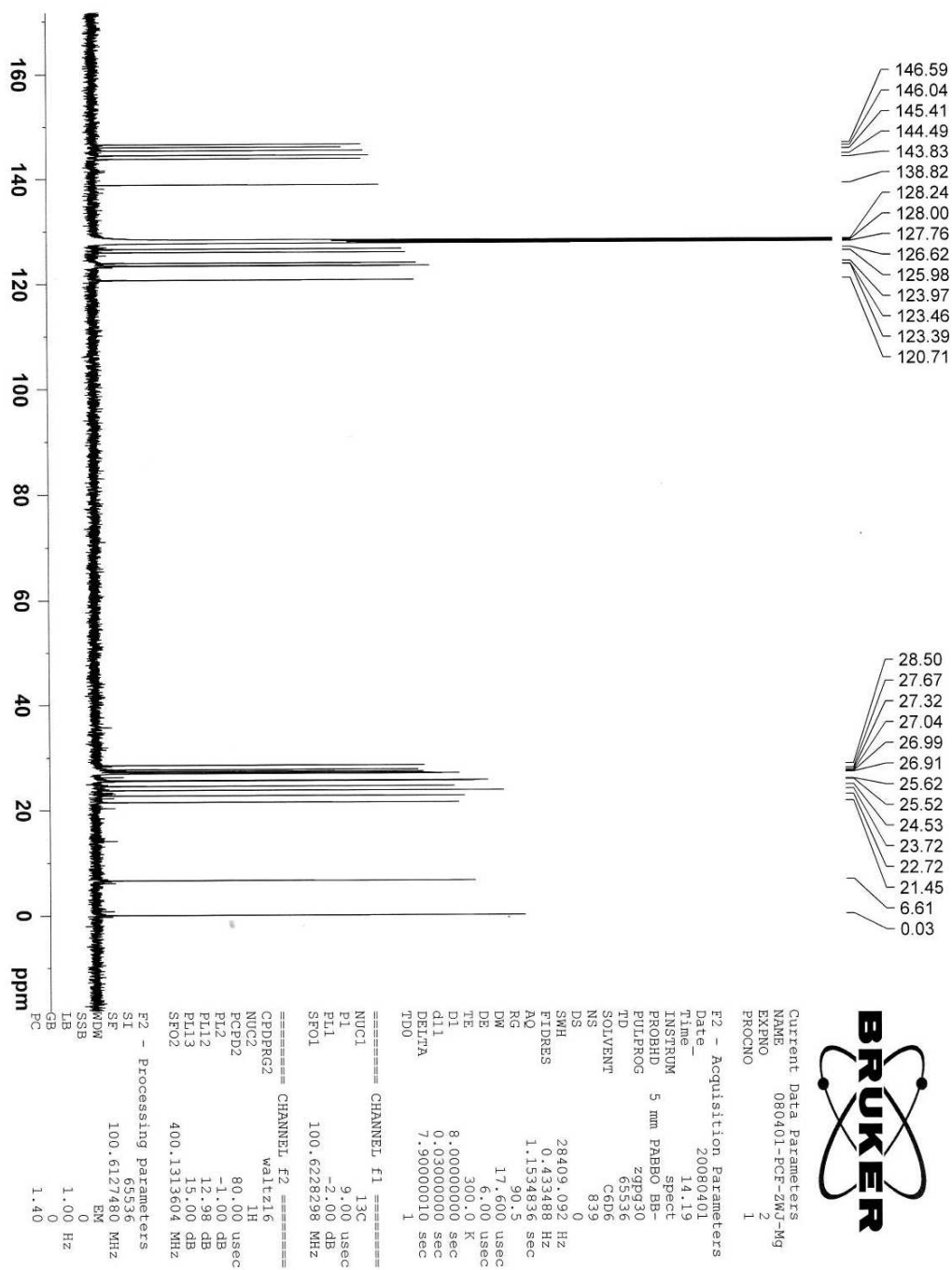
H(57B)	6371	7786	2553	53
H(58A)	6833	8628	2731	108
H(58B)	5811	8821	2691	108
H(59A)	7374	8704	3954	206
H(59B)	6357	8899	3914	206
H(60A)	6258	8199	4437	67
H(60B)	7204	7972	4366	67
H(61A)	-3664	4978	418	83
H(61B)	-3181	5564	497	83
H(62A)	-4303	5961	879	88
H(62B)	-4939	5535	248	88
H(63A)	-4911	5472	1628	84
H(63B)	-4921	4920	1172	84
H(64A)	-3378	5389	2361	83
H(64B)	-3516	4766	2114	83

Table 6. Torsion angles [deg] for 4.

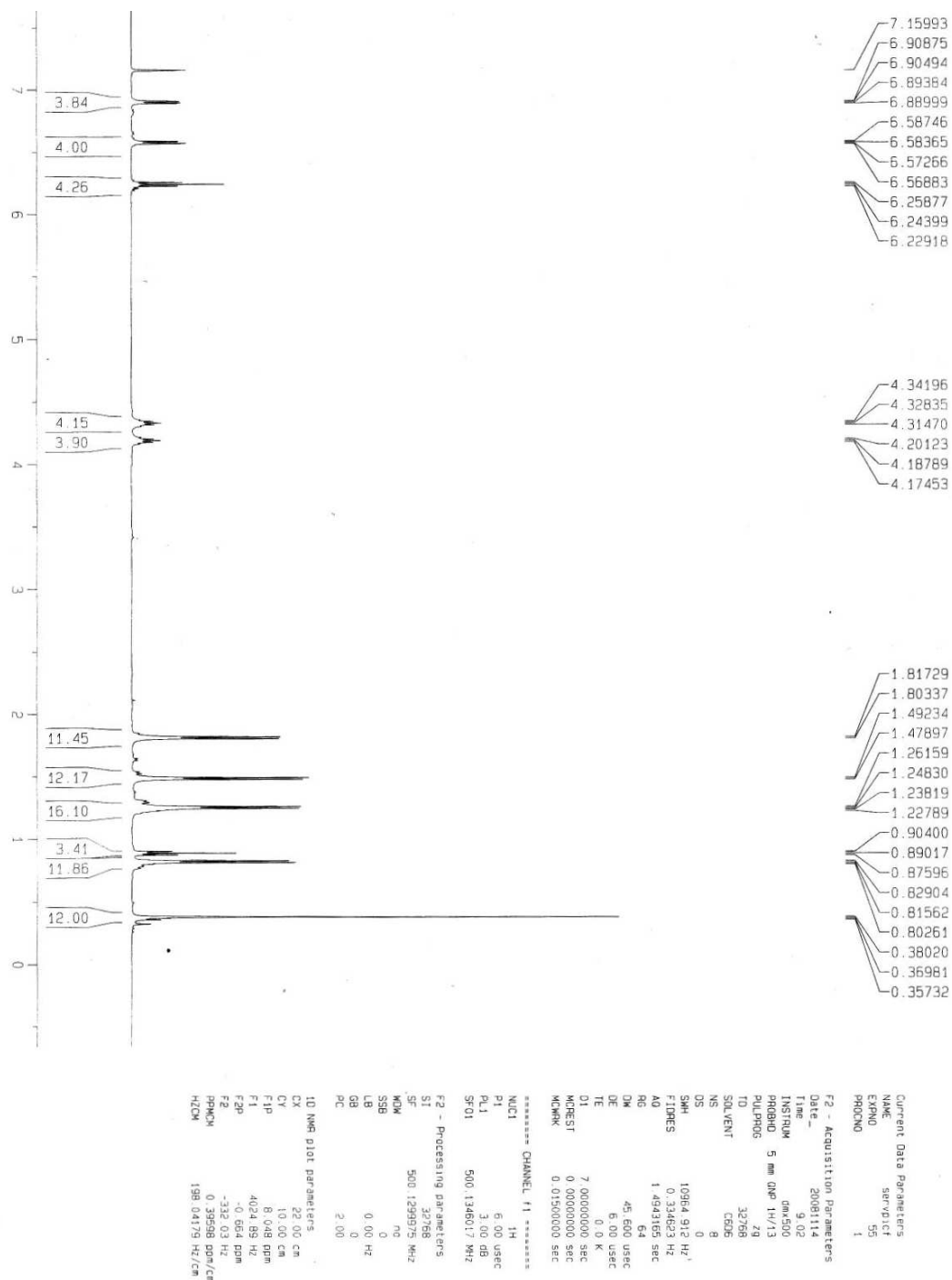
2. ^1H NMR spectrum of complex 2



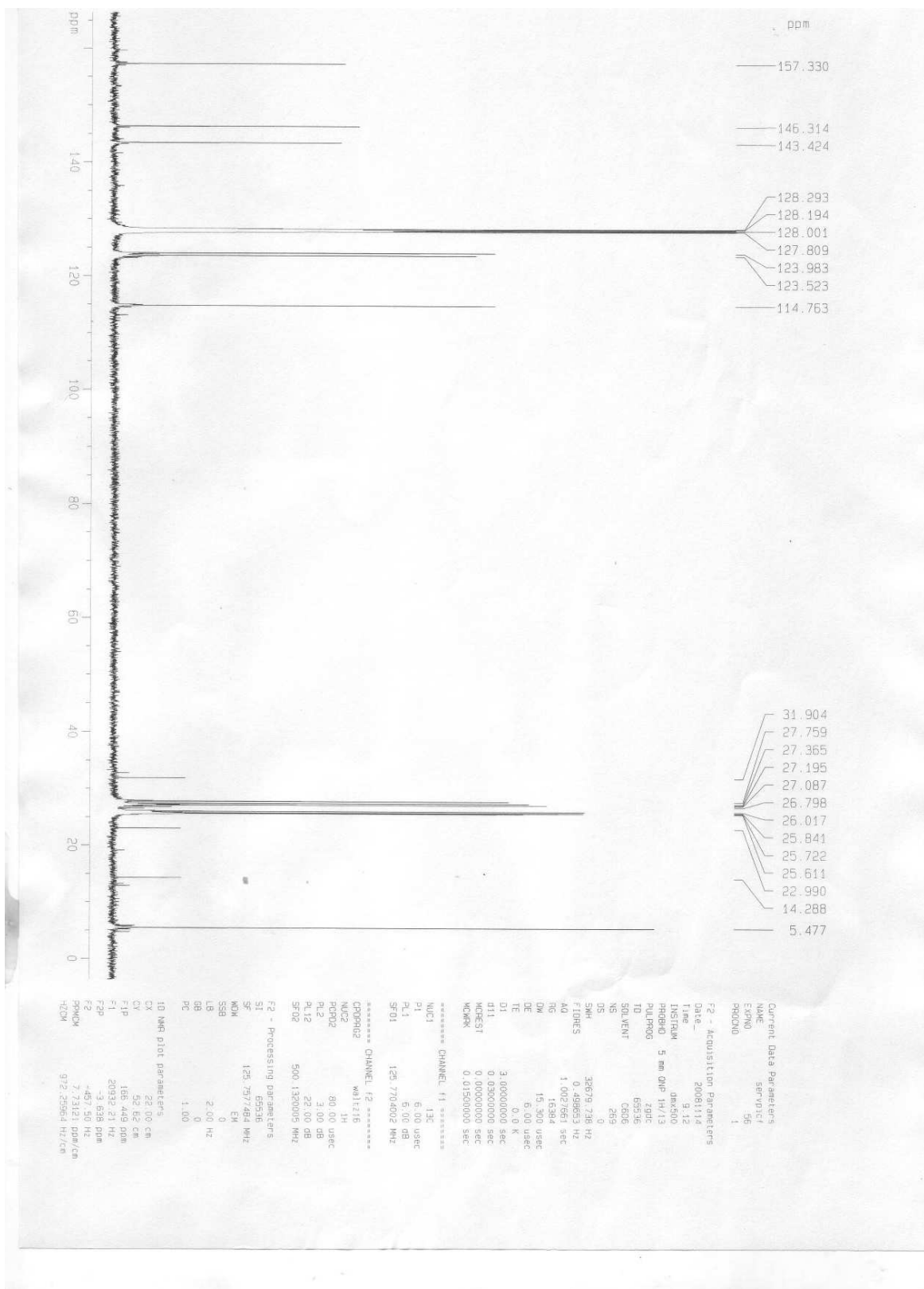
3. ^{13}C NMR spectrum of complex 2



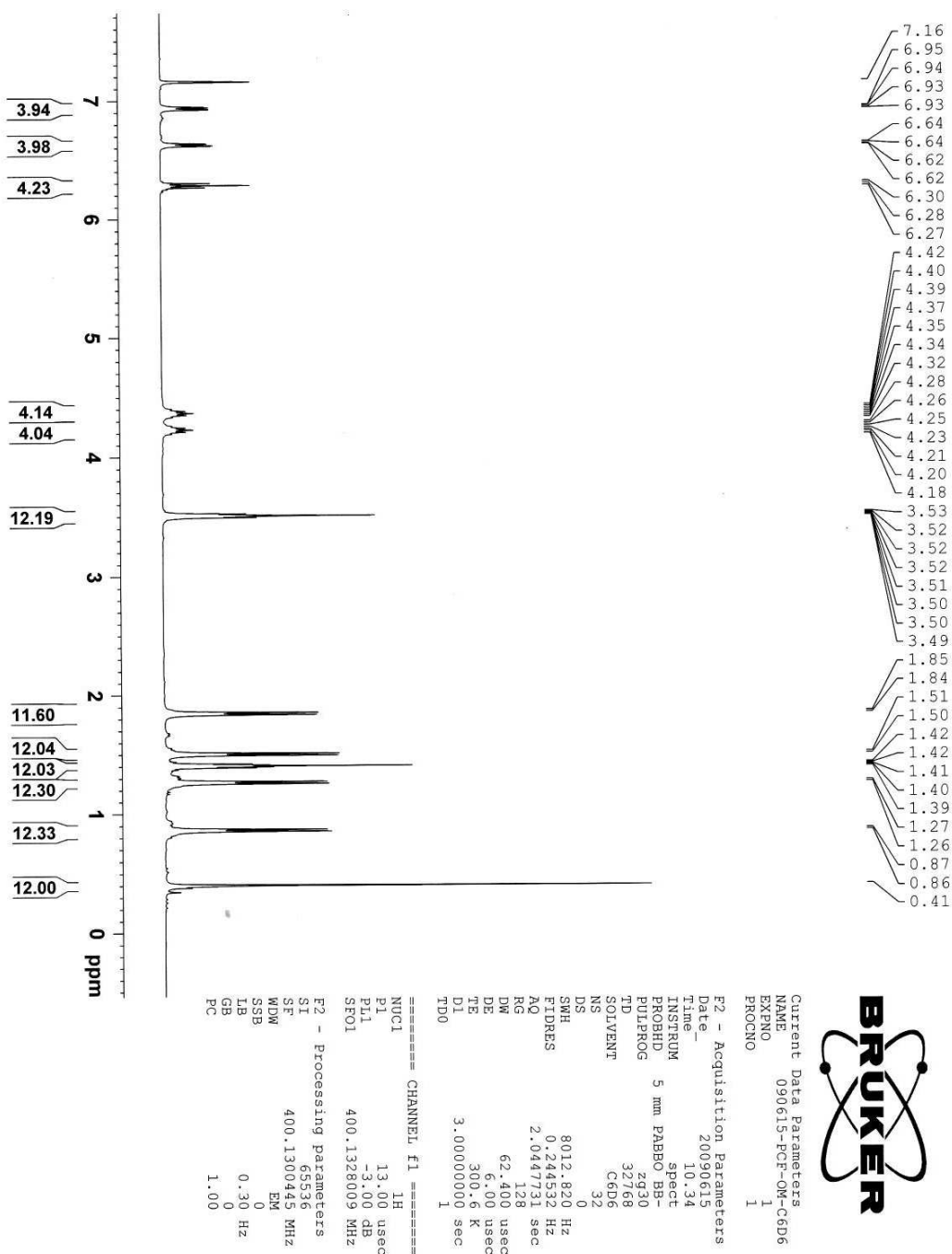
4. ^1H NMR spectrum of complex **3**



5. ^{13}C NMR spectrum of complex **3**



6. ^1H NMR spectrum of complex 4



7. ^{13}C NMR spectrum of complex 4

