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Electronic Supporting Information

for

Group 13 metal complexes containing the bis-(4-methylbenzoxazol-2-yl)-methanide ligand.

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1. Isolation and characterisation of side product 1a

Isolation of 1a:

Analogue procedure like stated in method 1 for **1**, but in a bigger scale.

2-Amino-3-methylphenol (11.28 g, 91.2 mmol, 2.00 eq.) and ethylbisimidate dihydrochloride (10.54 g, 45.6 mmol, 1.00 eq.) were dissolved in methanol (170 mL). Subsequently the reaction mixture was heated to reflux for 5 h and after cooling to rt stored at −32 °C in a refrigerator. The resulting crystalline material was filtered off, washed with saturated aqueous $NaHCO_3$ solution (3 x 50 mL) and water (6 x 50 mL) and dried under reduced pressure. 4.05 g of the crude impure product were isolated and 500 mg of this were purified via column chromatography (silica, PE/EtOAc = 5:1, 1st fraction, R_f = 0.26) to obtain compound **1** as brown powder (406 mg, 1.46 mmol, 26 % based on the applied amount of crude product). The 2nd fraction in the column chromatographic separation was isolated by using pure EtOAc as eluent since the 1st fraction was completely collected. This side product could be identified as **1a** (88 mg, 0.46 mmol, 8 %), which is a representative for the not completely proceeded cyclisation reaction. Crystals of **1a** suitable for X-ray diffraction experiments could be obtained upon recrystallisation from toluene.

Characterisation of 1a:

Anal. Calcd. for $C_{10}H_{10}N_2O_2$ (190.20 g/mol): C, 63.15; H, 5.30; N, 14.73. Found: C, 63.28; H, 5.45; N, 14.40; δ^1H (300 MHz, thf-d_8): 7.32 (d, $^3J_{HH}$ = 7.7 Hz, 1 H, H3), 7.17 (t, $^3J_{HH}$ = 7.8 Hz, 1 H, H4), 7.08 (d, $^3J_{HH}$ = 7.5 Hz, 1 H, H5), 7.10 – 6.90 (s_{br}, 1 H, NH_2), 6.70 – 6.45 (s_{br}, 1 H, NH_2), 3.80 (s, 2 H, H1'), 2.54 (s, 3 H, H9); δ^{13}C{^{1}H} (75 MHz, thf-d_8): 167.60 (s, 1 C, C8), 162.07 (s, 1 C, C1), 151.85 (s, 1 C, C2), 141.77 (s, 1 C, C7), 130.88 (s, 1 C, C6), 125.37 (s, 1 C, C4), 125.18 (s, 1 C, C5), 108.42 (s, 1 C, C3), 36.89 (s, 1 C, C1'), 16.41 (s, 1 C, C9); δ^{15}N{^{1}H} (75 MHz, thf-d_8): −279.92 (s, N2), −136.33 (s, N1); EI-MS, *m*/*z* (%):190 (35) $[M]^+$, 147 (100) $[M – C(O)NH_2]^+$.

2. Crystallographic details for 1a

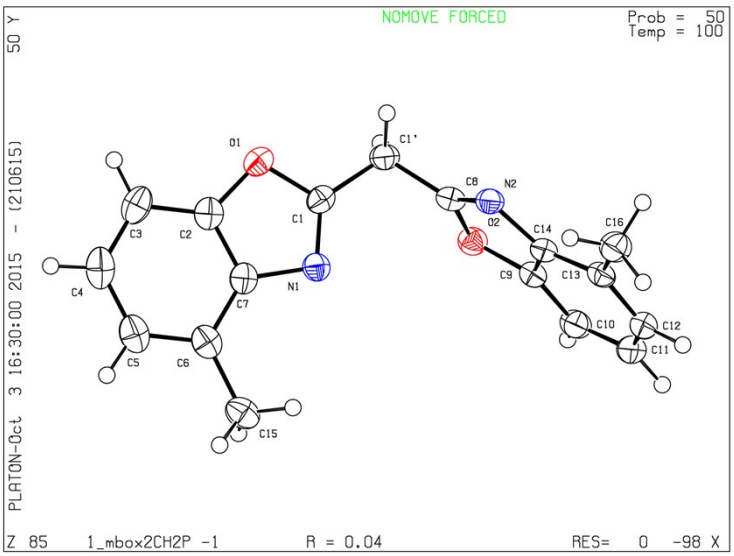
Table 1. Crystal structure data for **1a** at 100 K.

	1a
Formula	$C_{10}H_{10}N_2O_2$
Mol. w., g mol^{-1}	190.20
CCDC no.	1429356
Wavelength, Å	0.71073
Crystal system	triclinic
Space group	$P\bar{1}$
a, Å	7.790(2)
b, Å	7.974(2)
c, Å	8.279(3)
α, deg	93.24(2)
β, deg	115.09(3)
γ, deg	99.95(2)
V, Å^3	453.9(3)
Z	2
Refl. measured	7223
Refl. unique	1691
*R*1 [I>2*σ*(I)][a]	0.0496
w*R*2 (all refl.)[b]	0.1345
R_{int}	0.0406
$\Delta\rho_{fin}$, e Å^{-3}	0.408 / −0.228

[a] $R1 = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|}$ [b] $wR2 = \sqrt{\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}}$; $w = \frac{1}{\sigma^2(F_o^2) + (g_1P)^2 + g_2P}$; $P = \frac{(F_o^2 + 2F_c^2)}{3}$.

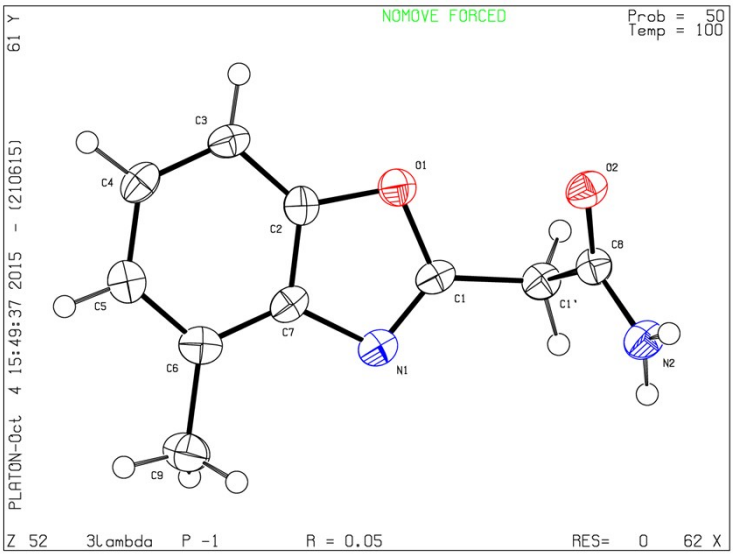
3. Bond lengths (Å) and angles (deg) for 1 - 7

3.1 Crystallographic parameters for 1



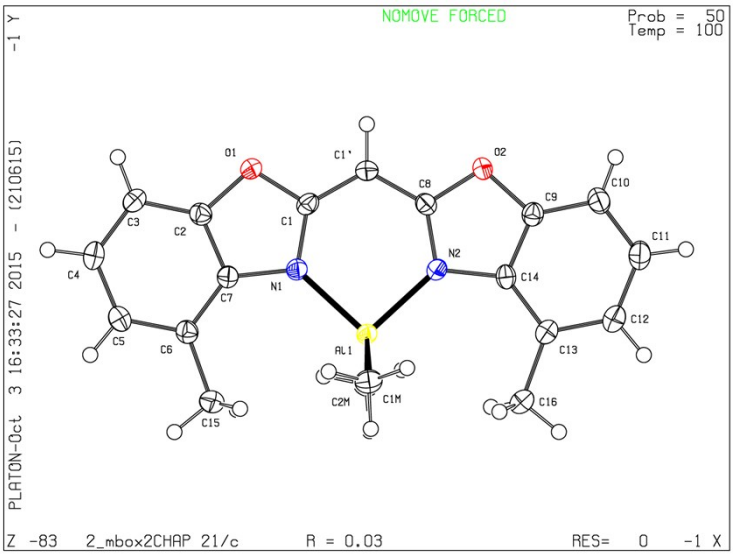
C(1')-C(8)	1.484(2)	C(3)-C(2)-C(7)	124.20(15)
C(1')-C(1)	1.489(2)	C(3)-C(2)-O(1)	128.21(14)
C(1)-N(1)	1.2896(19)	C(7)-C(2)-O(1)	107.58(12)
C(1)-O(1)	1.3740(17)	C(2)-C(3)-C(4)	114.72(15)
O(1)-C(2)	1.3859(18)	C(5)-C(4)-C(3)	121.87(15)
C(2)-C(3)	1.379(2)	C(6)-C(5)-C(4)	122.99(15)
C(2)-C(7)	1.383(2)	C(5)-C(6)-C(7)	115.10(15)
C(3)-C(4)	1.392(2)	C(5)-C(6)-C(15)	122.73(14)
C(4)-C(5)	1.390(2)	C(7)-C(6)-C(15)	122.16(13)
C(5)-C(6)	1.390(2)	C(2)-C(7)-C(6)	121.10(13)
C(6)-C(7)	1.398(2)	C(2)-C(7)-N(1)	108.80(13)
C(6)-C(15)	1.498(2)	C(6)-C(7)-N(1)	130.07(14)
C(7)-N(1)	1.4119(18)	C(1)-N(1)-C(7)	104.04(12)
C(8)-N(2)	1.2924(18)	N(2)-C(8)-O(2)	115.73(12)
C(8)-O(2)	1.3709(17)	N(2)-C(8)-C(1')	126.95(13)
O(2)-C(9)	1.3858(17)	O(2)-C(8)-C(1')	117.30(12)
C(9)-C(10)	1.381(2)	C(8)-O(2)-C(9)	103.66(11)
C(9)-C(14)	1.383(2)	C(10)-C(9)-C(14)	124.23(14)
C(10)-C(11)	1.384(2)	C(10)-C(9)-O(2)	128.10(13)
C(11)-C(12)	1.397(2)	C(14)-C(9)-O(2)	107.67(12)
C(12)-C(13)	1.388(2)	C(9)-C(10)-C(11)	114.65(14)
C(13)-C(14)	1.402(2)	C(10)-C(11)-C(12)	122.17(15)
C(13)-C(16)	1.499(2)	C(13)-C(12)-C(11)	122.76(14)
C(14)-N(2)	1.4049(18)	C(12)-C(13)-C(14)	115.03(14)
		C(12)-C(13)-C(16)	123.11(14)
C(8)-C(1')-C(1)	110.79(12)	C(14)-C(13)-C(16)	121.86(14)
N(1)-C(1)-O(1)	115.82(12)	C(9)-C(14)-C(13)	121.12(13)
N(1)-C(1)-C(1')	128.23(13)	C(9)-C(14)-N(2)	108.77(12)
O(1)-C(1)-C(1')	115.93(12)	C(13)-C(14)-N(2)	130.10(13)
C(1)-O(1)-C(2)	103.76(11)	C(8)-N(2)-C(14)	104.17(12)

3.2 Crystallographic parameters for 1a



C(1')-C(1)	1.498(3)	O(1)-C(1)-C(1')	116.18(18)
C(1')-C(8)	1.533(3)	C(1)-O(1)-C(2)	103.54(16)
C(1)-N(1)	1.279(3)	C(3)-C(2)-C(7)	124.1(2)
C(1)-O(1)	1.373(2)	C(3)-C(2)-O(1)	128.78(19)
O(1)-C(2)	1.390(3)	C(7)-C(2)-O(1)	107.13(18)
C(2)-C(3)	1.385(3)	C(4)-C(3)-C(2)	114.7(2)
C(2)-C(7)	1.386(3)	C(3)-C(4)-C(5)	121.9(2)
C(3)-C(4)	1.385(3)	C(6)-C(5)-C(4)	122.7(2)
C(4)-C(5)	1.399(3)	C(5)-C(6)-C(7)	115.6(2)
C(5)-C(6)	1.386(3)	C(5)-C(6)-C(9)	122.4(2)
C(6)-C(7)	1.390(3)	C(7)-C(6)-C(9)	122.0(2)
C(6)-C(9)	1.504(3)	C(2)-C(7)-C(6)	121.0(2)
C(7)-N(1)	1.411(3)	C(2)-C(7)-N(1)	108.98(19)
C(8)-O(2)	1.237(3)	C(6)-C(7)-N(1)	129.99(19)
C(8)-N(2)	1.316(3)	C(1)-N(1)-C(7)	103.92(17)
N(2)-H(1N)	0.90(3)	O(2)-C(8)-N(2)	123.7(2)
N(2)-H(2N)	0.93(3)	O(2)-C(8)-C(1')	120.16(19)
		N(2)-C(8)-C(1')	116.16(18)
C(1)-C(1')-C(8)	109.21(17)	H(1N)-N(2)-H(2N)	124(2)
N(1)-C(1)-O(1)	116.43(19)	H(1N)-N(2)-C(8)	119.9(17)
N(1)-C(1)-C(1')	127.30(19)	H(2N)-N(2)-C(8)	115.5(16)

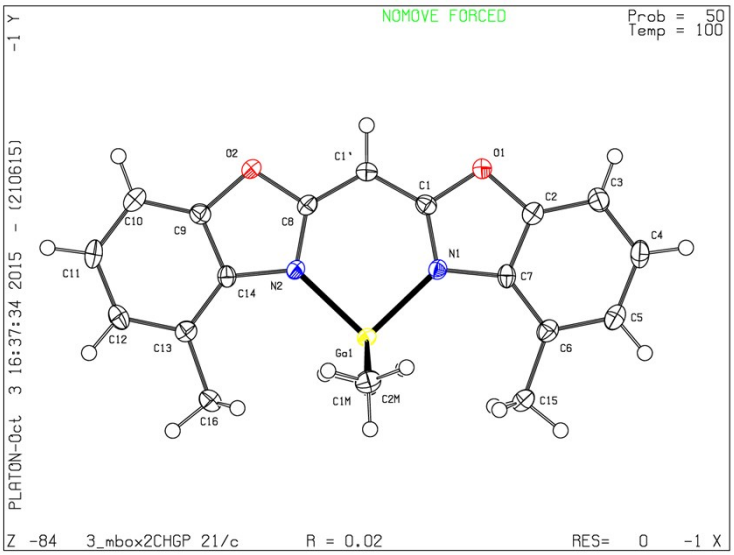
3.3 Crystallographic parameters for 2



Al(1)-N(2)	1.9395(14)	H(1')-C(1')-C(1)	119.4
Al(1)-N(1)	1.9405(14)	H(1')-C(1')-C(8)	119.4
Al(1)-C(1M)	1.9601(19)	C(1)-C(1')-C(8)	121.13(14)
Al(1)-C(2M)	1.970(2)	N(1)-C(1)-O(1)	112.45(14)
C(1')-H(1')	0.9500	N(1)-C(1)-C(1')	128.88(15)
C(1')-C(1)	1.383(2)	O(1)-C(1)-C(1')	118.67(14)
C(1')-C(8)	1.384(2)	C(3)-C(2)-O(1)	126.51(14)
C(1)-N(1)	1.350(2)	C(3)-C(2)-C(7)	124.77(15)
C(1)-O(1)	1.3578(19)	O(1)-C(2)-C(7)	108.71(13)
C(2)-C(3)	1.380(2)	C(2)-C(3)-C(4)	114.99(15)
C(2)-O(1)	1.3821(19)	C(5)-C(4)-C(3)	121.15(15)
C(2)-C(7)	1.390(2)	C(4)-C(5)-C(6)	123.28(16)
C(3)-C(4)	1.395(2)	C(7)-C(6)-C(5)	115.52(15)
C(4)-C(5)	1.392(2)	C(7)-C(6)-C(15)	124.02(14)
C(5)-C(6)	1.398(2)	C(5)-C(6)-C(15)	120.46(15)
C(6)-C(7)	1.395(2)	C(2)-C(7)-C(6)	120.28(14)
C(6)-C(15)	1.509(2)	C(2)-C(7)-N(1)	107.13(14)
C(7)-N(1)	1.418(2)	C(6)-C(7)-N(1)	132.58(14)
C(8)-N(2)	1.351(2)	C(1)-O(1)-C(2)	106.13(12)
C(8)-O(2)	1.3624(19)	C(1)-N(1)-C(7)	105.57(13)
C(9)-C(10)	1.376(2)	C(1)-N(1)-Al(1)	123.23(12)
C(9)-O(2)	1.381(2)	C(7)-N(1)-Al(1)	131.18(11)
C(9)-C(14)	1.387(2)	N(2)-C(8)-O(2)	112.59(13)
C(10)-C(11)	1.389(2)	N(2)-C(8)-C(1')	128.91(14)
C(11)-C(12)	1.396(3)	O(2)-C(8)-C(1')	118.50(13)
C(12)-C(13)	1.401(2)	C(10)-C(9)-O(2)	126.27(15)
C(13)-C(14)	1.398(2)	C(10)-C(9)-C(14)	124.73(15)
C(13)-C(16)	1.510(2)	O(2)-C(9)-C(14)	108.98(13)
C(14)-N(2)	1.416(2)	C(9)-C(10)-C(11)	115.33(16)
		C(10)-C(11)-C(12)	121.26(16)
N(2)-Al(1)-N(1)	94.68(6)	C(11)-C(12)-C(13)	122.81(16)
N(2)-Al(1)-C(1M)	109.08(8)	C(14)-C(13)-C(12)	115.63(16)
N(1)-Al(1)-C(1M)	110.68(7)	C(14)-C(13)-C(16)	123.76(15)
N(2)-Al(1)-C(2M)	110.85(8)	C(12)-C(13)-C(16)	120.61(15)
N(1)-Al(1)-C(2M)	109.53(8)	C(9)-C(14)-C(13)	120.22(14)
C(1M)-Al(1)-C(2M)	119.26(7)	C(9)-C(14)-N(2)	107.27(13)

C(13)-C(14)-N(2)	132.51(14)	C(8)-N(2)-Al(1)	123.17(10)
C(8)-O(2)-C(9)	105.72(12)	C(14)-N(2)-Al(1)	131.37(10)
C(8)-N(2)-C(14)	105.43(12)		

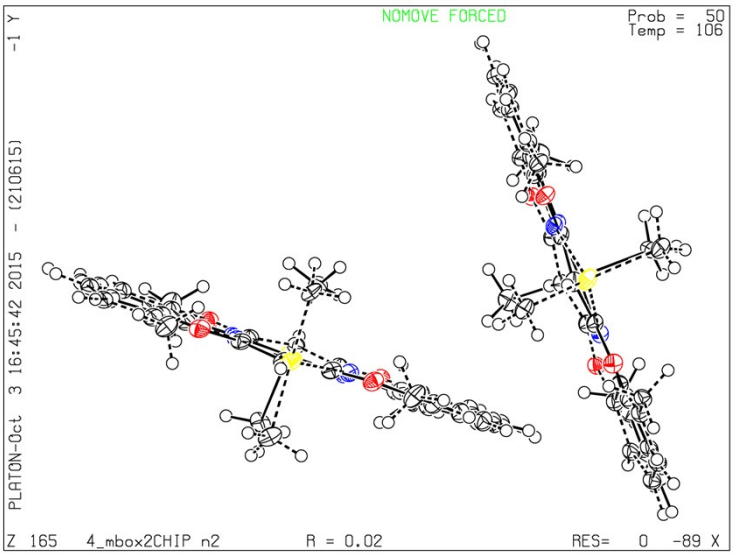
3.4 Crystallographic parameters for 3



C(1')-H(1')	0.9500	C(1)-O(1)-C(2)	105.86(14)
C(1')-C(1)	1.387(3)	C(3)-C(2)-O(1)	126.90(18)
C(1')-C(8)	1.389(3)	C(3)-C(2)-C(7)	124.46(18)
C(1)-N(1)	1.340(2)	O(1)-C(2)-C(7)	108.63(16)
C(1)-O(1)	1.360(2)	C(2)-C(3)-C(4)	115.62(19)
O(1)-C(2)	1.383(2)	C(5)-C(4)-C(3)	121.08(19)
C(2)-C(3)	1.371(3)	C(4)-C(5)-C(6)	122.93(19)
C(2)-C(7)	1.387(3)	C(7)-C(6)-C(5)	115.54(18)
C(3)-C(4)	1.392(3)	C(7)-C(6)-C(15)	123.74(18)
C(4)-C(5)	1.389(3)	C(5)-C(6)-C(15)	120.72(18)
C(5)-C(6)	1.402(3)	C(2)-C(7)-C(6)	120.36(18)
C(6)-C(7)	1.395(3)	C(2)-C(7)-N(1)	107.16(16)
C(6)-C(15)	1.505(3)	C(6)-C(7)-N(1)	132.48(18)
C(7)-N(1)	1.414(2)	C(1)-N(1)-C(7)	105.80(15)
N(1)-Ga(1)	2.0055(15)	C(1)-N(1)-Ga(1)	123.53(12)
Ga(1)-C(2M)	1.963(2)	C(7)-N(1)-Ga(1)	130.64(13)
Ga(1)-C(1M)	1.966(2)	C(2M)-Ga(1)-C(1M)	123.95(9)
Ga(1)-N(2)	2.0030(15)	C(2M)-Ga(1)-N(2)	109.42(8)
C(8)-N(2)	1.342(2)	C(1M)-Ga(1)-N(2)	108.57(8)
C(8)-O(2)	1.361(2)	C(2M)-Ga(1)-N(1)	108.37(8)
O(2)-C(9)	1.391(2)	C(1M)-Ga(1)-N(1)	109.32(7)
C(9)-C(10)	1.371(3)	N(2)-Ga(1)-N(1)	92.73(6)
C(9)-C(14)	1.386(3)	N(2)-C(8)-O(2)	112.58(16)
C(10)-C(11)	1.390(3)	N(2)-C(8)-C(1')	129.58(18)
C(11)-C(12)	1.392(3)	O(2)-C(8)-C(1')	117.83(16)
C(12)-C(13)	1.401(3)	C(8)-O(2)-C(9)	105.83(14)
C(13)-C(14)	1.397(3)	C(10)-C(9)-C(14)	125.19(18)
C(13)-C(16)	1.499(3)	C(10)-C(9)-O(2)	126.52(17)
C(14)-N(2)	1.413(2)	C(14)-C(9)-O(2)	108.28(16)
		C(9)-C(10)-C(11)	114.98(19)
H(1')-C(1')-C(1)	119.2	C(10)-C(11)-C(12)	121.07(18)
H(1')-C(1')-C(8)	119.2	C(11)-C(12)-C(13)	123.54(19)
C(1)-C(1')-C(8)	121.62(18)	C(14)-C(13)-C(12)	114.87(18)
N(1)-C(1)-O(1)	112.55(16)	C(14)-C(13)-C(16)	124.16(18)
N(1)-C(1)-C(1')	129.28(17)	C(12)-C(13)-C(16)	120.97(18)
O(1)-C(1)-C(1')	118.17(17)	C(9)-C(14)-C(13)	120.35(18)

C(9)-C(14)-N(2)	107.53(16)	C(8)-N(2)-Ga(1)	123.25(13)
C(13)-C(14)-N(2)	132.12(18)	C(14)-N(2)-Ga(1)	130.96(13)
C(8)-N(2)-C(14)	105.77(15)		

3.5 Crystallographic parameters for 4



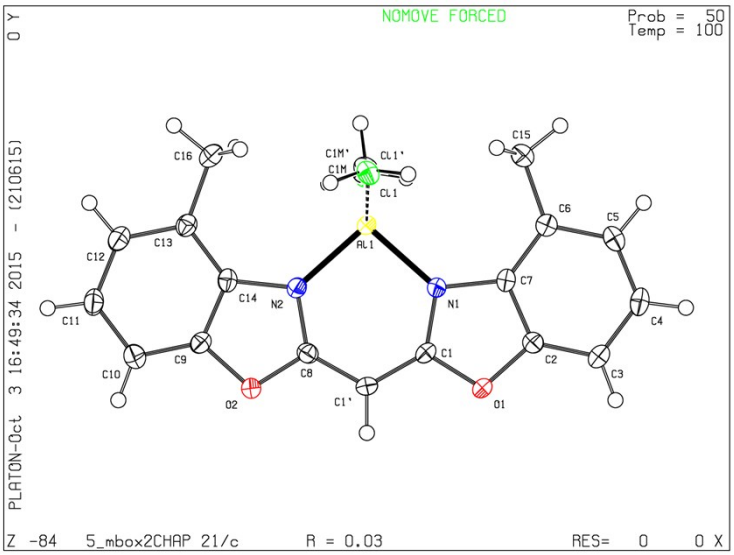
C(1')-C(1)	1.375(13)	C(4A)-C(5A)	1.349(12)
C(1')-C(8)	1.396(12)	C(5A)-C(6A)	1.405(12)
C(1)-N(1)	1.338(11)	C(6A)-C(7A)	1.396(12)
C(1)-O(1)	1.386(11)	C(6A)-C(15A)	1.503(13)
O(1)-C(2)	1.356(12)	C(7A)-N(1A)	1.425(11)
C(2)-C(7)	1.386(12)	N(1A)-In(1A)	2.215(9)
C(2)-C(3)	1.388(12)	In(1A)-C(1MA)	2.147(9)
C(3)-C(4)	1.398(12)	In(1A)-C(2MA)	2.161(11)
C(4)-C(5)	1.367(11)	In(1A)-N(2A)	2.225(9)
C(5)-C(6)	1.386(12)	C(8A)-N(2A)	1.333(12)
C(6)-C(7)	1.382(12)	C(8A)-O(2A)	1.392(12)
C(6)-C(15)	1.495(12)	O(2A)-C(9A)	1.365(12)
C(7)-N(1)	1.409(11)	C(9A)-C(14A)	1.383(13)
N(1)-In(1)	2.211(9)	C(9A)-C(10A)	1.395(12)
In(1)-C(2M)	2.152(10)	C(10A)-C(11A)	1.375(12)
In(1)-C(1M)	2.154(10)	C(11A)-C(12A)	1.399(12)
In(1)-N(2)	2.215(9)	C(12A)-C(13A)	1.391(12)
C(8)-N(2)	1.338(11)	C(13A)-C(14A)	1.380(12)
C(8)-O(2)	1.367(12)	C(13A)-C(16A)	1.522(13)
O(2)-C(9)	1.391(11)	C(14A)-N(2A)	1.405(11)
C(9)-C(14)	1.379(12)	C(1'B)-C(1B)	1.3668
C(9)-C(10)	1.380(12)	C(1'B)-C(8B)	1.3944
C(10)-C(11)	1.382(12)	C(1B)-N(1B)	1.3396
C(11)-C(12)	1.388(11)	C(1B)-O(1B)	1.3825
C(12)-C(13)	1.414(12)	O(1B)-C(2B)	1.3471
C(13)-C(14)	1.402(11)	C(2B)-C(7B)	1.3922
C(13)-C(16)	1.516(13)	C(2B)-C(3B)	1.3959
C(14)-N(2)	1.412(11)	C(3B)-C(4B)	1.3834
C(1'A)-C(1A)	1.370(13)	C(4B)-C(5B)	1.3745
C(1'A)-C(8A)	1.417(13)	C(5B)-C(6B)	1.3940
C(1A)-N(1A)	1.337(12)	C(6B)-C(7B)	1.3774
C(1A)-O(1A)	1.360(12)	C(6B)-C(15B)	1.4905
O(1A)-C(2A)	1.389(12)	C(7B)-N(1B)	1.3981
C(2A)-C(3A)	1.391(12)	N(1B)-In(1B)	2.2131
C(2A)-C(7A)	1.395(12)	In(1B)-C(1MB)	2.1540
C(3A)-C(4A)	1.396(11)	In(1B)-C(2MB)	2.1545

In(1B)-N(2B)	2.2144
C(8B)-N(2B)	1.3441
C(8B)-O(2B)	1.3643
O(2B)-C(9B)	1.3940
C(9B)-C(14B)	1.3666
C(9B)-C(10B)	1.3811
C(10B)-C(11B)	1.3943
C(11B)-C(12B)	1.3867
C(12B)-C(13B)	1.4166
C(13B)-C(14B)	1.4016
C(13B)-C(16B)	1.5259
C(14B)-N(2B)	1.4225
C(1'C)-C(1C)	1.3669
C(1'C)-C(8C)	1.3944
C(1C)-N(1C)	1.3396
C(1C)-O(1C)	1.3825
O(1C)-C(2C)	1.3472
C(2C)-C(7C)	1.3922
C(2C)-C(3C)	1.3958
C(3C)-C(4C)	1.3835
C(4C)-C(5C)	1.3744
C(5C)-C(6C)	1.3940
C(6C)-C(7C)	1.3774
C(6C)-C(15C)	1.4904
C(7C)-N(1C)	1.3981
N(1C)-In(1C)	2.2131
In(1C)-C(1MC)	2.1540
In(1C)-C(2MC)	2.1545
In(1C)-N(2C)	2.2144
C(8C)-N(2C)	1.3441
C(8C)-O(2C)	1.3643
O(2C)-C(9C)	1.3940
C(9C)-C(14C)	1.3666
C(9C)-C(10C)	1.3810
C(10C)-C(11C)	1.3943
C(11C)-C(12C)	1.3867
C(12C)-C(13C)	1.4166
C(13C)-C(14C)	1.4015
C(13C)-C(16C)	1.5259
C(14C)-N(2C)	1.4225

C(1)-C(1')-C(8)	123.3(5)
N(1)-C(1)-C(1')	131.0(9)
N(1)-C(1)-O(1)	112.0(9)
C(1')-C(1)-O(1)	116.8(10)
C(2)-O(1)-C(1)	105.0(9)
O(1)-C(2)-C(7)	110.4(9)
O(1)-C(2)-C(3)	127.3(10)
C(7)-C(2)-C(3)	122.3(10)
C(2)-C(3)-C(4)	113.3(10)
C(5)-C(4)-C(3)	124.8(10)
C(4)-C(5)-C(6)	121.1(10)
C(7)-C(6)-C(5)	115.3(9)
C(7)-C(6)-C(15)	124.5(10)
C(5)-C(6)-C(15)	120.3(11)
C(6)-C(7)-C(2)	123.1(9)
C(6)-C(7)-N(1)	130.5(10)
C(2)-C(7)-N(1)	106.4(8)
C(1)-N(1)-C(7)	106.2(8)
C(1)-N(1)-In(1)	123.5(7)
C(7)-N(1)-In(1)	130.0(7)
C(2M)-In(1)-C(1M)	130.10(19)
C(2M)-In(1)-N(1)	108.9(5)
C(1M)-In(1)-N(1)	108.3(5)
C(2M)-In(1)-N(2)	107.0(5)
C(1M)-In(1)-N(2)	107.1(5)
N(1)-In(1)-N(2)	86.77(13)
N(2)-C(8)-O(2)	112.2(9)
N(2)-C(8)-C(1')	130.5(10)
O(2)-C(8)-C(1')	117.1(10)
C(8)-O(2)-C(9)	106.2(9)
C(14)-C(9)-C(10)	125.9(10)
C(14)-C(9)-O(2)	107.7(8)
C(10)-C(9)-O(2)	126.4(10)
C(9)-C(10)-C(11)	116.6(10)
C(10)-C(11)-C(12)	119.1(9)
C(11)-C(12)-C(13)	124.2(10)
C(14)-C(13)-C(12)	115.9(10)
C(14)-C(13)-C(16)	121.0(10)
C(12)-C(13)-C(16)	123.1(10)
C(9)-C(14)-C(13)	118.2(9)
C(9)-C(14)-N(2)	108.2(8)
C(13)-C(14)-N(2)	133.5(10)
C(8)-N(2)-C(14)	105.7(8)
C(8)-N(2)-In(1)	123.7(7)
C(14)-N(2)-In(1)	130.6(7)
C(1A)-C(1'A)-C(8A)	123.8(6)
N(1A)-C(1A)-O(1A)	113.4(10)
N(1A)-C(1A)-C(1'A)	129.4(10)
O(1A)-C(1A)-C(1'A)	117.2(10)
C(1A)-O(1A)-C(2A)	106.3(10)
O(1A)-C(2A)-C(3A)	131.4(11)
O(1A)-C(2A)-C(7A)	107.3(9)
C(3A)-C(2A)-C(7A)	121.3(10)
C(2A)-C(3A)-C(4A)	116.9(10)
C(5A)-C(4A)-C(3A)	121.8(9)
C(4A)-C(5A)-C(6A)	122.2(10)
C(7A)-C(6A)-C(5A)	116.4(10)
C(7A)-C(6A)-C(15A)	123.8(10)
C(5A)-C(6A)-C(15A)	119.4(11)
C(2A)-C(7A)-C(6A)	120.9(9)
C(2A)-C(7A)-N(1A)	108.2(9)
C(6A)-C(7A)-N(1A)	130.9(10)
C(1A)-N(1A)-C(7A)	104.7(9)
C(1A)-N(1A)-In(1A)	124.9(7)
C(7A)-N(1A)-In(1A)	130.2(8)
C(1MA)-In(1A)-C(2MA)	126.85(18)
C(1MA)-In(1A)-N(1A)	108.1(5)
C(2MA)-In(1A)-N(1A)	109.8(5)
C(1MA)-In(1A)-N(2A)	112.3(5)
C(2MA)-In(1A)-N(2A)	105.6(5)
N(1A)-In(1A)-N(2A)	87.01(14)
N(2A)-C(8A)-O(2A)	111.5(9)
N(2A)-C(8A)-C(1'A)	131.5(10)
O(2A)-C(8A)-C(1'A)	116.9(10)
C(9A)-O(2A)-C(8A)	104.8(10)
O(2A)-C(9A)-C(14A)	110.2(9)
O(2A)-C(9A)-C(10A)	123.4(11)

C(14A)-C(9A)-C(10A)	126.4(10)	C(9B)-C(14B)-C(13B)	119.3
C(11A)-C(10A)-C(9A)	112.9(9)	C(9B)-C(14B)-N(2B)	108.5
C(10A)-C(11A)-C(12A)	121.4(9)	C(13B)-C(14B)-N(2B)	132.2
C(13A)-C(12A)-C(11A)	124.2(10)	C(8B)-N(2B)-C(14B)	105.7
C(14A)-C(13A)-C(12A)	114.7(10)	C(8B)-N(2B)-In(1B)	123.0
C(14A)-C(13A)-C(16A)	120.3(10)	C(14B)-N(2B)-In(1B)	131.1
C(12A)-C(13A)-C(16A)	124.6(11)	C(1C)-C(1'C)-C(8C)	123.9
C(13A)-C(14A)-C(9A)	119.9(9)	N(1C)-C(1C)-C(1'C)	130.4
C(13A)-C(14A)-N(2A)	133.7(10)	N(1C)-C(1C)-O(1C)	112.7
C(9A)-C(14A)-N(2A)	106.4(9)	C(1'C)-C(1C)-O(1C)	116.5
C(8A)-N(2A)-C(14A)	107.0(9)	C(2C)-O(1C)-C(1C)	104.1
C(8A)-N(2A)-In(1A)	122.0(8)	O(1C)-C(2C)-C(7C)	111.2
C(14A)-N(2A)-In(1A)	131.1(8)	O(1C)-C(2C)-C(3C)	127.1
C(1B)-C(1'B)-C(8B)	123.9	C(7C)-C(2C)-C(3C)	121.6
N(1B)-C(1B)-C(1'B)	130.4	C(4C)-C(3C)-C(2C)	114.6
N(1B)-C(1B)-O(1B)	112.7	C(5C)-C(4C)-C(3C)	124.1
C(1'B)-C(1B)-O(1B)	116.5	C(4C)-C(5C)-C(6C)	121.1
C(2B)-O(1B)-C(1B)	104.1	C(7C)-C(6C)-C(5C)	115.6
O(1B)-C(2B)-C(7B)	111.2	C(7C)-C(6C)-C(15C)	125.9
O(1B)-C(2B)-C(3B)	127.1	C(5C)-C(6C)-C(15C)	118.4
C(7B)-C(2B)-C(3B)	121.6	C(6C)-C(7C)-C(2C)	122.9
C(4B)-C(3B)-C(2B)	114.6	C(6C)-C(7C)-N(1C)	131.2
C(5B)-C(4B)-C(3B)	124.1	C(2C)-C(7C)-N(1C)	106.0
C(4B)-C(5B)-C(6B)	121.1	C(1C)-N(1C)-C(7C)	106.0
C(7B)-C(6B)-C(5B)	115.6	C(1C)-N(1C)-In(1C)	124.1
C(7B)-C(6B)-C(15B)	125.9	C(7C)-N(1C)-In(1C)	129.8
C(5B)-C(6B)-C(15B)	118.4	C(1MC)-In(1C)-C(2MC)	130.2
C(6B)-C(7B)-C(2B)	122.9	C(1MC)-In(1C)-N(1C)	107.6
C(6B)-C(7B)-N(1B)	131.2	C(2MC)-In(1C)-N(1C)	109.0
C(2B)-C(7B)-N(1B)	106.0	C(1MC)-In(1C)-N(2C)	107.4
C(1B)-N(1B)-C(7B)	106.0	C(2MC)-In(1C)-N(2C)	107.2
C(1B)-N(1B)-In(1B)	124.1	N(1C)-In(1C)-N(2C)	86.8
C(7B)-N(1B)-In(1B)	129.8	N(2C)-C(8C)-O(2C)	111.2
C(1MB)-In(1B)-C(2MB)	130.2	N(2C)-C(8C)-C(1'C)	130.6
C(1MB)-In(1B)-N(1B)	107.6	O(2C)-C(8C)-C(1'C)	117.9
C(2MB)-In(1B)-N(1B)	109.0	C(8C)-O(2C)-C(9C)	107.2
C(1MB)-In(1B)-N(2B)	107.4	C(14C)-C(9C)-C(10C)	126.4
C(2MB)-In(1B)-N(2B)	107.2	C(14C)-C(9C)-O(2C)	107.4
N(1B)-In(1B)-N(2B)	86.8	C(10C)-C(9C)-O(2C)	126.1
N(2B)-C(8B)-O(2B)	111.2	C(9C)-C(10C)-C(11C)	115.3
N(2B)-C(8B)-C(1'B)	130.6	C(12C)-C(11C)-C(10C)	119.5
O(2B)-C(8B)-C(1'B)	117.9	C(11C)-C(12C)-C(13C)	124.5
C(8B)-O(2B)-C(9B)	107.2	C(14C)-C(13C)-C(12C)	114.8
C(14B)-C(9B)-C(10B)	126.4	C(14C)-C(13C)-C(16C)	120.4
C(14B)-C(9B)-O(2B)	107.4	C(12C)-C(13C)-C(16C)	124.7
C(10B)-C(9B)-O(2B)	126.1	C(9C)-C(14C)-C(13C)	119.3
C(9B)-C(10B)-C(11B)	115.3	C(9C)-C(14C)-N(2C)	108.5
C(12B)-C(11B)-C(10B)	119.5	C(13C)-C(14C)-N(2C)	132.2
C(11B)-C(12B)-C(13B)	124.5	C(8C)-N(2C)-C(14C)	105.7
C(14B)-C(13B)-C(12B)	114.8	C(8C)-N(2C)-In(1C)	123.0
C(14B)-C(13B)-C(16B)	120.4	C(14C)-N(2C)-In(1C)	131.1
C(12B)-C(13B)-C(16B)	124.7		

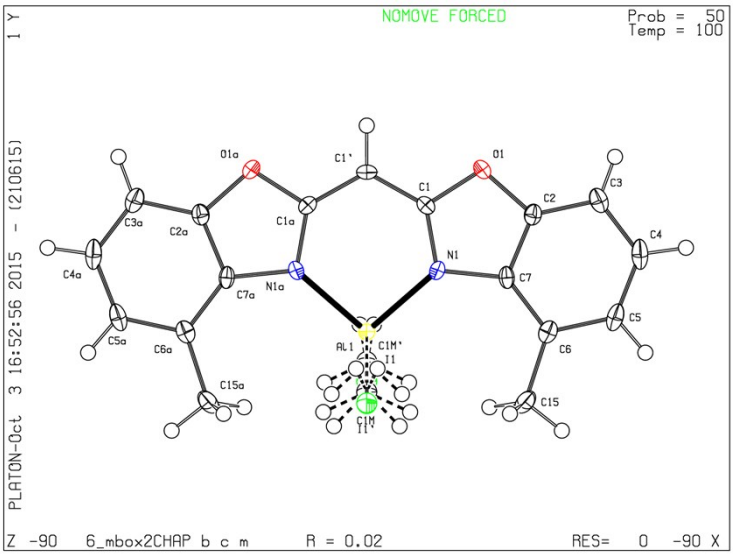
3.6 Crystallographic parameters for 5



C(1')-C(1)	1.379(2)	C(3)-C(2)-C(7)	125.26(16)
C(1')-C(8)	1.380(2)	C(3)-C(2)-O(1)	126.29(15)
C(1)-N(1)	1.349(2)	C(7)-C(2)-O(1)	108.44(14)
C(1)-O(1)	1.3560(19)	C(2)-C(3)-C(4)	114.85(16)
O(1)-C(2)	1.389(2)	C(5)-C(4)-C(3)	121.13(16)
C(2)-C(3)	1.372(2)	C(4)-C(5)-C(6)	123.49(17)
C(2)-C(7)	1.383(2)	C(7)-C(6)-C(5)	114.99(16)
C(3)-C(4)	1.390(3)	C(7)-C(6)-C(15)	124.61(15)
C(4)-C(5)	1.387(2)	C(5)-C(6)-C(15)	120.41(16)
C(5)-C(6)	1.402(2)	C(2)-C(7)-C(6)	120.27(15)
C(6)-C(7)	1.394(2)	C(2)-C(7)-N(1)	107.42(14)
C(6)-C(15)	1.499(2)	C(6)-C(7)-N(1)	132.31(15)
C(7)-N(1)	1.422(2)	C(1)-N(1)-C(7)	105.47(13)
N(1)-Al(1)	1.9107(14)	C(1)-N(1)-Al(1)	122.19(11)
Al(1)-N(2)	1.9086(14)	C(7)-N(1)-Al(1)	132.32(11)
Al(1)-C(1M)	1.984(11)	N(2)-Al(1)-N(1)	96.52(6)
Al(1)-C(1M')	1.986(11)	N(2)-Al(1)-C(1M)	112.4(4)
Al(1)-Cl(1)	2.092(4)	N(1)-Al(1)-C(1M)	112.1(4)
Al(1)-Cl(1')	2.096(4)	N(2)-Al(1)-C(1M')	111.4(4)
C(8)-N(2)	1.350(2)	N(1)-Al(1)-C(1M')	112.6(4)
C(8)-O(2)	1.3548(19)	N(2)-Al(1)-Cl(1)	108.91(13)
O(2)-C(9)	1.385(2)	N(1)-Al(1)-Cl(1)	108.93(13)
C(9)-C(10)	1.373(2)	C(1M)-Al(1)-Cl(1)	116.2(5)
C(9)-C(14)	1.381(2)	N(2)-Al(1)-Cl(1')	110.45(13)
C(10)-C(11)	1.387(2)	N(1)-Al(1)-Cl(1')	108.63(13)
C(11)-C(12)	1.389(3)	C(1M')-Al(1)-Cl(1')	115.6(5)
C(12)-C(13)	1.399(2)	N(2)-C(8)-O(2)	112.37(14)
C(13)-C(14)	1.399(2)	N(2)-C(8)-C(1')	128.65(15)
C(13)-C(16)	1.503(2)	O(2)-C(8)-C(1')	118.98(15)
C(14)-N(2)	1.419(2)	C(8)-O(2)-C(9)	106.09(12)
		C(10)-C(9)-C(14)	125.05(16)
C(1)-C(1')-C(8)	121.39(16)	C(10)-C(9)-O(2)	126.16(15)
N(1)-C(1)-O(1)	112.40(14)	C(14)-C(9)-O(2)	108.79(14)
N(1)-C(1)-C(1')	128.86(15)	C(9)-C(10)-C(11)	115.21(17)
O(1)-C(1)-C(1')	118.73(15)	C(10)-C(11)-C(12)	121.19(16)
C(1)-O(1)-C(2)	106.27(12)	C(11)-C(12)-C(13)	123.09(16)

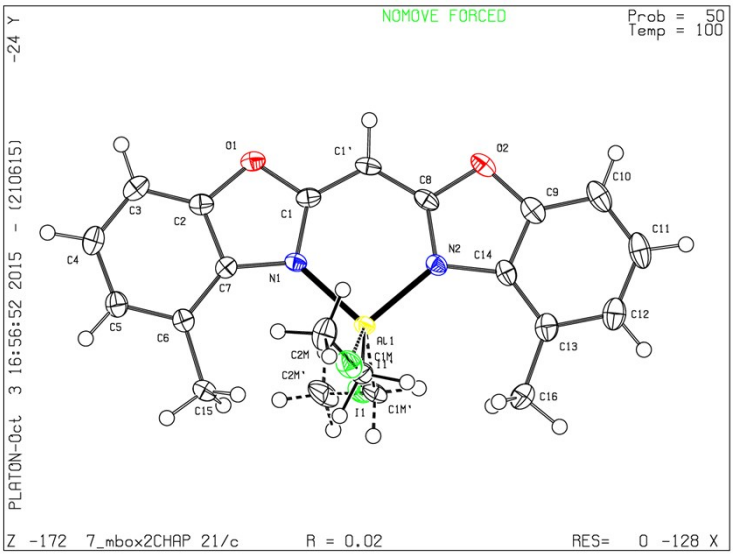
C(12)-C(13)-C(14)	115.45(16)	C(13)-C(14)-N(2)	132.77(16)
C(12)-C(13)-C(16)	120.80(15)	C(8)-N(2)-C(14)	105.53(13)
C(14)-C(13)-C(16)	123.75(15)	C(8)-N(2)-Al(1)	122.38(11)
C(9)-C(14)-C(13)	120.01(15)	C(14)-N(2)-Al(1)	132.09(11)
C(9)-C(14)-N(2)	107.23(14)		

3.7 Crystallographic parameters for 6



C(1')-C(1)#1	1.384(3)	C(3)-C(2)-C(7)	124.6(2)
C(1')-C(1)	1.384(3)	O(1)-C(2)-C(7)	109.09(18)
C(1)-N(1)	1.348(3)	C(2)-C(3)-C(4)	115.2(2)
C(1)-O(1)	1.361(3)	C(5)-C(4)-C(3)	121.4(2)
O(1)-C(2)	1.385(3)	C(4)-C(5)-C(6)	123.4(2)
C(2)-C(3)	1.377(3)	C(7)-C(6)-C(5)	115.0(2)
C(2)-C(7)	1.390(3)	C(7)-C(6)-C(15)	124.8(2)
C(3)-C(4)	1.386(4)	C(5)-C(6)-C(15)	120.1(2)
C(4)-C(5)	1.381(4)	C(2)-C(7)-C(6)	120.3(2)
C(5)-C(6)	1.406(3)	C(2)-C(7)-N(1)	106.75(19)
C(6)-C(7)	1.396(3)	C(6)-C(7)-N(1)	132.9(2)
C(6)-C(15)	1.502(3)	C(1)-N(1)-C(7)	105.73(18)
C(7)-N(1)	1.425(3)	C(1)-N(1)-Al(1)	121.18(15)
N(1)-Al(1)	1.909(2)	C(7)-N(1)-Al(1)	133.06(16)
Al(1)-N(1)#1	1.909(2)	N(1)-Al(1)-N(1)#1	97.84(12)
Al(1)-C(1M)	1.912(4)	N(1)-Al(1)-C(1M)	113.08(10)
Al(1)-C(1M')	1.957(18)	N(1)#1-Al(1)-C(1M)	113.08(10)
Al(1)-I(1')	2.256(8)	N(1)-Al(1)-C(1M')	104.0(11)
Al(1)-I(1)	2.5458(11)	N(1)#1-Al(1)-C(1M')	104.0(11)
		N(1)-Al(1)-I(1')	113.25(16)
C(1)#1-C(1')-C(1)	121.4(3)	N(1)#1-Al(1)-I(1')	113.25(16)
N(1)-C(1)-O(1)	112.58(19)	C(1M')-Al(1)-I(1')	121.4(17)
N(1)-C(1)-C(1')	129.2(2)	N(1)-Al(1)-I(1)	107.20(6)
O(1)-C(1)-C(1')	118.2(2)	N(1)#1-Al(1)-I(1)	107.20(6)
C(1)-O(1)-C(2)	105.85(17)	C(1M)-Al(1)-I(1)	116.63(14)
C(3)-C(2)-O(1)	126.3(2)		

3.8 Crystallographic parameters for 7



C(1')-C(8)	1.380(3)	C(1)-O(1)-C(2)	106.39(13)
C(1')-C(1)	1.381(2)	C(3)-C(2)-O(1)	126.02(16)
C(1)-N(1)	1.352(2)	C(3)-C(2)-C(7)	125.14(16)
C(1)-O(1)	1.355(2)	O(1)-C(2)-C(7)	108.83(14)
O(1)-C(2)	1.381(2)	C(2)-C(3)-C(4)	115.17(17)
C(2)-C(3)	1.371(2)	C(3)-C(4)-C(5)	121.07(17)
C(2)-C(7)	1.390(2)	C(4)-C(5)-C(6)	123.27(17)
C(3)-C(4)	1.391(3)	C(7)-C(6)-C(5)	115.30(16)
C(4)-C(5)	1.394(3)	C(7)-C(6)-C(15)	124.49(15)
C(5)-C(6)	1.402(2)	C(5)-C(6)-C(15)	120.20(15)
C(6)-C(7)	1.398(2)	C(2)-C(7)-C(6)	120.02(15)
C(6)-C(15)	1.501(2)	C(2)-C(7)-N(1)	106.80(14)
C(7)-N(1)	1.424(2)	C(6)-C(7)-N(1)	133.18(15)
N(1)-Al(1)	1.9115(16)	C(1)-N(1)-C(7)	105.66(14)
Al(1)-N(2)	1.9164(15)	C(1)-N(1)-Al(1)	121.41(12)
Al(1)-C(1M')	1.932(14)	C(7)-N(1)-Al(1)	132.91(11)
Al(1)-C(1M)	1.940(2)	N(1)-Al(1)-N(2)	97.38(7)
Al(1)-I(1)	2.5674(8)	N(1)-Al(1)-C(1M')	120.6(6)
Al(1)-I(1')	2.639(2)	N(2)-Al(1)-C(1M')	110.2(6)
C(1M)-C(2M)	1.556(4)	N(1)-Al(1)-C(1M)	112.07(8)
C(1M')-C(2M')	1.555(18)	N(2)-Al(1)-C(1M)	112.79(8)
C(8)-N(2)	1.350(2)	N(1)-Al(1)-I(1)	105.53(5)
C(8)-O(2)	1.357(2)	N(2)-Al(1)-I(1)	108.56(5)
O(2)-C(9)	1.383(2)	C(1M)-Al(1)-I(1)	118.28(7)
C(9)-C(10)	1.379(3)	N(1)-Al(1)-I(1')	100.29(7)
C(9)-C(14)	1.389(2)	N(2)-Al(1)-I(1')	109.30(6)
C(10)-C(11)	1.383(3)	C(1M')-Al(1)-I(1')	117.0(6)
C(11)-C(12)	1.401(3)	C(2M)-C(1M)-Al(1)	111.44(14)
C(12)-C(13)	1.406(2)	C(2M')-C(1M')-Al(1)	116.8(14)
C(13)-C(14)	1.390(3)	N(2)-C(8)-O(2)	112.77(15)
C(13)-C(16)	1.499(3)	N(2)-C(8)-C(1')	129.16(15)
C(14)-N(2)	1.431(2)	O(2)-C(8)-C(1')	118.07(15)
		C(8)-O(2)-C(9)	105.96(13)
C(8)-C(1')-C(1)	121.56(15)	C(10)-C(9)-O(2)	125.75(17)
N(1)-C(1)-O(1)	112.30(14)	C(10)-C(9)-C(14)	125.06(18)
N(1)-C(1)-C(1')	129.08(16)	O(2)-C(9)-C(14)	109.19(15)
O(1)-C(1)-C(1')	118.60(15)	C(9)-C(10)-C(11)	115.04(18)

C(10)-C(11)-C(12)	121.28(17)	C(9)-C(14)-N(2)	106.65(15)
C(11)-C(12)-C(13)	122.94(19)	C(13)-C(14)-N(2)	133.07(16)
C(14)-C(13)-C(12)	115.41(17)	C(8)-N(2)-C(14)	105.41(14)
C(14)-C(13)-C(16)	124.24(16)	C(8)-N(2)-Al(1)	121.33(12)
C(12)-C(13)-C(16)	120.35(18)	C(14)-N(2)-Al(1)	133.26(12)
C(9)-C(14)-C(13)	120.28(16)		