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Electronic Supporting Information

for

Bis-(benzothiazol-2-yl)-amines and their metal amides: a structural comparison in the solid state.

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1. Crystallographic details for 1 - 6 and 8

Table 1. Crystal structure data for **1** – **6** and **8**.

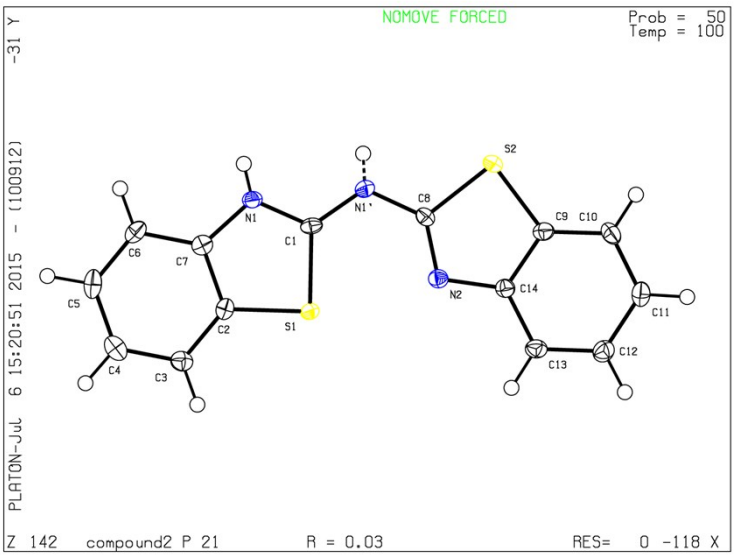
	1	**2** · 0.25 tol	**3** · 0.5 tol	**4**	**5**	**6** · 0.42 tol	**8** · 0.25 tol
Formula	$C_{14}H_9N_3S_2$	$C_{16}H_{13}N_3S_2$· 0.25 C_7H_8	$C_{16}H_{13}N_3O_2S_2$· 0.5 C_7H_8	$C_{16}H_{14}AlN_3S_2$	$C_{18}H_{18}AlN_3S_2$	$C_{21}H_{27}Al_2N_3O_2S_2$· 0.42 C_7H_8	$C_{16}H_{12}LiN_3S_2$· 0.25 C_7H_8
Mol. w., g mol^{-1}	283.37	334.45	389.48	339.40	367.47	509.92	340.38
CCDC no.	1042655	1042656	1042657	1042658	1042659	1042660	1042661
Wavelength, Å	0.71073	0.71073	0.71073	0.56086	0.56086	0.71073	0.71073
Crystal system	monoclinic	triclinic	monoclinic	triclinic	orthorhombic	monoclinic	triclinic
Space group	$P2_1$	$P\bar{1}$	$C2/c$	$P\bar{1}$	$Pccn$	$P2_1/c$	$P\bar{1}$
a, Å	10.853(3)	8.317(2)	28.107(4)	8.678(2)	16.013(3)	11.136(2)	14.094(2)
b, Å	4.587(2)	12.009(3)	12.581(2)	14.569(3)	16.930(3)	17.335(3)	16.125(3)
c, Å	12.513(4)	16.306(4)	21.980(3)	14.732(3)	12.855(2)	14.122(2)	16.706(3)
α, deg	90	85.55(2)	90	63.90(2)	90	90	71.00(3)
β, deg	93.90(2)	75.83(2)	112.93(3)	88.93(3)	90	95.96(2)	73.41(3)
γ, deg	90	89.23(3)	90	74.02(2)	90	90	69.20(2)
V, Å^3	621.5(4)	1574.3(7)	7158(2)	1596.6(7)	3485.0(10)	2711.4(8)	3293.3(13)
Z	2	4	16	4	8	4	8
Refl. measured	14858	25733	58842	38457	100934	23794	38560
Refl. unique	2785	7109	8090	7063	3588	5593	9464
$R1$ [I>2σ(I)][a]	0.0309	0.0344	0.0400	0.0349	0.0267	0.0432	0.0571
w$R2$ (all refl.)[b]	0.0801	0.0871	0.1027	0.0800	0.0725	0.1351	0.1491
R_{int}	0.0240	0.0358	0.0592	0.0280	0.0346	0.0351	0.0862
Abs. stru. para.[1]	0.02(2)	-	-	-	-	-	-
$\Delta\rho_{fin}$, e Å^{-3}	0.365 / −0.281	0.366 / −0.340	0.428 / −0.397	0.381 / −0.234	0.370 / −0.210	0.730 / −0.666	0.323 / −0.317

a $R1 = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|}$ b $wR2 = \sqrt{\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}}$; $w = \frac{1}{\sigma^2(F_o^2) + (g_1 P)^2 + g_2 P}$; $P = \frac{(F_o^2 + 2F_c^2)}{3}$.

1 S. Parsons, H. D. Flack and T. Wagner, *Acta Crystallogr., Sect. B*, 2013, **69**, 249-259.

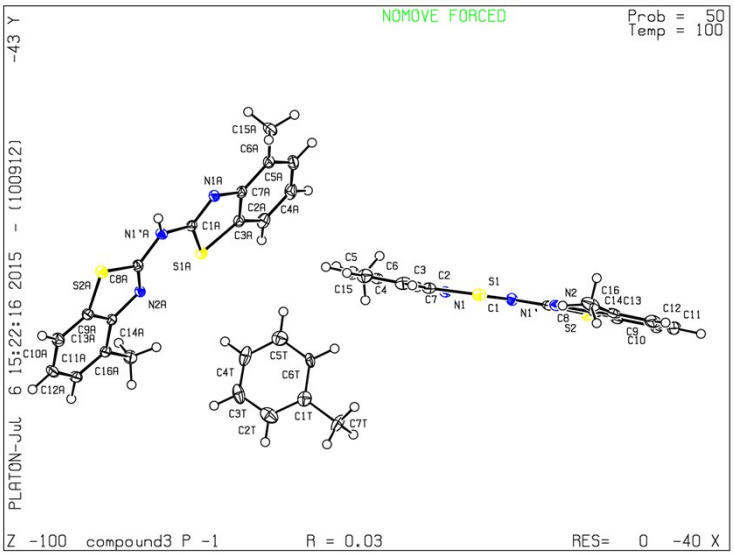
2. Bond lengths (Å) and angles (deg) for 1 - 6 and 8

2.1 Crystallographic parameters for 1



S(1)-C(2)	1.748(3)	H(1)-N(1)-C(1)	128(4)
S(1)-C(1)	1.760(3)	H(1)-N(1)-C(7)	119(4)
S(2)-C(9)	1.741(3)	C(1)-N(1)-C(7)	113.7(2)
S(2)-C(8)	1.768(3)	C(8)-N(2)-C(14)	110.0(2)
N(1')-H(1’)	0.77(5)	N(1)-C(1)-N(1')	121.2(2)
N(1')-C(1)	1.336(4)	N(1)-C(1)-S(1)	113.0(2)
N(1')-C(8)	1.367(4)	N(1')-C(1)-S(1)	125.8(2)
N(1)-H(1)	0.76(5)	C(3)-C(2)-C(7)	120.9(3)
N(1)-C(1)	1.331(4)	C(3)-C(2)-S(1)	127.9(2)
N(1)-C(7)	1.391(4)	C(7)-C(2)-S(1)	111.2(2)
N(2)-C(8)	1.301(4)	C(4)-C(3)-C(2)	118.5(3)
N(2)-C(14)	1.388(4)	C(3)-C(4)-C(5)	120.6(3)
C(2)-C(3)	1.392(4)	C(6)-C(5)-C(4)	121.0(3)
C(2)-C(7)	1.396(4)	C(5)-C(6)-C(7)	118.3(3)
C(3)-C(4)	1.385(4)	N(1)-C(7)-C(6)	126.6(3)
C(4)-C(5)	1.402(5)	N(1)-C(7)-C(2)	112.7(3)
C(5)-C(6)	1.386(4)	C(6)-C(7)-C(2)	120.7(3)
C(6)-C(7)	1.394(4)	N(2)-C(8)-N(1')	126.8(3)
C(9)-C(10)	1.385(4)	N(2)-C(8)-S(2)	116.2(2)
C(9)-C(14)	1.409(4)	N(1')-C(8)-S(2)	117.0(2)
C(10)-C(11)	1.391(4)	C(10)-C(9)-C(14)	122.4(3)
C(11)-C(12)	1.403(4)	C(10)-C(9)-S(2)	128.4(2)
C(12)-C(13)	1.385(4)	C(14)-C(9)-S(2)	109.1(2)
C(13)-C(14)	1.399(4)	C(9)-C(10)-C(11)	118.0(3)
		C(10)-C(11)-C(12)	120.4(3)
C(2)-S(1)-C(1)	89.35(15)	C(13)-C(12)-C(11)	121.2(3)
C(9)-S(2)-C(8)	88.62(14)	C(12)-C(13)-C(14)	119.1(3)
H(1’)-N(1')-C(1)	120(3)	N(2)-C(14)-C(13)	125.3(3)
H(1‘)-N(1')-C(8)	117(3)	N(2)-C(14)-C(9)	116.0(3)
C(1)-N(1')-C(8)	120.3(2)	C(13)-C(14)-C(9)	118.8(3)

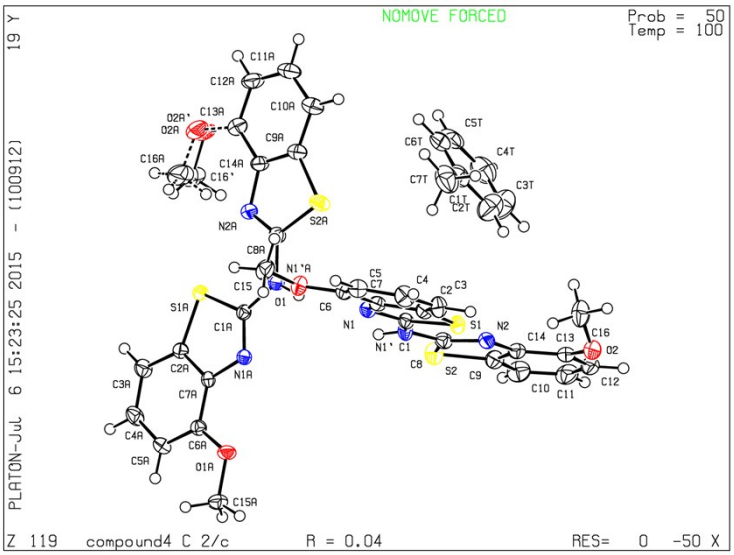
2.2 Crystallographic parameters for 2



N(1')-H(1)	0.846(16)	C(13A)-C(14A)	1.405(2)
N(1')-C(1)	1.370(2)	C(13A)-C(16A)	1.498(2)
N(1')-C(8)	1.372(2)	C(14A)-N(2A)	1.396(2)
C(8)-N(2)	1.293(2)	C(1A)-N(1A)	1.310(2)
C(8)-S(2)	1.7595(18)	C(1A)-S(1A)	1.7469(16)
S(2)-C(9)	1.7489(18)	S(1A)-C(2A)	1.7458(17)
C(9)-C(10)	1.393(3)	C(2A)-C(3A)	1.395(2)
C(9)-C(14)	1.398(3)	C(2A)-C(7A)	1.403(2)
C(10)-C(11)	1.393(3)	C(3A)-C(4A)	1.383(3)
C(11)-C(12)	1.391(3)	C(4A)-C(5A)	1.393(3)
C(12)-C(13)	1.386(3)	C(5A)-C(6A)	1.387(3)
C(13)-C(14)	1.410(2)	C(6A)-C(7A)	1.405(2)
C(13)-C(16)	1.497(3)	C(6A)-C(15A)	1.503(2)
C(14)-N(2)	1.396(2)	C(7A)-N(1A)	1.397(2)
C(1)-N(1)	1.304(2)	C(1T)-C(2T)	1.373(13)
C(1)-S(1)	1.7534(17)	C(1T)-C(6T)	1.381(14)
S(1)-C(2)	1.7441(18)	C(1T)-C(7T)	1.54(2)
C(2)-C(3)	1.391(2)	C(2T)-C(3T)	1.39(2)
C(2)-C(7)	1.407(2)	C(3T)-C(4T)	1.360(15)
C(3)-C(4)	1.382(3)	C(4T)-C(5T)	1.360(13)
C(4)-C(5)	1.398(3)	C(5T)-C(6T)	1.391(19)
C(5)-C(6)	1.390(2)		
C(6)-C(7)	1.405(2)	H(1)-N(1')-C(1)	118.0(13)
C(6)-C(15)	1.504(2)	H(1)-N(1')-C(8)	117.2(13)
C(7)-N(1)	1.396(2)	C(1)-N(1')-C(8)	124.82(14)
N(1'A)-H(1A)	0.843(16)	N(2)-C(8)-N(1')	123.74(16)
N(1'A)-C(1A)	1.370(2)	N(2)-C(8)-S(2)	117.27(13)
N(1'A)-C(8A)	1.376(2)	N(1')-C(8)-S(2)	118.99(12)
C(8A)-N(2A)	1.293(2)	C(9)-S(2)-C(8)	87.82(9)
C(8A)-S(2A)	1.7538(17)	C(10)-C(9)-C(14)	121.98(17)
S(2A)-C(9A)	1.7451(16)	C(10)-C(9)-S(2)	128.27(16)
C(9A)-C(10A)	1.389(2)	C(14)-C(9)-S(2)	109.75(13)
C(9A)-C(14A)	1.404(2)	C(11)-C(10)-C(9)	117.0(2)
C(10A)-C(11A)	1.387(2)	C(12)-C(11)-C(10)	121.21(18)
C(11A)-C(12A)	1.393(3)	C(13)-C(12)-C(11)	122.48(18)
C(12A)-C(13A)	1.390(2)	C(12)-C(13)-C(14)	116.59(19)

C(12)-C(13)-C(16)	123.02(17)	C(10A)-C(11A)-C(12A)	121.02(16)
C(14)-C(13)-C(16)	120.37(17)	C(13A)-C(12A)-C(11A)	122.35(15)
N(2)-C(14)-C(9)	115.45(15)	C(12A)-C(13A)-C(14A)	116.93(16)
N(2)-C(14)-C(13)	123.82(17)	C(12A)-C(13A)-C(16A)	122.39(15)
C(9)-C(14)-C(13)	120.73(16)	C(14A)-C(13A)-C(16A)	120.67(15)
C(8)-N(2)-C(14)	109.70(15)	N(2A)-C(14A)-C(9A)	115.55(13)
N(1)-C(1)-N(1')	120.31(14)	N(2A)-C(14A)-C(13A)	124.24(15)
N(1)-C(1)-S(1)	116.85(12)	C(9A)-C(14A)-C(13A)	120.21(15)
N(1')-C(1)-S(1)	122.84(12)	C(8A)-N(2A)-C(14A)	109.43(13)
C(2)-S(1)-C(1)	88.22(8)	N(1A)-C(1A)-N(1'A)	119.98(14)
C(3)-C(2)-C(7)	121.87(16)	N(1A)-C(1A)-S(1A)	116.88(12)
C(3)-C(2)-S(1)	128.06(13)	N(1'A)-C(1A)-S(1A)	123.13(11)
C(7)-C(2)-S(1)	110.03(13)	C(2A)-S(1A)-C(1A)	88.14(8)
C(4)-C(3)-C(2)	117.61(16)	C(3A)-C(2A)-C(7A)	121.86(15)
C(3)-C(4)-C(5)	120.95(17)	C(3A)-C(2A)-S(1A)	127.73(13)
C(6)-C(5)-C(4)	122.23(17)	C(7A)-C(2A)-S(1A)	110.36(12)
C(5)-C(6)-C(7)	117.01(15)	C(4A)-C(3A)-C(2A)	117.45(16)
C(5)-C(6)-C(15)	122.10(16)	C(3A)-C(4A)-C(5A)	120.97(17)
C(7)-C(6)-C(15)	120.85(15)	C(6A)-C(5A)-C(4A)	122.39(16)
N(1)-C(7)-C(6)	124.92(14)	C(5A)-C(6A)-C(7A)	117.04(16)
N(1)-C(7)-C(2)	114.76(15)	C(5A)-C(6A)-C(15A)	121.39(15)
C(6)-C(7)-C(2)	120.26(15)	C(7A)-C(6A)-C(15A)	121.46(15)
C(1)-N(1)-C(7)	110.07(13)	N(1A)-C(7A)-C(2A)	114.46(14)
H(1A)-N(1'A)-C(1A)	117.0(13)	N(1A)-C(7A)-C(6A)	125.22(15)
H(1A)-N(1'A)-C(8A)	118.0(13)	C(2A)-C(7A)-C(6A)	120.29(15)
C(1A)-N(1'A)-C(8A)	124.96(14)	C(1A)-N(1A)-C(7A)	110.13(13)
N(2A)-C(8A)-N(1'A)	124.02(15)	C(2T)-C(1T)-C(6T)	118.6(15)
N(2A)-C(8A)-S(2A)	117.52(12)	C(2T)-C(1T)-C(7T)	120.3(10)
N(1'A)-C(8A)-S(2A)	118.45(12)	C(6T)-C(1T)-C(7T)	121.0(8)
C(9A)-S(2A)-C(8A)	88.07(8)	C(1T)-C(2T)-C(3T)	121.6(13)
C(10A)-C(9A)-C(14A)	122.21(15)	C(4T)-C(3T)-C(2T)	117.9(10)
C(10A)-C(9A)-S(2A)	128.35(13)	C(3T)-C(4T)-C(5T)	122.8(17)
C(14A)-C(9A)-S(2A)	109.43(12)	C(4T)-C(5T)-C(6T)	118.4(10)
C(11A)-C(10A)-C(9A)	117.27(16)	C(1T)-C(6T)-C(5T)	120.7(9)

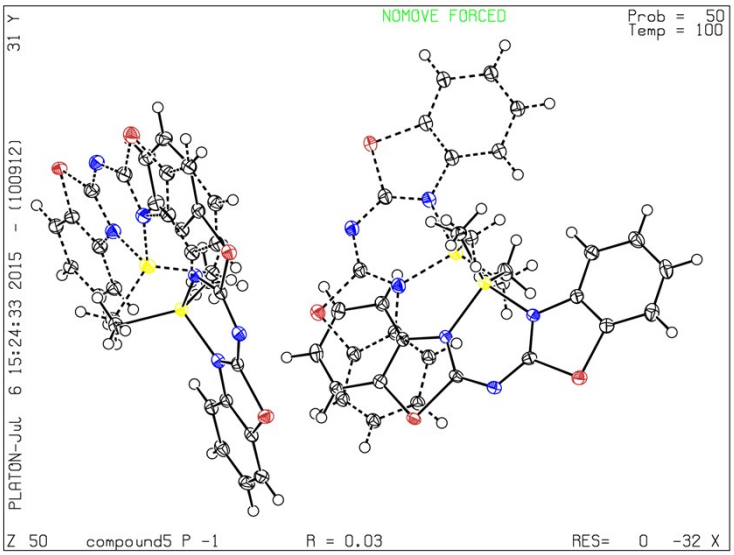
2.3 Crystallographic parameters for 3



N(1')-H(1)	0.842(19)	C(11A)-C(12A)	1.377(3)
N(1')-C(8)	1.360(3)	C(12A)-C(13A)	1.391(3)
N(1')-C(1)	1.365(2)	C(13A)-O(2A)	1.365(11)
C(8)-N(2)	1.297(2)	C(13A)-O(2A')	1.369(9)
C(8)-S(2)	1.748(2)	C(13A)-C(14A)	1.410(3)
S(2)-C(9)	1.738(2)	C(14A)-N(2A)	1.398(2)
C(9)-C(10)	1.383(3)	O(2A)-C(16A)	1.395(16)
C(9)-C(14)	1.401(3)	O(2A')-C(16')	1.408(12)
C(10)-C(11)	1.377(3)	C(1A)-N(1A)	1.305(2)
C(11)-C(12)	1.381(3)	C(1A)-S(1A)	1.7468(19)
C(12)-C(13)	1.378(3)	S(1A)-C(2A)	1.7411(18)
C(13)-O(2)	1.363(3)	C(2A)-C(7A)	1.393(2)
C(13)-C(14)	1.407(3)	C(2A)-C(3A)	1.394(3)
C(14)-N(2)	1.394(3)	C(3A)-C(4A)	1.374(3)
O(2)-C(16)	1.420(3)	C(4A)-C(5A)	1.398(3)
C(1)-N(1)	1.297(2)	C(5A)-C(6A)	1.377(3)
C(1)-S(1)	1.7551(19)	C(6A)-O(1A)	1.359(2)
S(1)-C(2)	1.740(2)	C(6A)-C(7A)	1.400(2)
C(2)-C(3)	1.394(3)	C(7A)-N(1A)	1.387(2)
C(2)-C(7)	1.397(3)	O(1A)-C(15A)	1.429(2)
C(3)-C(4)	1.373(3)	C(1T)-C(2T)	1.376(3)
C(4)-C(5)	1.393(3)	C(1T)-C(6T)	1.392(4)
C(5)-C(6)	1.379(3)	C(1T)-C(7T)	1.499(4)
C(6)-O(1)	1.362(2)	C(2T)-C(3T)	1.369(4)
C(6)-C(7)	1.400(3)	C(3T)-C(4T)	1.377(4)
C(7)-N(1)	1.385(2)	C(4T)-C(5T)	1.370(4)
O(1)-C(15)	1.428(2)	C(5T)-C(6T)	1.375(4)
N(1'A)-H(1A)	0.844(19)		
N(1'A)-C(1A)	1.365(2)	H(1)-N(1')-C(8)	117.8(16)
N(1'A)-C(8A)	1.366(2)	H(1)-N(1')-C(1)	116.0(16)
C(8A)-N(2A)	1.286(2)	C(8)-N(1')-C(1)	125.80(17)
C(8A)-S(2A)	1.7512(19)	N(2)-C(8)-N(1')	124.96(18)
S(2A)-C(9A)	1.741(2)	N(2)-C(8)-S(2)	117.28(15)
C(9A)-C(10A)	1.392(3)	N(1')-C(8)-S(2)	117.76(14)
C(9A)-C(14A)	1.400(3)	C(9)-S(2)-C(8)	88.08(10)
C(10A)-C(11A)	1.378(3)	C(10)-C(9)-C(14)	123.0(2)

C(10)-C(9)-S(2)	127.00(18)	C(11A)-C(10A)-C(9A)	116.9(2)
C(14)-C(9)-S(2)	109.96(15)	C(12A)-C(11A)-C(10A)	121.48(19)
C(11)-C(10)-C(9)	117.5(2)	C(11A)-C(12A)-C(13A)	121.8(2)
C(10)-C(11)-C(12)	120.9(2)	O(2A)-C(13A)-C(12A)	114.0(6)
C(13)-C(12)-C(11)	121.8(2)	O(2A')-C(13A)-C(12A)	115.8(5)
O(2)-C(13)-C(12)	116.54(19)	O(2A)-C(13A)-C(14A)	126.8(6)
O(2)-C(13)-C(14)	124.59(19)	O(2A')-C(13A)-C(14A)	125.5(5)
C(12)-C(13)-C(14)	118.8(2)	C(12A)-C(13A)-C(14A)	118.3(2)
N(2)-C(14)-C(9)	115.04(17)	N(2A)-C(14A)-C(9A)	114.98(17)
N(2)-C(14)-C(13)	127.02(19)	N(2A)-C(14A)-C(13A)	126.92(19)
C(9)-C(14)-C(13)	117.93(19)	C(9A)-C(14A)-C(13A)	118.09(17)
C(8)-N(2)-C(14)	109.65(17)	C(8A)-N(2A)-C(14A)	110.17(16)
C(13)-O(2)-C(16)	118.63(16)	C(13A)-O(2A)-C(16A)	116.8(12)
N(1)-C(1)-N(1')	120.97(17)	C(13A)-O(2A')-C(16')	123.1(10)
N(1)-C(1)-S(1)	116.78(14)	N(1A)-C(1A)-N(1'A)	120.78(16)
N(1')-C(1)-S(1)	122.21(14)	N(1A)-C(1A)-S(1A)	116.70(13)
C(2)-S(1)-C(1)	88.23(9)	N(1'A)-C(1A)-S(1A)	122.52(13)
C(3)-C(2)-C(7)	121.91(19)	C(2A)-S(1A)-C(1A)	88.37(8)
C(3)-C(2)-S(1)	128.73(16)	C(7A)-C(2A)-C(3A)	121.79(17)
C(7)-C(2)-S(1)	109.35(14)	C(7A)-C(2A)-S(1A)	109.52(13)
C(4)-C(3)-C(2)	117.29(19)	C(3A)-C(2A)-S(1A)	128.69(15)
C(3)-C(4)-C(5)	121.96(19)	C(4A)-C(3A)-C(2A)	117.18(18)
C(6)-C(5)-C(4)	120.62(19)	C(3A)-C(4A)-C(5A)	122.30(18)
O(1)-C(6)-C(5)	125.88(18)	C(6A)-C(5A)-C(4A)	120.01(17)
O(1)-C(6)-C(7)	115.36(17)	O(1A)-C(6A)-C(5A)	125.70(16)
C(5)-C(6)-C(7)	118.74(18)	O(1A)-C(6A)-C(7A)	115.28(16)
N(1)-C(7)-C(2)	115.98(17)	C(5A)-C(6A)-C(7A)	119.02(17)
N(1)-C(7)-C(6)	124.56(17)	N(1A)-C(7A)-C(2A)	115.81(15)
C(2)-C(7)-C(6)	119.46(17)	N(1A)-C(7A)-C(6A)	124.50(16)
C(1)-N(1)-C(7)	109.64(16)	C(2A)-C(7A)-C(6A)	119.69(16)
C(6)-O(1)-C(15)	116.61(16)	C(1A)-N(1A)-C(7A)	109.60(15)
H(1A)-N(1'A)-C(1A)	117.0(16)	C(6A)-O(1A)-C(15A)	117.09(15)
H(1A)-N(1'A)-C(8A)	117.5(16)	C(2T)-C(1T)-C(6T)	117.6(3)
C(1A)-N(1'A)-C(8A)	125.37(16)	C(2T)-C(1T)-C(7T)	120.7(3)
N(2A)-C(8A)-N(1'A)	124.84(17)	C(6T)-C(1T)-C(7T)	121.7(2)
N(2A)-C(8A)-S(2A)	116.95(14)	C(3T)-C(2T)-C(1T)	121.3(3)
N(1'A)-C(8A)-S(2A)	118.20(14)	C(2T)-C(3T)-C(4T)	120.5(3)
C(9A)-S(2A)-C(8A)	88.33(9)	C(5T)-C(4T)-C(3T)	119.3(3)
C(10A)-C(9A)-C(14A)	123.34(19)	C(4T)-C(5T)-C(6T)	120.1(3)
C(10A)-C(9A)-S(2A)	127.09(17)	C(5T)-C(6T)-C(1T)	121.2(2)
C(14A)-C(9A)-S(2A)	109.57(14)		

2.4 Crystallographic parameters for 4



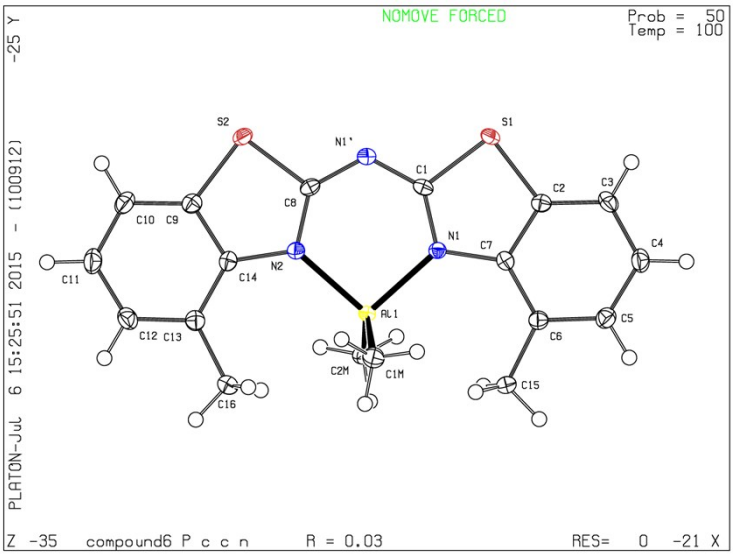
Al(1)-N(1)	1.9279(17)	C(2A)-C(7A)	1.402(3)
Al(1)-N(2)	1.9286(17)	C(3A)-C(4A)	1.387(3)
Al(1)-C(2M)	1.958(2)	C(4A)-C(5A)	1.392(3)
Al(1)-C(1M)	1.960(2)	C(5A)-C(6A)	1.385(3)
N(1')-C(8)	1.330(3)	C(6A)-C(7A)	1.390(3)
N(1')-C(1)	1.337(2)	C(7A)-N(1A)	1.403(2)
C(1)-N(1)	1.337(2)	C(8A)-N(2A)	1.348(3)
C(1)-S(1)	1.7527(18)	C(8A)-S(2A)	1.744(2)
S(1)-C(2)	1.7415(19)	S(2A)-C(9A)	1.738(2)
C(2)-C(3)	1.395(3)	C(9A)-C(10A)	1.393(3)
C(2)-C(7)	1.400(3)	C(9A)-C(14A)	1.398(3)
C(3)-C(4)	1.386(3)	C(10A)-C(11A)	1.387(3)
C(4)-C(5)	1.394(3)	C(11A)-C(12A)	1.394(3)
C(5)-C(6)	1.387(3)	C(12A)-C(13A)	1.384(3)
C(6)-C(7)	1.393(3)	C(13A)-C(14A)	1.397(3)
C(7)-N(1)	1.400(2)	C(14A)-N(2A)	1.401(3)
C(8)-N(2)	1.345(3)	Al(1B)-N(1B)	1.926(14)
C(8)-S(2)	1.745(2)	Al(1B)-N(2B)	1.928(13)
S(2)-C(9)	1.737(2)	Al(1B)-C(1MB)	1.948(15)
C(9)-C(10)	1.396(3)	Al(1B)-C(2MB)	1.966(15)
C(9)-C(14)	1.397(3)	N(1'B)-C(1B)	1.335(14)
C(10)-C(11)	1.383(3)	N(1'B)-C(8B)	1.335(14)
C(11)-C(12)	1.393(3)	C(1B)-N(1B)	1.343(14)
C(12)-C(13)	1.387(3)	C(1B)-S(1B)	1.748(14)
C(13)-C(14)	1.397(3)	S(1B)-C(2B)	1.736(15)
C(14)-N(2)	1.402(2)	C(2B)-C(3B)	1.395(15)
Al(1A)-N(2A)	1.925(2)	C(2B)-C(7B)	1.401(14)
Al(1A)-N(1A)	1.9303(17)	C(3B)-C(4B)	1.390(16)
Al(1A)-C(2MA)	1.954(3)	C(4B)-C(5B)	1.390(16)
Al(1A)-C(1MA)	1.959(2)	C(5B)-C(6B)	1.388(16)
N(1'A)-C(1A)	1.331(2)	C(6B)-C(7B)	1.400(15)
N(1'A)-C(8A)	1.334(3)	C(7B)-N(1B)	1.398(14)
C(1A)-N(1A)	1.341(2)	C(8B)-N(2B)	1.350(14)
C(1A)-S(1A)	1.7523(18)	C(8B)-S(2B)	1.754(14)
S(1A)-C(2A)	1.742(2)	S(2B)-C(9B)	1.746(14)
C(2A)-C(3A)	1.390(3)	C(9B)-C(10B)	1.395(15)

C(9B)-C(14B)	1.406(14)
C(10B)-C(11B)	1.389(16)
C(11B)-C(12B)	1.392(16)
C(12B)-C(13B)	1.389(15)
C(13B)-C(14B)	1.404(15)
C(14B)-N(2B)	1.406(14)
Al(1C)-N(1C)	1.929(13)
Al(1C)-N(2C)	1.937(13)
Al(1C)-C(2MC)	1.947(14)
Al(1C)-C(1MC)	1.963(15)
N(1'C)-C(1C)	1.335(14)
N(1'C)-C(8C)	1.342(14)
C(1C)-N(1C)	1.347(14)
C(1C)-S(1C)	1.752(14)
S(1C)-C(2C)	1.726(14)
C(2C)-C(3C)	1.395(15)
C(2C)-C(7C)	1.402(14)
C(3C)-C(4C)	1.385(16)
C(4C)-C(5C)	1.380(15)
C(5C)-C(6C)	1.394(15)
C(6C)-C(7C)	1.394(15)
C(7C)-N(1C)	1.398(14)
C(8C)-N(2C)	1.355(14)
C(8C)-S(2C)	1.742(14)
S(2C)-C(9C)	1.743(14)
C(9C)-C(10C)	1.398(14)
C(9C)-C(14C)	1.398(14)
C(10C)-C(11C)	1.391(15)
C(11C)-C(12C)	1.383(15)
C(12C)-C(13C)	1.386(15)
C(13C)-C(14C)	1.406(14)
C(14C)-N(2C)	1.408(14)

N(1)-Al(1)-N(2)	91.48(7)
N(1)-Al(1)-C(2M)	110.16(8)
N(2)-Al(1)-C(2M)	111.22(8)
N(1)-Al(1)-C(1M)	110.24(8)
N(2)-Al(1)-C(1M)	109.38(9)
C(2M)-Al(1)-C(1M)	120.54(10)
C(8)-N(1')-C(1)	119.73(16)
N(1)-C(1)-N(1')	129.87(16)
N(1)-C(1)-S(1)	113.42(13)
N(1')-C(1)-S(1)	116.70(13)
C(2)-S(1)-C(1)	90.41(9)
C(3)-C(2)-C(7)	121.04(17)
C(3)-C(2)-S(1)	129.19(15)
C(7)-C(2)-S(1)	109.76(14)
C(4)-C(3)-C(2)	118.25(18)
C(3)-C(4)-C(5)	120.98(18)
C(6)-C(5)-C(4)	120.81(19)
C(5)-C(6)-C(7)	118.81(18)
C(6)-C(7)-C(2)	120.11(17)
C(6)-C(7)-N(1)	125.48(17)
C(2)-C(7)-N(1)	114.40(16)
C(1)-N(1)-C(7)	112.01(15)
C(1)-N(1)-Al(1)	124.53(12)
C(7)-N(1)-Al(1)	123.45(12)
N(1')-C(8)-N(2)	129.83(18)
N(1')-C(8)-S(2)	116.88(15)
N(2)-C(8)-S(2)	113.27(15)
C(9)-S(2)-C(8)	90.75(10)
C(10)-C(9)-C(14)	121.33(18)
C(10)-C(9)-S(2)	128.87(16)
C(14)-C(9)-S(2)	109.79(14)
C(11)-C(10)-C(9)	118.18(19)
C(10)-C(11)-C(12)	120.81(18)
C(13)-C(12)-C(11)	121.23(19)
C(12)-C(13)-C(14)	118.47(19)
C(9)-C(14)-C(13)	119.96(17)
C(9)-C(14)-N(2)	114.48(16)
C(13)-C(14)-N(2)	125.56(17)
C(8)-N(2)-C(14)	111.72(16)
C(8)-N(2)-Al(1)	124.35(13)
C(14)-N(2)-Al(1)	123.91(13)
N(2A)-Al(1A)-N(1A)	91.61(8)
N(2A)-Al(1A)-C(2MA)	110.13(10)
N(1A)-Al(1A)-C(2MA)	111.87(9)
N(2A)-Al(1A)-C(1MA)	110.73(10)
N(1A)-Al(1A)-C(1MA)	110.00(9)
C(2MA)-Al(1A)-C(1MA)	119.11(11)
C(1A)-N(1'A)-C(8A)	119.85(17)
N(1'A)-C(1A)-N(1A)	129.84(17)
N(1'A)-C(1A)-S(1A)	116.72(14)
N(1A)-C(1A)-S(1A)	113.44(14)
C(2A)-S(1A)-C(1A)	90.38(9)
C(3A)-C(2A)-C(7A)	121.15(19)
C(3A)-C(2A)-S(1A)	128.85(16)
C(7A)-C(2A)-S(1A)	109.99(14)
C(4A)-C(3A)-C(2A)	118.07(19)
C(3A)-C(4A)-C(5A)	121.08(19)
C(6A)-C(5A)-C(4A)	120.8(2)
C(5A)-C(6A)-C(7A)	118.80(19)
C(6A)-C(7A)-C(2A)	120.05(18)
C(6A)-C(7A)-N(1A)	125.82(17)
C(2A)-C(7A)-N(1A)	114.12(17)
C(1A)-N(1A)-C(7A)	112.03(16)
C(1A)-N(1A)-Al(1A)	124.33(13)
C(7A)-N(1A)-Al(1A)	123.57(13)
N(1'A)-C(8A)-N(2A)	129.72(19)
N(1'A)-C(8A)-S(2A)	116.63(16)
N(2A)-C(8A)-S(2A)	113.61(15)
C(9A)-S(2A)-C(8A)	90.55(10)
C(10A)-C(9A)-C(14A)	121.26(18)
C(10A)-C(9A)-S(2A)	128.85(16)
C(14A)-C(9A)-S(2A)	109.89(14)
C(11A)-C(10A)-C(9A)	118.14(19)
C(10A)-C(11A)-C(12A)	120.80(19)
C(13A)-C(12A)-C(11A)	121.22(19)
C(12A)-C(13A)-C(14A)	118.45(19)
C(13A)-C(14A)-C(9A)	120.13(18)
C(13A)-C(14A)-N(2A)	125.30(18)
C(9A)-C(14A)-N(2A)	114.56(17)
C(8A)-N(2A)-C(14A)	111.37(18)
C(8A)-N(2A)-Al(1A)	124.12(15)
C(14A)-N(2A)-Al(1A)	124.42(14)
N(1B)-Al(1B)-N(2B)	91.1(10)
N(1B)-Al(1B)-C(1MB)	112.7(16)
N(2B)-Al(1B)-C(1MB)	111.6(16)

N(1B)-Al(1B)-C(2MB)	109.6(15)
N(2B)-Al(1B)-C(2MB)	111.0(16)
C(1MB)-Al(1B)-C(2MB)	117.8(17)
C(1B)-N(1'B)-C(8B)	121(2)
N(1'B)-C(1B)-N(1B)	128.9(16)
N(1'B)-C(1B)-S(1B)	118.0(15)
N(1B)-C(1B)-S(1B)	113.0(11)
C(2B)-S(1B)-C(1B)	91.4(10)
C(3B)-C(2B)-C(7B)	122.5(17)
C(3B)-C(2B)-S(1B)	128(2)
C(7B)-C(2B)-S(1B)	108.4(13)
C(4B)-C(3B)-C(2B)	116(2)
C(3B)-C(4B)-C(5B)	119(2)
C(6B)-C(5B)-C(4B)	123(2)
C(5B)-C(6B)-C(7B)	114.9(19)
N(1B)-C(7B)-C(6B)	123(2)
N(1B)-C(7B)-C(2B)	115.7(14)
C(6B)-C(7B)-C(2B)	120.8(16)
C(1B)-N(1B)-C(7B)	111.3(14)
C(1B)-N(1B)-Al(1B)	125.2(14)
C(7B)-N(1B)-Al(1B)	122.3(16)
N(1'B)-C(8B)-N(2B)	128.6(17)
N(1'B)-C(8B)-S(2B)	116.5(15)
N(2B)-C(8B)-S(2B)	114.8(12)
C(9B)-S(2B)-C(8B)	90.2(10)
C(10B)-C(9B)-C(14B)	122.3(17)
C(10B)-C(9B)-S(2B)	128.5(16)
C(14B)-C(9B)-S(2B)	109.2(12)
C(11B)-C(10B)-C(9B)	117(2)
C(10B)-C(11B)-C(12B)	121(2)
C(13B)-C(12B)-C(11B)	123(2)
C(12B)-C(13B)-C(14B)	117.1(19)
C(13B)-C(14B)-C(9B)	119.7(17)
C(13B)-C(14B)-N(2B)	123.7(19)
C(9B)-C(14B)-N(2B)	116.0(14)
C(8B)-N(2B)-C(14B)	109.7(13)
C(8B)-N(2B)-Al(1B)	125.2(13)
C(14B)-N(2B)-Al(1B)	124.9(14)
N(1C)-Al(1C)-N(2C)	91.3(9)
N(1C)-Al(1C)-C(2MC)	112.3(14)
N(2C)-Al(1C)-C(2MC)	110.8(14)
N(1C)-Al(1C)-C(1MC)	109.4(15)
N(2C)-Al(1C)-C(1MC)	110.6(16)
C(2MC)-Al(1C)-C(1MC)	119.0(17)
C(1C)-N(1'C)-C(8C)	120.8(18)
N(1'C)-C(1C)-N(1C)	128.0(16)
N(1'C)-C(1C)-S(1C)	118.3(13)
N(1C)-C(1C)-S(1C)	113.0(11)
C(2C)-S(1C)-C(1C)	91.3(9)
C(3C)-C(2C)-C(7C)	123.1(16)
C(3C)-C(2C)-S(1C)	128.1(15)
C(7C)-C(2C)-S(1C)	108.6(12)
C(4C)-C(3C)-C(2C)	116.1(19)
C(5C)-C(4C)-C(3C)	120.0(19)
C(4C)-C(5C)-C(6C)	125.1(19)
C(5C)-C(6C)-C(7C)	114.6(18)
C(6C)-C(7C)-N(1C)	123.4(15)
C(6C)-C(7C)-C(2C)	120.6(14)
N(1C)-C(7C)-C(2C)	116.0(13)
C(1C)-N(1C)-C(7C)	110.6(12)
C(1C)-N(1C)-Al(1C)	125.0(12)
C(7C)-N(1C)-Al(1C)	123.1(13)
N(1'C)-C(8C)-N(2C)	128.5(16)
N(1'C)-C(8C)-S(2C)	116.2(13)
N(2C)-C(8C)-S(2C)	114.9(11)
C(8C)-S(2C)-C(9C)	90.7(9)
C(10C)-C(9C)-C(14C)	124.9(15)
C(10C)-C(9C)-S(2C)	126.5(15)
C(14C)-C(9C)-S(2C)	108.6(12)
C(11C)-C(10C)-C(9C)	116.1(17)
C(12C)-C(11C)-C(10C)	118.8(19)
C(11C)-C(12C)-C(13C)	126(2)
C(12C)-C(13C)-C(14C)	115.8(18)
C(9C)-C(14C)-C(13C)	118.4(14)
C(9C)-C(14C)-N(2C)	116.7(13)
C(13C)-C(14C)-N(2C)	124.8(16)
C(8C)-N(2C)-C(14C)	108.9(12)
C(8C)-N(2C)-Al(1C)	124.1(12)
C(14C)-N(2C)-Al(1C)	126.2(13)

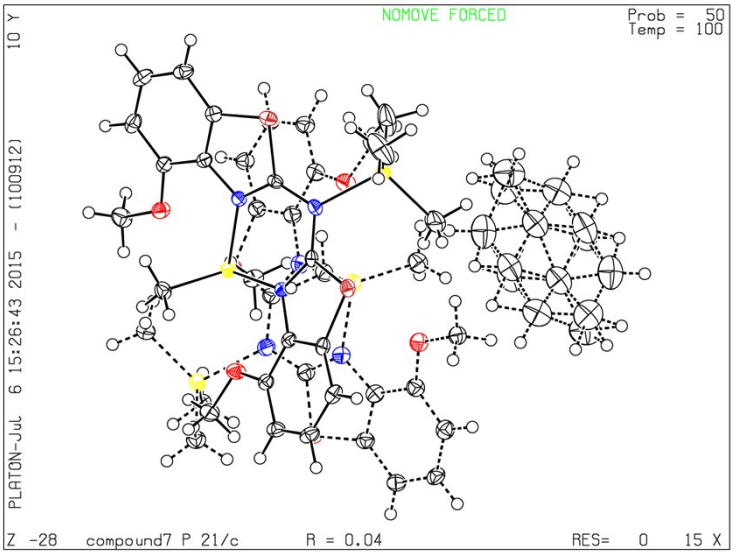
2.5 Crystallographic parameters for 5



Al(1)-N(1)	1.9556(13)	N(1')-C(1)-N(1)	131.20(13)
Al(1)-C(1M)	1.9602(15)	N(1')-C(1)-S(1)	114.38(10)
Al(1)-C(2M)	1.9625(15)	N(1)-C(1)-S(1)	114.42(10)
Al(1)-N(2)	1.9670(12)	C(2)-S(1)-C(1)	90.31(7)
N(1')-C(8)	1.3305(19)	C(3)-C(2)-C(7)	123.24(13)
N(1')-C(1)	1.3320(18)	C(3)-C(2)-S(1)	126.22(11)
C(1)-N(1)	1.3405(17)	C(7)-C(2)-S(1)	110.48(10)
C(1)-S(1)	1.7419(14)	C(4)-C(3)-C(2)	117.54(13)
S(1)-C(2)	1.7368(14)	C(3)-C(4)-C(5)	120.21(14)
C(2)-C(3)	1.386(2)	C(4)-C(5)-C(6)	123.03(14)
C(2)-C(7)	1.4066(19)	C(5)-C(6)-C(7)	117.06(13)
C(3)-C(4)	1.384(2)	C(5)-C(6)-C(15)	118.42(13)
C(4)-C(5)	1.390(2)	C(7)-C(6)-C(15)	124.50(13)
C(5)-C(6)	1.397(2)	C(2)-C(7)-C(6)	118.87(13)
C(6)-C(7)	1.4099(19)	C(2)-C(7)-N(1)	113.47(12)
C(6)-C(15)	1.504(2)	C(6)-C(7)-N(1)	127.64(12)
C(7)-N(1)	1.4193(17)	C(1)-N(1)-C(7)	111.29(11)
C(8)-N(2)	1.3435(18)	C(1)-N(1)-Al(1)	119.20(9)
C(8)-S(2)	1.7445(14)	C(7)-N(1)-Al(1)	129.42(9)
S(2)-C(9)	1.7354(15)	N(1')-C(8)-N(2)	131.00(13)
C(9)-C(10)	1.391(2)	N(1')-C(8)-S(2)	114.57(10)
C(9)-C(14)	1.4087(19)	N(2)-C(8)-S(2)	114.42(10)
C(10)-C(11)	1.376(2)	C(9)-S(2)-C(8)	90.29(7)
C(11)-C(12)	1.394(2)	C(10)-C(9)-C(14)	122.82(14)
C(12)-C(13)	1.396(2)	C(10)-C(9)-S(2)	126.55(11)
C(13)-C(14)	1.409(2)	C(14)-C(9)-S(2)	110.61(11)
C(13)-C(16)	1.504(2)	C(11)-C(10)-C(9)	117.86(14)
C(14)-N(2)	1.4197(18)	C(10)-C(11)-C(12)	120.32(14)
		C(11)-C(12)-C(13)	122.80(14)
N(1)-Al(1)-C(1M)	104.73(6)	C(12)-C(13)-C(14)	117.29(13)
N(1)-Al(1)-C(2M)	109.19(6)	C(12)-C(13)-C(16)	118.54(13)
C(1M)-Al(1)-C(2M)	126.65(7)	C(14)-C(13)-C(16)	124.15(13)
N(1)-Al(1)-N(2)	96.52(5)	C(9)-C(14)-C(13)	118.87(13)
C(1M)-Al(1)-N(2)	108.41(6)	C(9)-C(14)-N(2)	113.47(12)
C(2M)-Al(1)-N(2)	107.24(6)	C(13)-C(14)-N(2)	127.61(12)
C(8)-N(1')-C(1)	122.97(12)	C(8)-N(2)-C(14)	111.19(11)

C(8)-N(2)-Al(1)	118.87(9)	C(14)-N(2)-Al(1)	129.56(9)

2.6 Crystallographic parameters for 6

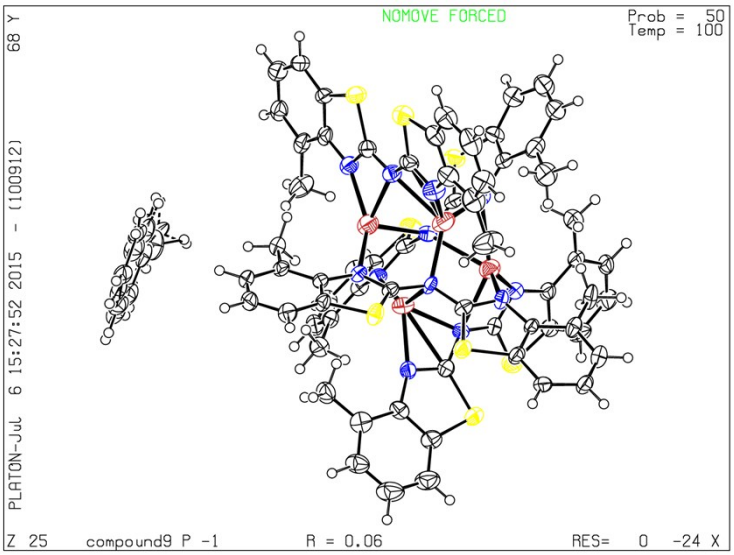


Al(1)-C(1M)	1.960(2)	Al(1A)-C(2MA)	1.969(15)
Al(1)-C(2M)	1.967(2)	Al(1A)-N(2A)	1.991(13)
Al(1)-N(1)	1.9948(18)	Al(1A)-N(1A)	2.002(13)
Al(1)-N(2)	1.9957(19)	N(1'A)-C(1A)	1.362(14)
N(1')-C(8)	1.365(3)	N(1'A)-C(8A)	1.367(14)
N(1')-C(1)	1.366(3)	N(1'A)-Al(2A)	2.074(16)
N(1')-Al(2)	2.0660(19)	C(1A)-N(1A)	1.323(14)
C(1)-N(1)	1.334(3)	C(1A)-S(1A)	1.746(14)
C(1)-S(1)	1.747(2)	S(1A)-C(2A)	1.742(15)
S(1)-C(2)	1.736(2)	C(2A)-C(7A)	1.389(15)
C(2)-C(7)	1.389(3)	C(2A)-C(3A)	1.407(15)
C(2)-C(3)	1.404(3)	C(3A)-C(4A)	1.383(16)
C(3)-C(4)	1.380(3)	C(4A)-C(5A)	1.402(16)
C(4)-C(5)	1.401(3)	C(5A)-C(6A)	1.390(16)
C(5)-C(6)	1.388(3)	C(6A)-O(1A)	1.357(15)
C(6)-O(1)	1.360(3)	C(6A)-C(7A)	1.409(15)
C(6)-C(7)	1.403(3)	C(7A)-N(1A)	1.400(14)
C(7)-N(1)	1.408(3)	O(1A)-C(15A)	1.442(16)
O(1)-C(15)	1.436(3)	C(8A)-N(2A)	1.326(14)
C(8)-N(2)	1.328(3)	C(8A)-S(2A)	1.767(14)
C(8)-S(2)	1.750(2)	S(2A)-C(9A)	1.740(14)
S(2)-C(9)	1.739(3)	C(9A)-C(14A)	1.388(15)
C(9)-C(14)	1.389(3)	C(9A)-C(10A)	1.409(15)
C(9)-C(10)	1.399(3)	C(10A)-C(11A)	1.379(16)
C(10)-C(11)	1.384(3)	C(11A)-C(12A)	1.396(16)
C(11)-C(12)	1.397(3)	C(12A)-C(13A)	1.393(16)
C(12)-C(13)	1.385(3)	C(13A)-O(2A)	1.359(15)
C(13)-O(2)	1.359(3)	C(13A)-C(14A)	1.410(15)
C(13)-C(14)	1.407(3)	C(14A)-N(2A)	1.408(14)
C(14)-N(2)	1.408(3)	O(2A)-C(16A)	1.447(17)
O(2)-C(16)	1.437(3)	Al(2A)-C(4MA)	1.943(18)
Al(2)-C(4M)	1.956(3)	Al(2A)-C(3MA)	1.957(15)
Al(2)-C(5M)	1.963(3)	Al(2A)-C(5MA)	1.958(15)
Al(2)-C(3M)	1.967(3)	C(1T)-C(6T)	1.368(11)
Al(1A)-C(1MA)	1.968(15)	C(1T)-C(2T)	1.395(10)

C(1T)-C(7T)	1.511(12)
C(2T)-C(3T)	1.414(10)
C(3T)-C(4T)	1.395(11)
C(4T)-C(5T)	1.348(10)
C(5T)-C(6T)	1.370(11)
C(1M)-Al(1)-C(2M)	129.57(11)
C(1M)-Al(1)-N(1)	109.22(9)
C(2M)-Al(1)-N(1)	107.42(9)
C(1M)-Al(1)-N(2)	108.64(9)
C(2M)-Al(1)-N(2)	106.23(9)
N(1)-Al(1)-N(2)	87.75(8)
C(8)-N(1')-C(1)	118.44(18)
C(8)-N(1')-Al(2)	120.40(14)
C(1)-N(1')-Al(2)	120.34(14)
N(1)-C(1)-N(1')	128.17(19)
N(1)-C(1)-S(1)	114.35(16)
N(1')-C(1)-S(1)	117.41(16)
C(2)-S(1)-C(1)	90.42(10)
C(7)-C(2)-C(3)	121.7(2)
C(7)-C(2)-S(1)	109.26(16)
C(3)-C(2)-S(1)	128.97(18)
C(4)-C(3)-C(2)	117.1(2)
C(3)-C(4)-C(5)	122.1(2)
C(6)-C(5)-C(4)	120.2(2)
O(1)-C(6)-C(5)	126.4(2)
O(1)-C(6)-C(7)	115.03(18)
C(5)-C(6)-C(7)	118.6(2)
C(2)-C(7)-C(6)	120.1(2)
C(2)-C(7)-N(1)	115.66(19)
C(6)-C(7)-N(1)	124.13(19)
C(1)-N(1)-C(7)	110.26(17)
C(1)-N(1)-Al(1)	126.56(14)
C(7)-N(1)-Al(1)	122.75(14)
C(6)-O(1)-C(15)	117.81(17)
N(2)-C(8)-N(1')	128.03(19)
N(2)-C(8)-S(2)	114.53(16)
N(1')-C(8)-S(2)	117.36(15)
C(9)-S(2)-C(8)	90.15(11)
C(14)-C(9)-C(10)	122.1(2)
C(14)-C(9)-S(2)	109.35(17)
C(10)-C(9)-S(2)	128.43(19)
C(11)-C(10)-C(9)	117.0(2)
C(10)-C(11)-C(12)	122.2(2)
C(13)-C(12)-C(11)	120.1(2)
O(2)-C(13)-C(12)	126.4(2)
O(2)-C(13)-C(14)	114.58(19)
C(12)-C(13)-C(14)	119.0(2)
C(9)-C(14)-C(13)	119.5(2)
C(9)-C(14)-N(2)	115.53(19)
C(13)-C(14)-N(2)	124.82(19)
C(8)-N(2)-C(14)	110.39(17)
C(8)-N(2)-Al(1)	126.95(15)
C(14)-N(2)-Al(1)	122.35(14)
C(13)-O(2)-C(16)	118.16(18)
C(4M)-Al(2)-C(5M)	115.58(18)
C(4M)-Al(2)-C(3M)	106.65(17)
C(5M)-Al(2)-C(3M)	118.07(16)
C(4M)-Al(2)-N(1')	105.83(11)
C(5M)-Al(2)-N(1')	104.90(11)
C(3M)-Al(2)-N(1')	104.57(11)
C(1MA)-Al(1A)-C(2MA)	131.5(14)
C(1MA)-Al(1A)-N(2A)	107.0(12)
C(2MA)-Al(1A)-N(2A)	106.6(11)
C(1MA)-Al(1A)-N(1A)	108.8(12)
C(2MA)-Al(1A)-N(1A)	106.8(11)
N(2A)-Al(1A)-N(1A)	87.4(8)
C(1A)-N(1'A)-C(8A)	116.0(14)
C(1A)-N(1'A)-Al(2A)	121.2(12)
C(8A)-N(1'A)-Al(2A)	121.5(12)
N(1A)-C(1A)-N(1'A)	129.1(14)
N(1A)-C(1A)-S(1A)	114.6(10)
N(1'A)-C(1A)-S(1A)	116.3(12)
C(2A)-S(1A)-C(1A)	90.1(8)
C(7A)-C(2A)-C(3A)	122.8(14)
C(7A)-C(2A)-S(1A)	109.0(12)
C(3A)-C(2A)-S(1A)	128.2(14)
C(4A)-C(3A)-C(2A)	116.0(17)
C(3A)-C(4A)-C(5A)	122.0(18)
C(6A)-C(5A)-C(4A)	121.6(18)
O(1A)-C(6A)-C(5A)	125.8(17)
O(1A)-C(6A)-C(7A)	116.6(16)
C(5A)-C(6A)-C(7A)	117.1(15)
C(2A)-C(7A)-N(1A)	115.8(13)
C(2A)-C(7A)-C(6A)	120.4(13)
N(1A)-C(7A)-C(6A)	123.8(14)
C(1A)-N(1A)-C(7A)	110.5(12)
C(1A)-N(1A)-Al(1A)	126.9(11)
C(7A)-N(1A)-Al(1A)	122.1(11)
C(6A)-O(1A)-C(15A)	118.8(19)
N(2A)-C(8A)-N(1'A)	130.3(14)
N(2A)-C(8A)-S(2A)	114.6(10)
N(1'A)-C(8A)-S(2A)	115.2(12)
C(9A)-S(2A)-C(8A)	89.6(8)
C(14A)-C(9A)-C(10A)	122.2(14)
C(14A)-C(9A)-S(2A)	109.8(11)
C(10A)-C(9A)-S(2A)	128.0(14)
C(11A)-C(10A)-C(9A)	115.4(18)
C(10A)-C(11A)-C(12A)	124.4(19)
C(13A)-C(12A)-C(11A)	119.2(18)
O(2A)-C(13A)-C(12A)	127.0(16)
O(2A)-C(13A)-C(14A)	114.7(15)
C(12A)-C(13A)-C(14A)	118.2(15)
C(9A)-C(14A)-N(2A)	115.7(12)
C(9A)-C(14A)-C(13A)	120.4(13)
N(2A)-C(14A)-C(13A)	123.6(14)
C(8A)-N(2A)-C(14A)	110.3(12)
C(8A)-N(2A)-Al(1A)	126.0(11)
C(14A)-N(2A)-Al(1A)	123.1(11)
C(13A)-O(2A)-C(16A)	121(2)
C(4MA)-Al(2A)-C(3MA)	113.2(13)
C(4MA)-Al(2A)-C(5MA)	114.1(13)
C(3MA)-Al(2A)-C(5MA)	114.4(14)
C(4MA)-Al(2A)-N(1'A)	101.4(18)
C(3MA)-Al(2A)-N(1'A)	106.0(13)
C(5MA)-Al(2A)-N(1'A)	106.3(13)
C(6T)-C(1T)-C(2T)	118.7(8)
C(6T)-C(1T)-C(7T)	120.7(8)

C(2T)-C(1T)-C(7T)	120.7(8)	C(5T)-C(4T)-C(3T)	118.0(8)
C(1T)-C(2T)-C(3T)	118.3(9)	C(4T)-C(5T)-C(6T)	121.8(9)
C(4T)-C(3T)-C(2T)	121.3(9)	C(1T)-C(6T)-C(5T)	121.8(9)

2.7 Crystallographic parameters for 8

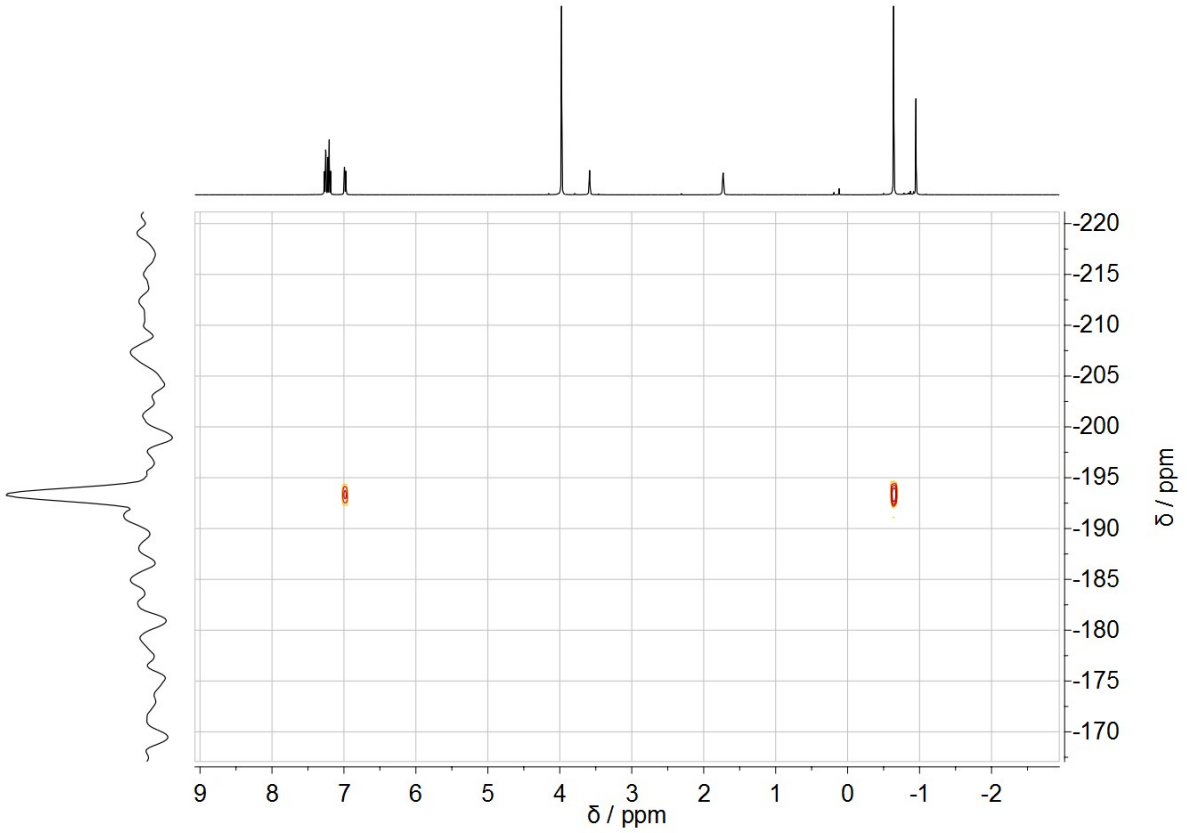


C(1)-N(1)	1.327(6)	Li(3)-C(1A)	2.745(10)
C(1)-N(1')	1.345(6)	Li(3)-Li(4)	2.998(13)
C(1)-S(1)	1.769(5)	C(4)-C(5)	1.395(7)
C(1)-Li(1)	2.482(10)	Li(4)-N(2B)	2.062(9)
N(1')-C(8)	1.347(6)	Li(4)-N(2C)	2.073(9)
N(1')-Li(1)	2.235(10)	Li(4)-N(1'C)	2.144(9)
N(1')-Li(2)	2.251(9)	Li(4)-N(1'A)	2.274(9)
S(1)-C(2)	1.753(5)	Li(4)-C(8C)	2.439(9)
Li(1)-N(1)	2.039(9)	Li(4)-N(2A)	2.483(9)
Li(1)-N(2A)	2.112(9)	Li(4)-N(1'B)	2.518(9)
Li(1)-N(1'B)	2.204(9)	Li(4)-C(8A)	2.564(9)
Li(1)-C(8B)	2.584(10)	Li(4)-C(8B)	2.626(9)
Li(1)-N(2B)	2.642(10)	C(5)-C(6)	1.381(6)
C(2)-C(3)	1.388(6)	C(6)-C(7)	1.395(7)
C(2)-C(7)	1.392(6)	C(6)-C(15)	1.519(7)
N(1)-C(7)	1.401(6)	C(9)-C(10)	1.388(7)
S(2)-C(9)	1.750(5)	C(9)-C(14)	1.398(7)
S(2)-C(8)	1.763(5)	C(10)-C(11)	1.398(8)
Li(2)-N(2)	1.950(10)	C(11)-C(12)	1.365(7)
Li(2)-N(1'A)	2.056(10)	C(12)-C(13)	1.366(7)
Li(2)-N(1B)	2.096(10)	C(13)-C(14)	1.416(7)
Li(2)-C(8)	2.418(10)	C(13)-C(16)	1.477(7)
Li(2)-C(1B)	2.633(10)	C(1A)-N(1A)	1.324(6)
Li(2)-N(1'B)	2.643(10)	C(1A)-N(1'A)	1.359(5)
Li(2)-Li(4)	3.484(13)	C(1A)-S(1A)	1.769(5)
C(3)-C(4)	1.379(7)	N(1'A)-C(8A)	1.358(5)
N(2)-C(8)	1.324(6)	S(1A)-C(2A)	1.739(5)
N(2)-C(14)	1.382(6)	C(2A)-C(3A)	1.373(6)
Li(3)-N(1C)	1.999(9)	C(2A)-C(7A)	1.414(6)
Li(3)-N(1A)	2.074(10)	N(1A)-C(7A)	1.377(5)
Li(3)-N(1B)	2.280(9)	S(2A)-C(9A)	1.747(5)
Li(3)-N(1'C)	2.357(10)	S(2A)-C(8A)	1.763(5)
Li(3)-N(1'B)	2.429(9)	C(3A)-C(4A)	1.390(6)
Li(3)-C(1C)	2.502(10)	N(2A)-C(8A)	1.333(5)
Li(3)-C(1B)	2.573(9)	N(2A)-C(14A)	1.391(5)
Li(3)-N(1'A)	2.712(9)	C(4A)-C(5A)	1.371(7)

C(5A)-C(6A)	1.372(6)	C(1T)-C(6T)	1.392(11)
C(6A)-C(7A)	1.402(6)	C(1T)-C(7T)	1.491(11)
C(6A)-C(15A)	1.497(7)	C(2T)-C(3T)	1.345(11)
C(9A)-C(10A)	1.382(6)	C(3T)-C(4T)	1.412(11)
C(9A)-C(14A)	1.394(6)	C(4T)-C(5T)	1.403(10)
C(10A)-C(11A)	1.365(6)	C(5T)-C(6T)	1.361(10)
C(11A)-C(12A)	1.378(7)	C(1')-C(2')	1.380(14)
C(12A)-C(13A)	1.382(6)	C(1')-C(6')	1.384(14)
C(13A)-C(14A)	1.406(6)	C(1')-C(7')	1.505(15)
C(13A)-C(16A)	1.491(6)	C(2')-C(3')	1.361(15)
C(1B)-N(1B)	1.319(6)	C(3')-C(4')	1.390(15)
C(1B)-N(1'B)	1.347(6)	C(4')-C(5')	1.405(15)
C(1B)-S(1B)	1.763(5)	C(5')-C(6')	1.366(14)
N(1'B)-C(8B)	1.348(6)		
S(1B)-C(2B)	1.755(5)	N(1)-C(1)-N(1')	118.2(4)
C(2B)-C(3B)	1.368(7)	N(1)-C(1)-S(1)	114.1(4)
C(2B)-C(7B)	1.391(7)	N(1')-C(1)-S(1)	127.7(4)
N(1B)-C(7B)	1.395(6)	N(1)-C(1)-Li(1)	55.1(3)
S(2B)-C(9B)	1.740(5)	N(1')-C(1)-Li(1)	63.5(3)
S(2B)-C(8B)	1.761(5)	S(1)-C(1)-Li(1)	167.4(4)
C(3B)-C(4B)	1.354(7)	C(1)-N(1')-C(8)	125.2(4)
N(2B)-C(8B)	1.320(6)	C(1)-N(1')-Li(1)	83.9(4)
N(2B)-C(14B)	1.390(6)	C(8)-N(1')-Li(1)	148.0(4)
C(4B)-C(5B)	1.359(7)	C(1)-N(1')-Li(2)	149.3(4)
C(5B)-C(6B)	1.389(7)	C(8)-N(1')-Li(2)	80.2(4)
C(6B)-C(7B)	1.404(7)	Li(1)-N(1')-Li(2)	77.8(3)
C(6B)-C(15B)	1.495(7)	C(2)-S(1)-C(1)	89.4(2)
C(9B)-C(14B)	1.403(6)	N(1)-Li(1)-N(2A)	143.3(5)
C(9B)-C(10B)	1.404(7)	N(1)-Li(1)-N(1'B)	104.5(4)
C(10B)-C(11B)	1.351(7)	N(2A)-Li(1)-N(1'B)	110.6(4)
C(11B)-C(12B)	1.396(7)	N(1)-Li(1)-N(1')	64.7(3)
C(12B)-C(13B)	1.379(7)	N(2A)-Li(1)-N(1')	101.1(4)
C(13B)-C(14B)	1.384(6)	N(1'B)-Li(1)-N(1')	95.6(4)
C(13B)-C(16B)	1.510(7)	N(1)-Li(1)-C(1)	32.3(2)
C(1C)-N(1C)	1.313(6)	N(2A)-Li(1)-C(1)	124.4(4)
C(1C)-N(1'C)	1.350(6)	N(1'B)-Li(1)-C(1)	104.3(4)
C(1C)-S(1C)	1.765(5)	N(1')-Li(1)-C(1)	32.58(19)
N(1'C)-C(8C)	1.338(6)	N(1)-Li(1)-C(8B)	99.8(4)
S(1C)-C(2C)	1.736(5)	N(2A)-Li(1)-C(8B)	115.6(4)
C(2C)-C(3C)	1.386(7)	N(1'B)-Li(1)-C(8B)	31.43(18)
C(2C)-C(7C)	1.390(6)	N(1')-Li(1)-C(8B)	122.3(4)
N(1C)-C(7C)	1.400(6)	C(1)-Li(1)-C(8B)	116.9(4)
S(2C)-C(9C)	1.733(5)	N(1)-Li(1)-N(2B)	115.1(4)
S(2C)-C(8C)	1.770(5)	N(2A)-Li(1)-N(2B)	93.8(3)
C(3C)-C(4C)	1.361(7)	N(1'B)-Li(1)-N(2B)	55.2(2)
N(2C)-C(8C)	1.328(6)	N(1')-Li(1)-N(2B)	150.6(4)
N(2C)-C(14C)	1.378(6)	C(1)-Li(1)-N(2B)	141.8(4)
C(4C)-C(5C)	1.366(7)	C(8B)-Li(1)-N(2B)	29.22(16)
C(5C)-C(6C)	1.397(6)	C(3)-C(2)-C(7)	122.6(5)
C(6C)-C(7C)	1.384(6)	C(3)-C(2)-S(1)	127.6(4)
C(6C)-C(15C)	1.508(7)	C(7)-C(2)-S(1)	109.8(3)
C(9C)-C(10C)	1.375(7)	C(1)-N(1)-C(7)	111.5(4)
C(9C)-C(14C)	1.398(6)	C(1)-N(1)-Li(1)	92.6(4)
C(10C)-C(11C)	1.369(8)	C(7)-N(1)-Li(1)	154.9(4)
C(11C)-C(12C)	1.380(7)	C(9)-S(2)-C(8)	89.5(3)
C(12C)-C(13C)	1.380(7)	N(2)-Li(2)-N(1'A)	114.3(5)
C(13C)-C(14C)	1.404(7)	N(2)-Li(2)-N(1B)	121.0(5)
C(13C)-C(16C)	1.480(7)	N(1'A)-Li(2)-N(1B)	122.1(4)
C(1T)-C(2T)	1.375(10)	N(2)-Li(2)-N(1')	65.5(3)

N(1'A)-Li(2)-N(1')	121.4(5)	N(1'C)-Li(3)-C(1A)	79.6(3)
N(1B)-Li(2)-N(1')	97.0(4)	N(1'B)-Li(3)-C(1A)	104.7(3)
N(2)-Li(2)-C(8)	33.1(2)	C(1C)-Li(3)-C(1A)	105.0(3)
N(1'A)-Li(2)-C(8)	129.5(5)	C(1B)-Li(3)-C(1A)	120.6(3)
N(1B)-Li(2)-C(8)	106.8(4)	N(1'A)-Li(3)-C(1A)	28.83(15)
N(1')-Li(2)-C(8)	33.30(19)	N(1C)-Li(3)-Li(4)	101.5(4)
N(2)-Li(2)-C(1B)	133.9(4)	N(1A)-Li(3)-Li(4)	90.9(4)
N(1'A)-Li(2)-C(1B)	110.3(4)	N(1B)-Li(3)-Li(4)	106.4(3)
N(1B)-Li(2)-C(1B)	29.72(19)	N(1'C)-Li(3)-Li(4)	45.3(2)
N(1')-Li(2)-C(1B)	81.8(3)	N(1'B)-Li(3)-Li(4)	54.1(2)
C(8)-Li(2)-C(1B)	105.7(3)	C(1C)-Li(3)-Li(4)	74.8(3)
N(2)-Li(2)-N(1'B)	149.3(4)	C(1B)-Li(3)-Li(4)	84.7(3)
N(1'A)-Li(2)-N(1'B)	84.0(3)	N(1'A)-Li(3)-Li(4)	46.6(2)
N(1B)-Li(2)-N(1'B)	56.8(3)	C(1A)-Li(3)-Li(4)	65.4(3)
N(1')-Li(2)-N(1'B)	84.0(3)	C(3)-C(4)-C(5)	121.0(5)
C(8)-Li(2)-N(1'B)	116.2(4)	N(2B)-Li(4)-N(2C)	124.1(4)
C(1B)-Li(2)-N(1'B)	29.58(17)	N(2B)-Li(4)-N(1'C)	102.6(4)
N(2)-Li(2)-Li(4)	141.7(5)	N(2C)-Li(4)-N(1'C)	66.2(3)
N(1'A)-Li(2)-Li(4)	38.6(2)	N(2B)-Li(4)-N(1'A)	136.5(4)
N(1B)-Li(2)-Li(4)	95.9(4)	N(2C)-Li(4)-N(1'A)	99.3(4)
N(1')-Li(2)-Li(4)	102.7(4)	N(1'C)-Li(4)-N(1'A)	95.3(4)
C(8)-Li(2)-Li(4)	131.1(4)	N(2B)-Li(4)-C(8C)	118.2(4)
C(1B)-Li(2)-Li(4)	74.6(3)	N(2C)-Li(4)-C(8C)	32.99(18)
N(1'B)-Li(2)-Li(4)	46.0(2)	N(1'C)-Li(4)-C(8C)	33.17(18)
C(4)-C(3)-C(2)	117.3(5)	N(1'A)-Li(4)-C(8C)	98.2(3)
C(8)-N(2)-C(14)	112.3(4)	N(2B)-Li(4)-N(2A)	99.9(3)
C(8)-N(2)-Li(2)	93.2(4)	N(2C)-Li(4)-N(2A)	111.9(4)
C(14)-N(2)-Li(2)	149.9(4)	N(1'C)-Li(4)-N(2A)	153.1(4)
N(1C)-Li(3)-N(1A)	119.5(4)	N(1'A)-Li(4)-N(2A)	58.0(2)
N(1C)-Li(3)-N(1B)	117.5(4)	C(8C)-Li(4)-N(2A)	138.6(4)
N(1A)-Li(3)-N(1B)	114.7(4)	N(2B)-Li(4)-N(1'B)	58.7(2)
N(1C)-Li(3)-N(1'C)	63.1(3)	N(2C)-Li(4)-N(1'B)	155.1(4)
N(1A)-Li(3)-N(1'C)	89.7(3)	N(1'C)-Li(4)-N(1'B)	88.9(3)
N(1B)-Li(3)-N(1'C)	144.8(4)	N(1'A)-Li(4)-N(1'B)	82.7(3)
N(1C)-Li(3)-N(1'B)	101.4(4)	C(8C)-Li(4)-N(1'B)	122.1(4)
N(1A)-Li(3)-N(1'B)	131.5(4)	N(2A)-Li(4)-N(1'B)	90.4(3)
N(1B)-Li(3)-N(1'B)	58.5(2)	N(2B)-Li(4)-C(8A)	129.0(4)
N(1'C)-Li(3)-N(1'B)	86.4(3)	N(2C)-Li(4)-C(8A)	96.1(3)
N(1C)-Li(3)-C(1C)	31.47(19)	N(1'C)-Li(4)-C(8A)	123.2(4)
N(1A)-Li(3)-C(1C)	103.3(4)	N(1'A)-Li(4)-C(8A)	31.90(17)
N(1B)-Li(3)-C(1C)	141.8(4)	C(8C)-Li(4)-C(8A)	112.5(3)
N(1'C)-Li(3)-C(1C)	32.10(17)	N(2A)-Li(4)-C(8A)	30.57(15)
N(1'B)-Li(3)-C(1C)	98.5(3)	N(1'B)-Li(4)-C(8A)	98.2(3)
N(1C)-Li(3)-C(1B)	102.1(4)	N(2B)-Li(4)-C(8B)	29.71(18)
N(1A)-Li(3)-C(1B)	138.2(4)	N(2C)-Li(4)-C(8B)	142.1(4)
N(1B)-Li(3)-C(1B)	30.81(18)	N(1'C)-Li(4)-C(8B)	90.4(3)
N(1'C)-Li(3)-C(1B)	114.7(4)	N(1'A)-Li(4)-C(8B)	112.7(4)
N(1'B)-Li(3)-C(1B)	31.08(17)	C(8C)-Li(4)-C(8B)	118.7(4)
C(1C)-Li(3)-C(1B)	115.4(4)	N(2A)-Li(4)-C(8B)	102.4(3)
N(1C)-Li(3)-N(1'A)	143.0(4)	N(1'B)-Li(4)-C(8B)	30.28(16)
N(1A)-Li(3)-N(1'A)	55.8(2)	C(8A)-Li(4)-C(8B)	121.8(3)
N(1B)-Li(3)-N(1'A)	93.0(3)	N(2B)-Li(4)-Li(3)	102.4(4)
N(1'C)-Li(3)-N(1'A)	79.9(3)	N(2C)-Li(4)-Li(3)	108.2(4)
N(1'B)-Li(3)-N(1'A)	76.0(3)	N(1'C)-Li(4)-Li(3)	51.4(3)
C(1C)-Li(3)-N(1'A)	111.6(4)	N(1'A)-Li(4)-Li(3)	60.0(3)
C(1B)-Li(3)-N(1'A)	93.9(3)	C(8C)-Li(4)-Li(3)	79.1(3)
N(1C)-Li(3)-C(1A)	132.4(4)	N(2A)-Li(4)-Li(3)	109.4(3)
N(1A)-Li(3)-C(1A)	27.67(18)	N(1'B)-Li(4)-Li(3)	51.4(2)
N(1B)-Li(3)-C(1A)	110.0(3)	C(8A)-Li(4)-Li(3)	91.4(3)

C(8B)-Li(4)-Li(3)	73.7(3)
N(2B)-Li(4)-Li(2)	103.1(3)
N(2C)-Li(4)-Li(2)	132.2(4)
N(1'C)-Li(4)-Li(2)	99.1(3)
N(1'A)-Li(4)-Li(2)	34.3(2)
C(8C)-Li(4)-Li(2)	119.3(4)
N(2A)-Li(4)-Li(2)	61.3(2)
N(1'B)-Li(4)-Li(2)	49.1(2)
C(8A)-Li(4)-Li(2)	52.6(2)
C(8B)-Li(4)-Li(2)	78.5(3)
Li(3)-Li(4)-Li(2)	48.6(2)
C(6)-C(5)-C(4)	121.3(5)
C(5)-C(6)-C(7)	118.4(5)
C(5)-C(6)-C(15)	120.0(5)
C(7)-C(6)-C(15)	121.6(4)
C(2)-C(7)-C(6)	119.4(4)
C(2)-C(7)-N(1)	115.1(5)
C(6)-C(7)-N(1)	125.5(5)
N(2)-C(8)-N(1')	117.8(4)
N(2)-C(8)-S(2)	113.7(4)
N(1')-C(8)-S(2)	128.5(4)
N(2)-C(8)-Li(2)	53.6(3)
N(1')-C(8)-Li(2)	66.5(3)
S(2)-C(8)-Li(2)	159.3(4)
C(10)-C(9)-C(14)	121.6(5)
C(10)-C(9)-S(2)	128.9(4)
C(14)-C(9)-S(2)	109.5(4)
C(9)-C(10)-C(11)	116.6(5)
C(12)-C(11)-C(10)	121.6(6)
C(11)-C(12)-C(13)	123.2(6)
C(12)-C(13)-C(14)	116.4(5)
C(12)-C(13)-C(16)	122.5(5)
C(14)-C(13)-C(16)	121.1(5)
N(2)-C(14)-C(9)	115.0(5)
N(2)-C(14)-C(13)	124.4(5)
C(9)-C(14)-C(13)	120.6(5)
N(1A)-C(1A)-N(1'A)	118.7(4)
N(1A)-C(1A)-S(1A)	114.6(3)
N(1'A)-C(1A)-S(1A)	126.7(4)
N(1A)-C(1A)-Li(3)	46.7(3)
N(1'A)-C(1A)-Li(3)	74.2(3)
S(1A)-C(1A)-Li(3)	154.1(3)
C(8A)-N(1'A)-C(1A)	124.1(4)
C(8A)-N(1'A)-Li(2)	108.7(4)
C(1A)-N(1'A)-Li(2)	112.1(4)
C(8A)-N(1'A)-Li(4)	85.9(3)
C(1A)-N(1'A)-Li(4)	115.5(3)
Li(2)-N(1'A)-Li(4)	107.0(4)
C(8A)-N(1'A)-Li(3)	155.9(3)
C(1A)-N(1'A)-Li(3)	76.9(3)
Li(2)-N(1'A)-Li(3)	67.6(3)
Li(4)-N(1'A)-Li(3)	73.3(3)
C(2A)-S(1A)-C(1A)	88.9(2)
C(3A)-C(2A)-C(7A)	122.1(4)
C(3A)-C(2A)-S(1A)	127.7(4)
C(7A)-C(2A)-S(1A)	110.1(3)
C(1A)-N(1A)-C(7A)	111.7(4)
C(1A)-N(1A)-Li(3)	105.7(4)
C(7A)-N(1A)-Li(3)	136.3(4)
C(9A)-S(2A)-C(8A)	89.4(2)
C(2A)-C(3A)-C(4A)	117.6(5)
C(8A)-N(2A)-C(14A)	111.1(4)
C(8A)-N(2A)-Li(1)	121.6(4)
C(14A)-N(2A)-Li(1)	122.8(4)
C(8A)-N(2A)-Li(4)	78.1(3)
C(14A)-N(2A)-Li(4)	139.3(3)
Li(1)-N(2A)-Li(4)	75.6(3)
C(5A)-C(4A)-C(3A)	120.4(4)
C(4A)-C(5A)-C(6A)	123.4(5)
C(5A)-C(6A)-C(7A)	117.2(5)
C(5A)-C(6A)-C(15A)	122.2(4)
C(7A)-C(6A)-C(15A)	120.6(4)
N(1A)-C(7A)-C(6A)	126.2(4)
N(1A)-C(7A)-C(2A)	114.6(4)
C(6A)-C(7A)-C(2A)	119.2(4)
N(2A)-C(8A)-N(1'A)	118.5(4)
N(2A)-C(8A)-S(2A)	114.3(3)
N(1'A)-C(8A)-S(2A)	127.1(3)
N(2A)-C(8A)-Li(4)	71.3(3)
N(1'A)-C(8A)-Li(4)	62.2(3)
S(2A)-C(8A)-Li(4)	141.2(3)
C(10A)-C(9A)-C(14A)	122.5(4)
C(10A)-C(9A)-S(2A)	127.6(4)
C(14A)-C(9A)-S(2A)	109.9(3)
C(11A)-C(10A)-C(9A)	117.2(5)
C(10A)-C(11A)-C(12A)	121.3(5)
C(11A)-C(12A)-C(13A)	122.9(4)
C(12A)-C(13A)-C(14A)	116.3(4)
C(12A)-C(13A)-C(16A)	122.6(4)
C(14A)-C(13A)-C(16A)	121.1(4)
N(2A)-C(14A)-C(9A)	115.3(4)
N(2A)-C(14A)-C(13A)	124.8(4)
C(9A)-C(14A)-C(13A)	119.9(4)
N(1B)-C(1B)-N(1'B)	119.6(4)
N(1B)-C(1B)-S(1B)	114.6(4)
N(1'B)-C(1B)-S(1B)	125.8(4)
N(1B)-C(1B)-Li(3)	62.3(3)
N(1'B)-C(1B)-Li(3)	68.6(3)
S(1B)-C(1B)-Li(3)	147.1(3)
N(1B)-C(1B)-Li(2)	52.0(3)
N(1'B)-C(1B)-Li(2)	75.6(3)
S(1B)-C(1B)-Li(2)	144.4(3)
Li(3)-C(1B)-Li(2)	62.6(3)
C(1B)-N(1'B)-C(8B)	124.7(4)
C(1B)-N(1'B)-Li(1)	115.0(4)
C(8B)-N(1'B)-Li(1)	90.1(4)
C(1B)-N(1'B)-Li(3)	80.3(3)
C(8B)-N(1'B)-Li(3)	124.8(3)
Li(1)-N(1'B)-Li(3)	125.9(4)
C(1B)-N(1'B)-Li(4)	152.8(4)
C(8B)-N(1'B)-Li(4)	79.3(3)
Li(1)-N(1'B)-Li(4)	73.3(3)
Li(3)-N(1'B)-Li(4)	74.6(3)
C(1B)-N(1'B)-Li(2)	74.8(3)
C(8B)-N(1'B)-Li(2)	157.8(4)
Li(1)-N(1'B)-Li(2)	70.4(3)
Li(3)-N(1'B)-Li(2)	64.3(3)
Li(4)-N(1'B)-Li(2)	84.9(3)

C(2B)-S(1B)-C(1B)	89.3(3)
C(3B)-C(2B)-C(7B)	123.1(5)
C(3B)-C(2B)-S(1B)	127.6(4)
C(7B)-C(2B)-S(1B)	109.3(4)
C(1B)-N(1B)-C(7B)	111.1(4)
C(1B)-N(1B)-Li(2)	98.3(4)
C(7B)-N(1B)-Li(2)	130.6(4)
C(1B)-N(1B)-Li(3)	86.9(4)
C(7B)-N(1B)-Li(3)	141.3(4)
Li(2)-N(1B)-Li(3)	76.2(3)
C(9B)-S(2B)-C(8B)	89.4(2)
C(4B)-C(3B)-C(2B)	116.5(6)
C(8B)-N(2B)-C(14B)	111.3(4)
C(8B)-N(2B)-Li(4)	99.5(4)
C(14B)-N(2B)-Li(4)	139.1(4)
C(8B)-N(2B)-Li(1)	72.9(3)
C(14B)-N(2B)-Li(1)	140.9(3)
Li(4)-N(2B)-Li(1)	72.8(3)
C(3B)-C(4B)-C(5B)	123.2(6)
C(4B)-C(5B)-C(6B)	121.0(5)
C(5B)-C(6B)-C(7B)	117.2(5)
C(5B)-C(6B)-C(15B)	122.9(5)
C(7B)-C(6B)-C(15B)	119.9(5)
C(2B)-C(7B)-N(1B)	115.6(5)
C(2B)-C(7B)-C(6B)	118.9(5)
N(1B)-C(7B)-C(6B)	125.5(5)
N(2B)-C(8B)-N(1'B)	117.5(4)
N(2B)-C(8B)-S(2B)	114.6(4)
N(1'B)-C(8B)-S(2B)	127.8(4)
N(2B)-C(8B)-Li(1)	77.8(3)
N(1'B)-C(8B)-Li(1)	58.5(3)
S(2B)-C(8B)-Li(1)	139.4(3)
N(2B)-C(8B)-Li(4)	50.8(3)
N(1'B)-C(8B)-Li(4)	70.5(3)
S(2B)-C(8B)-Li(4)	152.5(3)
Li(1)-C(8B)-Li(4)	65.8(3)
C(14B)-C(9B)-C(10B)	121.0(5)
C(14B)-C(9B)-S(2B)	109.7(4)
C(10B)-C(9B)-S(2B)	129.3(4)
C(11B)-C(10B)-C(9B)	118.1(5)
C(10B)-C(11B)-C(12B)	120.8(5)
C(13B)-C(12B)-C(11B)	122.3(5)
C(12B)-C(13B)-C(14B)	117.4(5)
C(12B)-C(13B)-C(16B)	123.1(5)
C(14B)-C(13B)-C(16B)	119.4(5)
C(13B)-C(14B)-N(2B)	124.7(4)
C(13B)-C(14B)-C(9B)	120.4(5)
N(2B)-C(14B)-C(9B)	115.0(4)
N(1C)-C(1C)-N(1'C)	119.4(4)
N(1C)-C(1C)-S(1C)	115.2(4)
N(1'C)-C(1C)-S(1C)	125.3(4)
N(1C)-C(1C)-Li(3)	52.6(3)
N(1'C)-C(1C)-Li(3)	68.0(3)
S(1C)-C(1C)-Li(3)	164.8(3)
C(8C)-N(1'C)-C(1C)	124.3(4)
C(8C)-N(1'C)-Li(4)	85.6(4)
C(1C)-N(1'C)-Li(4)	147.8(4)
C(8C)-N(1'C)-Li(3)	139.8(4)
C(1C)-N(1'C)-Li(3)	79.9(3)
Li(4)-N(1'C)-Li(3)	83.4(3)
C(2C)-S(1C)-C(1C)	88.5(2)
C(3C)-C(2C)-C(7C)	120.7(5)
C(3C)-C(2C)-S(1C)	128.3(4)
C(7C)-C(2C)-S(1C)	111.0(4)
C(1C)-N(1C)-C(7C)	111.1(4)
C(1C)-N(1C)-Li(3)	95.9(4)
C(7C)-N(1C)-Li(3)	150.6(4)
C(9C)-S(2C)-C(8C)	89.0(2)
C(4C)-C(3C)-C(2C)	118.2(5)
C(8C)-N(2C)-C(14C)	111.5(4)
C(8C)-N(2C)-Li(4)	88.8(4)
C(14C)-N(2C)-Li(4)	158.8(4)
C(3C)-C(4C)-C(5C)	121.6(5)
C(4C)-C(5C)-C(6C)	121.6(5)
C(7C)-C(6C)-C(5C)	116.8(5)
C(7C)-C(6C)-C(15C)	120.1(4)
C(5C)-C(6C)-C(15C)	123.1(5)
C(6C)-C(7C)-C(2C)	121.1(4)
C(6C)-C(7C)-N(1C)	124.7(4)
C(2C)-C(7C)-N(1C)	114.2(4)
N(2C)-C(8C)-N(1'C)	119.4(4)
N(2C)-C(8C)-S(2C)	114.1(4)
N(1'C)-C(8C)-S(2C)	126.2(4)
N(2C)-C(8C)-Li(4)	58.2(3)
N(1'C)-C(8C)-Li(4)	61.2(3)
S(2C)-C(8C)-Li(4)	170.1(3)
C(10C)-C(9C)-C(14C)	121.4(5)
C(10C)-C(9C)-S(2C)	128.1(4)
C(14C)-C(9C)-S(2C)	110.4(4)
C(11C)-C(10C)-C(9C)	117.6(5)
C(10C)-C(11C)-C(12C)	122.1(5)
C(13C)-C(12C)-C(11C)	121.2(5)
C(12C)-C(13C)-C(14C)	117.2(5)
C(12C)-C(13C)-C(16C)	120.4(5)
C(14C)-C(13C)-C(16C)	122.3(5)
N(2C)-C(14C)-C(9C)	115.0(4)
N(2C)-C(14C)-C(13C)	124.7(4)
C(9C)-C(14C)-C(13C)	120.3(5)
C(2T)-C(1T)-C(6T)	118.9(10)
C(2T)-C(1T)-C(7T)	121.3(10)
C(6T)-C(1T)-C(7T)	119.6(10)
C(3T)-C(2T)-C(1T)	122.6(10)
C(2T)-C(3T)-C(4T)	117.9(9)
C(5T)-C(4T)-C(3T)	120.9(9)
C(6T)-C(5T)-C(4T)	118.4(9)
C(5T)-C(6T)-C(1T)	121.2(10)
C(2')-C(1')-C(6')	118.9(16)
C(2')-C(1')-C(7')	118.4(16)
C(6')-C(1')-C(7')	121.9(17)
C(3')-C(2')-C(1')	121.1(16)
C(2')-C(3')-C(4')	118.9(16)
C(3')-C(4')-C(5')	121.4(17)
C(6')-C(5')-C(4')	117.3(16)
C(5')-C(6')-C(1')	122.1(17)

3. ^{1}H, ^{15}N-HMBC for 6