Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Heterocyclic substituted methanides as promising alternatives to the ubiquitous *nacnac* ligand?

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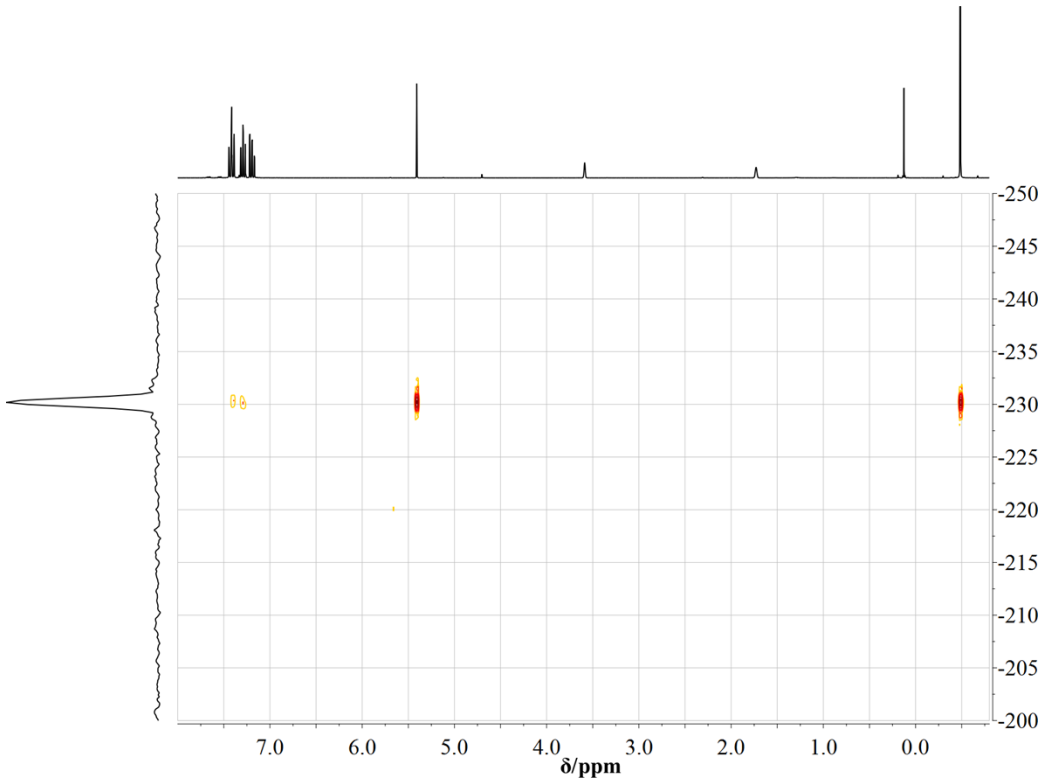
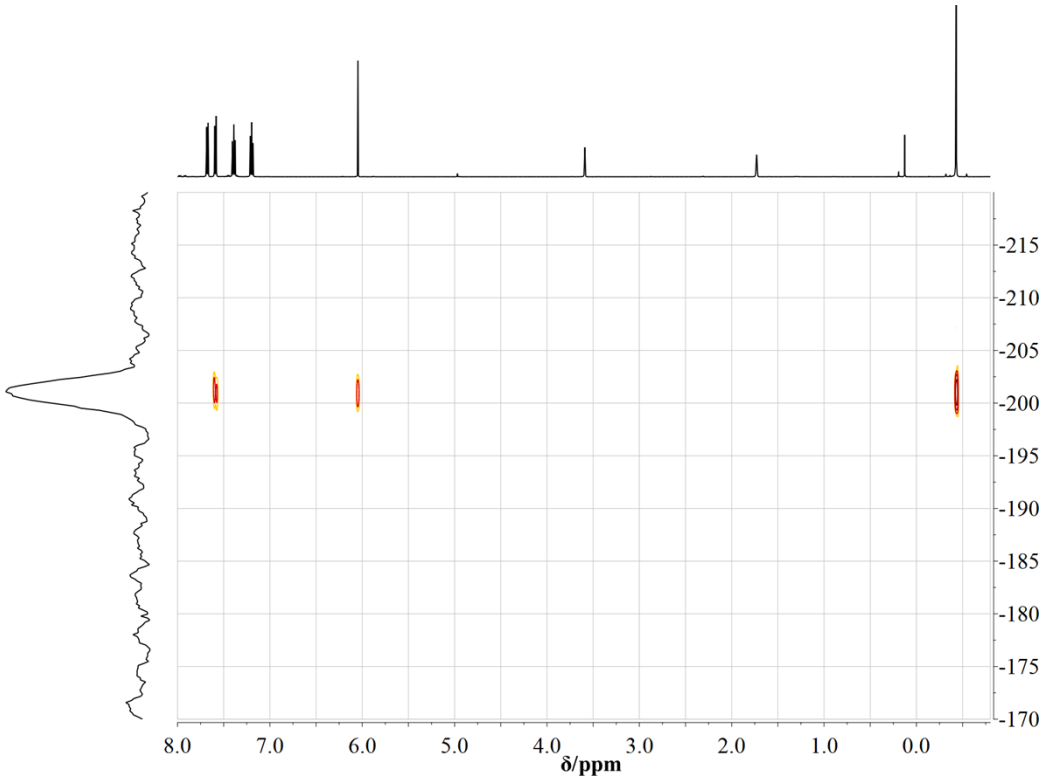
Content:

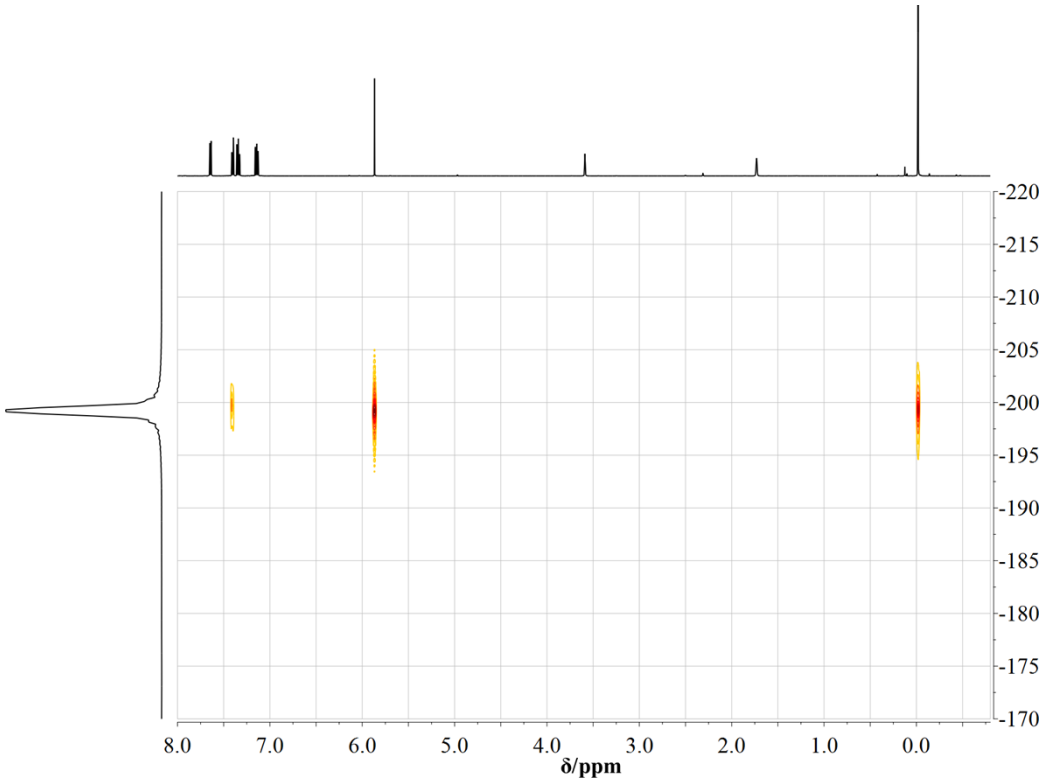
1.1 $^{1}H,^{15}N$-NMR data of 3



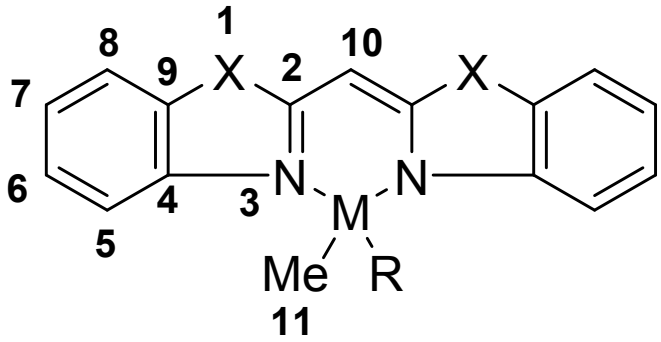
1.2 $^{1}H,^{15}N$-NMR data of 4



1.3 $^{1}H,^{15}N$-NMR data of 8



1.4 Scheme for assignment of the NMR spectroscopic data



2. Crystallographic data

Table S1. Data collection parameters for compounds **1** – **9** at 100 K.

		1	**2**	**3**	**4**
CCDC no.		995110	995111	995112	995113
Crystal system		monoclinic	monoclinic	triclinic	triclinic
Space group		$P2_1/c$	$C2/c$	$P\bar{1}$	$P\bar{1}$
Empirical formula		$C_{15}H_{10}N_2O_2$	$C_{15}H_{10}N_2S_2$	$C_{17}H_{15}AlN_2O_2$	$C_{17}H_{15}AlN_2S_2$
Z		4	4	2	2
Formula mass [g mol^{-1}]		250.25	282.37	306.29	338.41
Unit cell lengths [Å]	*a*	9.066(1)	25.412(3)	7.998(2)	7.126(1)
	b	9.457(1)	4.536(1)	8.336(2)	7.696(1)
	c	14.172(2)	11.165(2)	13.294(3)	14.730(2)
Unit cell angles [deg]	α	90	90	93.54(2)	90.50(1)
	β	104.23(2)	102.76(2)	103.31(2)	93.12(1)
	γ	90	90	117.86(3)	93.44(2)
Volume [Å^3]		1177.8(3)	1255.2(4)	747.6(3)	805.11(19)
ρ_{calc} [Mg/m^{-3}]		1.411	1.494	1.361	1.396
μ [mm^{-1}]		0.096	0.409	0.144	0.382
F(000)		520	584	320	352
crystal size [mm^3]		0.20x0.20x0.08	0.12x0.10x0.10	0.12x0.08x0.08	0.12x0.10x0.10
θ-min, max [deg]		2.32 - 29.69	1.64 - 27.10	1.61 - 25.42	1.39-26.47
max., min. transm.		0.7459, 0.6934	0.7461, 0.7084	0.9705, 0.8155	0.7454, 0.6837
refl. collected		18686	24628	12679	34844
unique refl.		3321	1379	2745	3313
parameters		245	87	201	201
restraints		422	0	24	231
R1, wR2 [$I \geq 2\sigma(I)$][a, b]		0.0390, 0.0978	0.0245, 0.00631	0.0447, 0.1071	0.0320, 0.0867
R1, wR2 (all data)		0.0459, 0.1014	0.0249, 0.0634	0.0676, 0.1181	0.0354, 0.0897
Goodness-of-fit		1.049	1.091	1.025	1.034

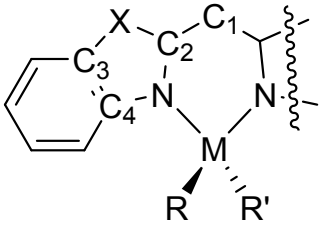
		5	**6**	**7**	**8**
CCDC no.		995114	995115	995116	995117
Crystal system		monoclinic	monoclinic	monoclinic	orthorhombic
Space group		$C2/m$	$P\bar{1}$	$P2_1$	$Pnma$
Empirical formula		$C_{16}H_{12}AlClN_2O_2$	$C_{16}H_{12}AlClN_2S_2$	$C_{17}H_{15}GaN_2O_2$	$C_{17}H_{15}GaN_2S_2$
Z		12	2	4	4
Formula mass [g mol^{-1}]		326.71	358.83	349.03	381.15
Unit cell lengths [Å]	*a*	21.226(3)	7.074(2)	8.386(2)	15.446(3)
	b	15.558(2)	7.694(2)	13.944(3)	15.177(3)
	c	14.163(3)	14.664(3)	13.838(3)	6.929(2)
Unit cell angles [deg]	α	90	89.97(2)	90	90
	β	112.76(2)	85.29(2)	107.60(2)	90
	γ	90	85.89(2)	90	90
Volume [Å^3]		4312.9(12)	793.4(3)	1542.4(6)	1624.3(6)
ρ_{calc} [Mg/m^{-3}]		1.400	1.502	1.503	1.559
μ [mm^{-1}]		0.287	0.555	1.792	1.023
F(000)		1880	368	712	776
crystal size [mm^3]		0.24x0.19x0.09	0.11x0.11x0.08	0.09x0.07x0.07	0.42x0.27x0.26
θ-min, max [deg]		1.56 - 26.37	1.39 - 25.38	1.46 - 28.32	2.08 - 23.68
max., min. transm.		0.7454, 0.7066	0.9143, 0.7544	0.7457, 0.7031	0.7449, 0.6769
refl. collected		49655	21727	46102	40129
unique refl.		4564	2882	7674	2580
parameters		449	209	402	108
restraints		729	32	176	103
R1, wR2 [$I \geq 2\sigma(I)$][a, b]		0.0414, 0.1003	0.0348, 0.00761	0.0339, 0.0790	0.0251, 0.596
R1, wR2 (all data)		0.0464, 0.1025	0.0453, 0.0801	0.0353, 0.0799	0.265, 0.602
Goodness-of-fit		1.118	1.054	1.026	1.268

		9
CCDC no.		995118
Crystal system		monoclinic
Space group		C2/*c*
Empirical formula		$C_{25}H_{19}N_3O_3$
Z		8
Formula mass [g mol^{-1}]		409.43
Unit cell lengths [Å]	*a*	31.997(3)
	b	8.907(1)
	c	15.673(2)
Unit cell angles [deg]	α	90
	β	117.53(1)
	γ	90
Volume [Å^3]		3961.0(8)
ρ_{calc} [Mg/m^{-3}]		1.373
μ [mm^{-1}]		0.092
F(000)		1712
crystal size [mm^3]		0.20 x 0.20 x 0.20
θ-min, max [deg]		1.44 - 27.12
max., min. transm.		0.9703, 0.9216
refl. collected		19537
unique refl.		4360
parameters		358
restraints		594
R1, wR2 [$I \geq 2\sigma(I)$][a, b]		0.0347, 0.0839
R1, wR2 (all data)		0.0429, 0.0891
Goodness-of-fit		1.043

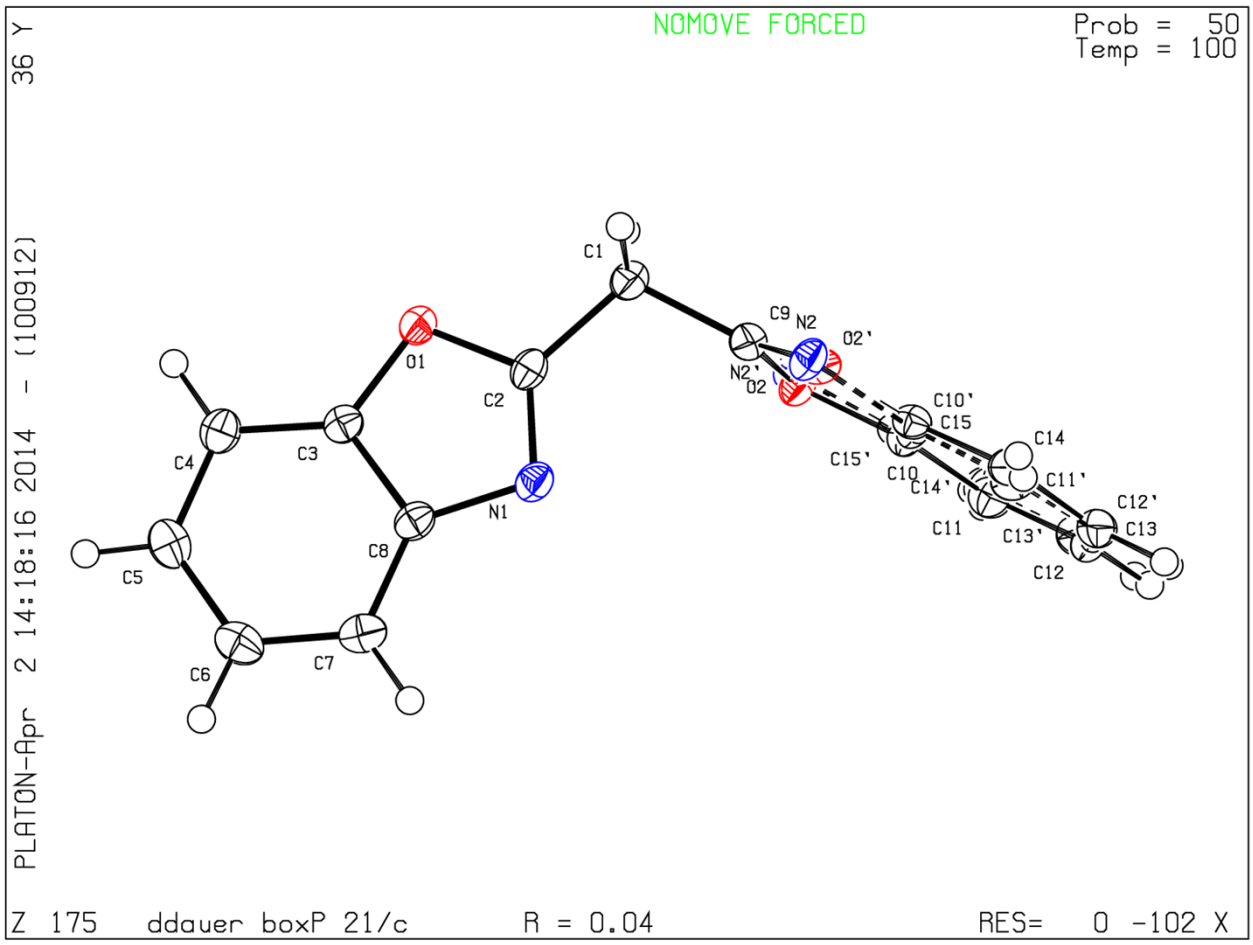
a) $R1 = \frac{\sum \| F_o | - | F_c \|}{\sum | F_o |}$; b) $wR2 = \sqrt{\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}}$ with $w = \frac{1}{\sigma^2(F_o^2) + (g_1 P)^2 + g_2 P}; P = \frac{(F_o^2 + 2F_c^2)}{3}$.

Table S2. Additional bond lengths [pm] and angles [deg] for compounds **1** - **8**

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
C2−X	137.16(13)	174.98(12)	136.8(3)	174.59(16)	136.3(2)	174.5(2)	137.0(8)	175.14(16)
C3−X	138.63(13)	173.49(12)	139.3(3)	173.86(16)	139.0(3)	174.5(2)	139.5(8)	174.04(18)
C3−C4	139.24(15)	140.72(16)	138.3(3)	140.10(20)	138.3(3)	139.7(3)	138.7(10)	140.10(20)
M−C	-	-	195.5(2)	196.14(16)	no statement due to disorder		196.9(7)	196.70(20)
M−Cl	-	-	-	-			-	-
X−C2−N	116.54(10)	116.67(9)	111.90(19)	113.16(12)	112.23(17)	113.01(17)	112.8(6)	112.99(11)
X−C2−C1	117.38(9)	119.68(7)	120.10(20)	120.49(12)	119.76(18)	121.00(17)	118.6(6)	119.78(12)
N−C2−C1	126.06(10)	123.51(10)	128.00(20)	126.36(14)	128.00(19)	126.00(20)	128.6(6)	127.20(15)
C2−X−C3	103.36(8)	88.82(6)	105.98(17)	90.72(7)	105.71(16)	90.83(11)	105.3(5)	90.60(8)
C2−N−M	-	-	125.36(15)	124.31(11)	124.33(14)	123.37(16)	126.7(5)	123.78(11)
C4−N−M	-	-	128.43(15)	123.73(10)	129.60(14)	124.74(15)	126.9(5)	123.92(10)
R−M−R	-	-	115.89(11)	117.96(7)	112.5(6)	113.2(5)	122.6(3)	125.57(10)



2.1 Bond lengths [Å] and angles [deg] for 1.



Bond lengths [Å] and angles [deg] for **1**.

C(1)-C(9)	1.4864(15)	C(10)-C(15)	1.391(3)
C(1)-C(2)	1.4917(15)	C(11)-C(12)	1.396(3)
C(1)-H(1A)	0.9900	C(11)-H(11)	0.9500
C(1)-H(1B)	0.9900	C(12)-C(13)	1.402(3)
C(9)-N(2)	1.284(5)	C(12)-H(12)	0.9500
C(9)-N(2')	1.309(15)	C(13)-C(14)	1.392(4)
C(9)-O(2')	1.335(13)	C(13)-H(13)	0.9500
C(9)-O(2)	1.372(3)	C(14)-C(15)	1.389(4)
O(2)-C(10)	1.390(3)	C(14)-H(14)	0.9500
N(2)-C(15)	1.414(4)	O(2')-C(10')	1.393(13)
C(10)-C(11)	1.385(4)	N(2')-C(15')	1.385(14)

C(10')-C(15')	1.353(12)
C(10')-C(11')	1.416(14)
C(11')-C(12')	1.384(13)
C(11')-H(11')	0.9500
C(12')-C(13')	1.371(10)
C(12')-H(12')	0.9500
C(13')-C(14')	1.352(12)
C(13')-H(13')	0.9500
C(14')-C(15')	1.396(14)
C(14')-H(14')	0.9500
C(2)-N(1)	1.2888(14)
C(2)-O(1)	1.3712(13)
O(1)-C(3)	1.3826(13)
N(1)-C(8)	1.4062(14)
C(3)-C(4)	1.3831(15)
C(3)-C(8)	1.3938(15)
C(4)-C(5)	1.3920(17)
C(4)-H(4)	0.9500
C(5)-C(6)	1.4035(18)
C(5)-H(5)	0.9500
C(6)-C(7)	1.3916(17)
C(6)-H(6)	0.9500
C(7)-C(8)	1.3904(16)
C(7)-H(7)	0.9500

C(9)-C(1)-C(2)	111.23(9)
C(9)-C(1)-H(1A)	109.4
C(2)-C(1)-H(1A)	109.4
C(9)-C(1)-H(1B)	109.4
C(2)-C(1)-H(1B)	109.4
H(1A)-C(1)-H(1B)	108.0
N(2')-C(9)-O(2')	116.5(10)
N(2)-C(9)-O(2)	116.4(3)
N(2)-C(9)-C(1)	124.9(2)
N(2')-C(9)-C(1)	112.9(8)
O(2')-C(9)-C(1)	130.6(7)
O(2)-C(9)-C(1)	118.69(18)
C(9)-O(2)-C(10)	103.4(3)
C(9)-N(2)-C(15)	104.2(4)
C(11)-C(10)-O(2)	127.9(3)
C(11)-C(10)-C(15)	124.4(3)
O(2)-C(10)-C(15)	107.7(3)
C(10)-C(11)-C(12)	115.6(3)
C(10)-C(11)-H(11)	122.2
C(12)-C(11)-H(11)	122.2
C(11)-C(12)-C(13)	121.0(3)
C(11)-C(12)-H(12)	119.5
C(13)-C(12)-H(12)	119.5
C(14)-C(13)-C(12)	122.2(3)
C(14)-C(13)-H(13)	118.9
C(12)-C(13)-H(13)	118.9
C(15)-C(14)-C(13)	117.2(3)
C(15)-C(14)-H(14)	121.4
C(13)-C(14)-H(14)	121.4
C(14)-C(15)-C(10)	119.7(3)
C(14)-C(15)-N(2)	132.0(3)
C(10)-C(15)-N(2)	108.3(3)
C(9)-O(2')-C(10')	102.7(11)
C(9)-N(2')-C(15')	103.1(13)
C(15')-C(10')-O(2')	108.1(13)
C(15')-C(10')-C(11')	125.0(13)
O(2')-C(10')-C(11')	126.8(12)
C(12')-C(11')-C(10')	113.9(12)
C(12')-C(11')-H(11')	123.1
C(10')-C(11')-H(11')	123.1
C(13')-C(12')-C(11')	120.3(13)
C(13')-C(12')-H(12')	119.9
C(11')-C(12')-H(12')	119.9
C(14')-C(13')-C(12')	125.4(13)
C(14')-C(13')-H(13')	117.3
C(12')-C(13')-H(13')	117.3
C(13')-C(14')-C(15')	115.8(13)
C(13')-C(14')-H(14')	122.1
C(15')-C(14')-H(14')	122.1

C(10')-C(15')-N(2')	109.4(13)	C(7)-C(6)-C(5)	121.48(11)
C(10')-C(15')-C(14')	119.5(13)	C(7)-C(6)-H(6)	119.3
N(2')-C(15')-C(14')	131.1(13)	C(5)-C(6)-H(6)	119.3
N(1)-C(2)-O(1)	116.67(10)	C(8)-C(7)-C(6)	117.26(11)
N(1)-C(2)-C(1)	127.22(10)	C(8)-C(7)-H(7)	121.4
O(1)-C(2)-C(1)	116.07(9)	C(6)-C(7)-H(7)	121.4
C(2)-O(1)-C(3)	103.31(8)	C(7)-C(8)-C(3)	120.10(10)
C(2)-N(1)-C(8)	103.63(9)	C(7)-C(8)-N(1)	131.11(10)
O(1)-C(3)-C(4)	128.54(10)	C(3)-C(8)-N(1)	108.78(9)
O(1)-C(3)-C(8)	107.59(9)		
C(4)-C(3)-C(8)	123.87(10)		
C(3)-C(4)-C(5)	115.53(11)		
C(3)-C(4)-H(4)	122.2		
C(5)-C(4)-H(4)	122.2		
C(4)-C(5)-C(6)	121.74(11)		
C(4)-C(5)-H(5)	119.1		
C(6)-C(5)-H(5)	119.1		

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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_2

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_2

```
Bond precision:  C-C = 0.0017 A          Wavelength=0.71073

Cell:             a=9.066(1)     b=9.457(1)          c=14.172(2)
                  alpha=90       beta=104.23(1)      gamma=90
Temperature:      100 K

                 Calculated                Reported  Volume
                 1177.8(3)                 1177.8(3)  Space
group            P 21/c                    P   21/c   Hall
group            -P 2ybc                   -P 2ybc
```

Moiety formula	C15 H10 N2 O2	C15 H10 N2 O2
Sum formula	C15 H10 N2 O2	C15 H10 N2 O2
Mr	250.25	250.25
Dx,g cm-3	1.411	1.411
Z	4	4
Mu (mm-1)	0.096	0.096
F000	520.0	520.0
F000'	520.23	
h,k,lmax	12,13,19	12,13,19
Nref	3341	3321
Tmin,Tmax	0.981,0.992	0.693,0.746
Tmin'	0.981	

Correction method= MULTI-SCAN

Data completeness= 0.994 Theta(max)= 29.687

R(reflections)= 0.0390(2852) wR2(reflections)= 0.1014(3321) S = 1.049 Npar= Npar = 245

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT019_ALERT_1_C	_diffrn_measured_fraction_theta_full/_max < 1.0	0.998	Why ?
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	3.267	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	16	Why ?

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	27	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	17	Why ?
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O2 -- C9 ..	5.8	su
PLAT301_ALERT_3_G	Main Residue Disorder ..... Percentage =	42	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	422	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	4	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check	

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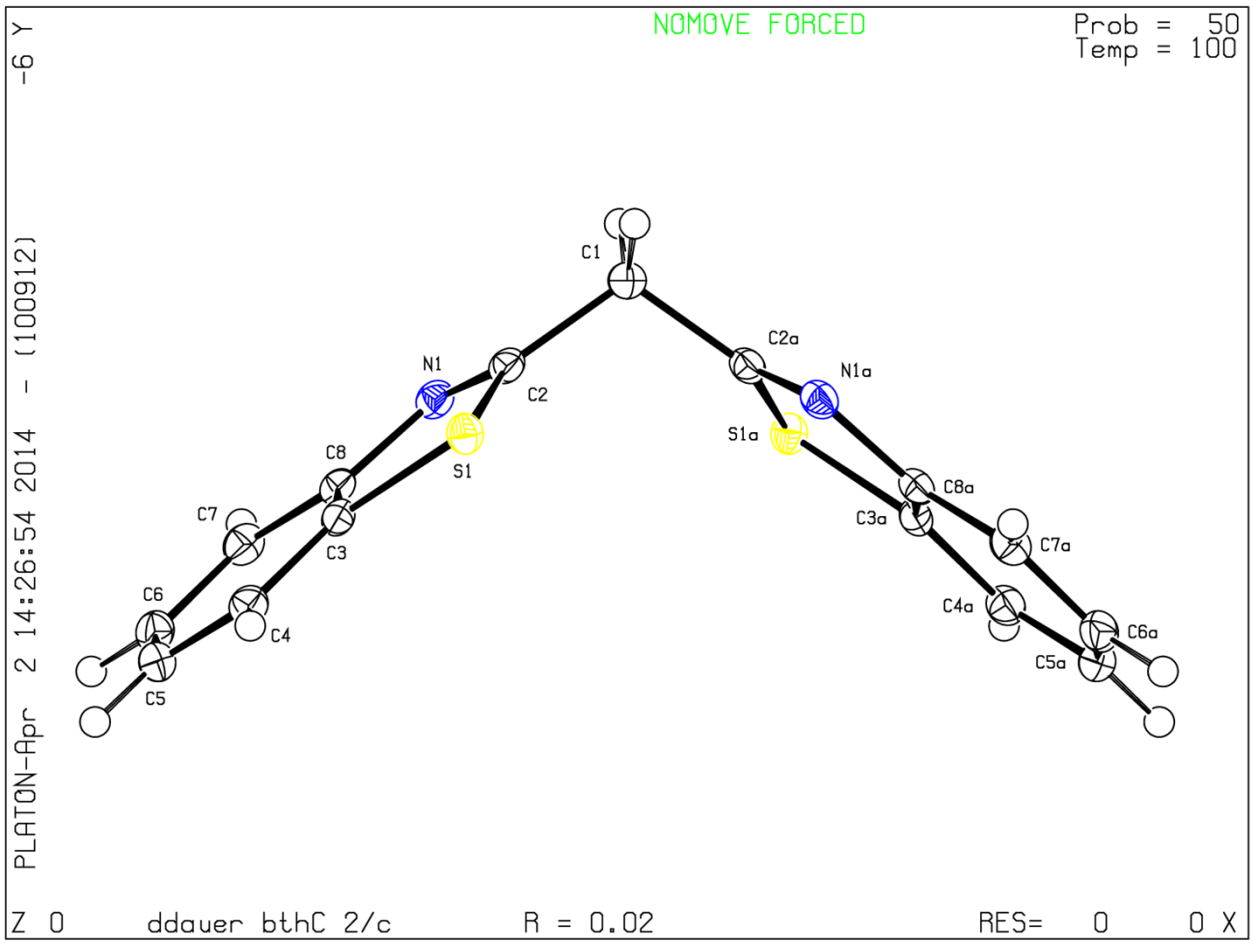
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

2.2 Bond lengths [Å] and angles [deg] for 2.



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

S(1)-C(3)	1.7349(12)	C(4)-C(5)	1.3859(18)
S(1)-C(2)	1.7498(12)	C(4)-H(4)	0.9500
N(1)-C(2)	1.2955(16)	C(5)-C(6)	1.4034(18)
N(1)-C(8)	1.3943(16)	C(5)-H(5)	0.9500
C(1)-C(2)	1.5106(15)	C(7)-C(6)	1.3821(18)
C(1)-C(2)#1	1.5106(15)	C(7)-H(7)	0.9500
C(1)-H(00A)	0.9900	C(6)-H(00C)	0.9500
C(1)-H(00B)	0.9900		
C(8)-C(7)	1.4022(17)	C(3)-S(1)-C(2)	88.82(6)
C(8)-C(3)	1.4072(16)	C(2)-N(1)-C(8)	109.96(10)
C(3)-C(4)	1.3970(17)	C(2)-C(1)-C(2)#1	109.59(14)

C(2)-C(1)-H(00A)	109.8	C(4)-C(5)-C(6)	120.98(12)
C(2)#1-C(1)-H(00A)	109.8	C(4)-C(5)-H(5)	119.5
C(2)-C(1)-H(00B)	109.8	C(6)-C(5)-H(5)	119.5
C(2)#1-C(1)-H(00B)	109.8	C(6)-C(7)-C(8)	118.92(11)
H(00A)-C(1)-H(00B)	108.2	C(6)-C(7)-H(7)	120.5
N(1)-C(2)-C(1)	123.51(10)	C(8)-C(7)-H(7)	120.5
N(1)-C(2)-S(1)	116.67(9)	C(7)-C(6)-C(5)	121.14(11)
C(1)-C(2)-S(1)	119.68(7)	C(7)-C(6)-H(00C)	119.4
N(1)-C(8)-C(7)	125.38(11)	C(5)-C(6)-H(00C)	119.4
N(1)-C(8)-C(3)	115.30(10)		
C(7)-C(8)-C(3)	119.31(11)		
C(4)-C(3)-C(8)	121.87(11)		
C(4)-C(3)-S(1)	128.86(9)		
C(8)-C(3)-S(1)	109.26(9)		
C(5)-C(4)-C(3)	117.77(11)		
C(5)-C(4)-H(4)	121.1		
C(3)-C(4)-H(4)	121.1		

Symmetry transformations used to generate equivalent atoms:

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

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_2

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_2

```
Bond precision:  C-C = 0.0018 A          Wavelength=0.71073

Cell:            a=25.412(3)     b=4.536(1)          c=11.165(2)
                 alpha=90        beta=102.76(2)      gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	1255.2(4)	1255.2(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C15 H10 N2 S2	C15 H10 N2 S2
Sum formula	C15 H10 N2 S2	C15 H10 N2 S2
Mr	282.39	282.37
Dx,g cm-3	1.494	1.494
Z	4	4
Mu (mm-1)	0.409	0.409
F000	584.0	584.0
F000'	585.15	
h,k,lmax	32,5,14	32,5,14
Nref	1385	1379
Tmin,Tmax	0.952,0.960	0.708,0.746
Tmin'	0.952	

Correction method= MULTI-SCAN

Data completeness= 0.996 Theta(max)= 27.097

R(reflections)= 0.0245(1347) wR2(reflections)= 0.0634(1379)

S = 1.091 Npar= Npar = 87

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Why ?

Alert level G

PLAT128_ALERT_4_G Alternate Setting for Input Space-Group C2/c I2/a Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 3 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check

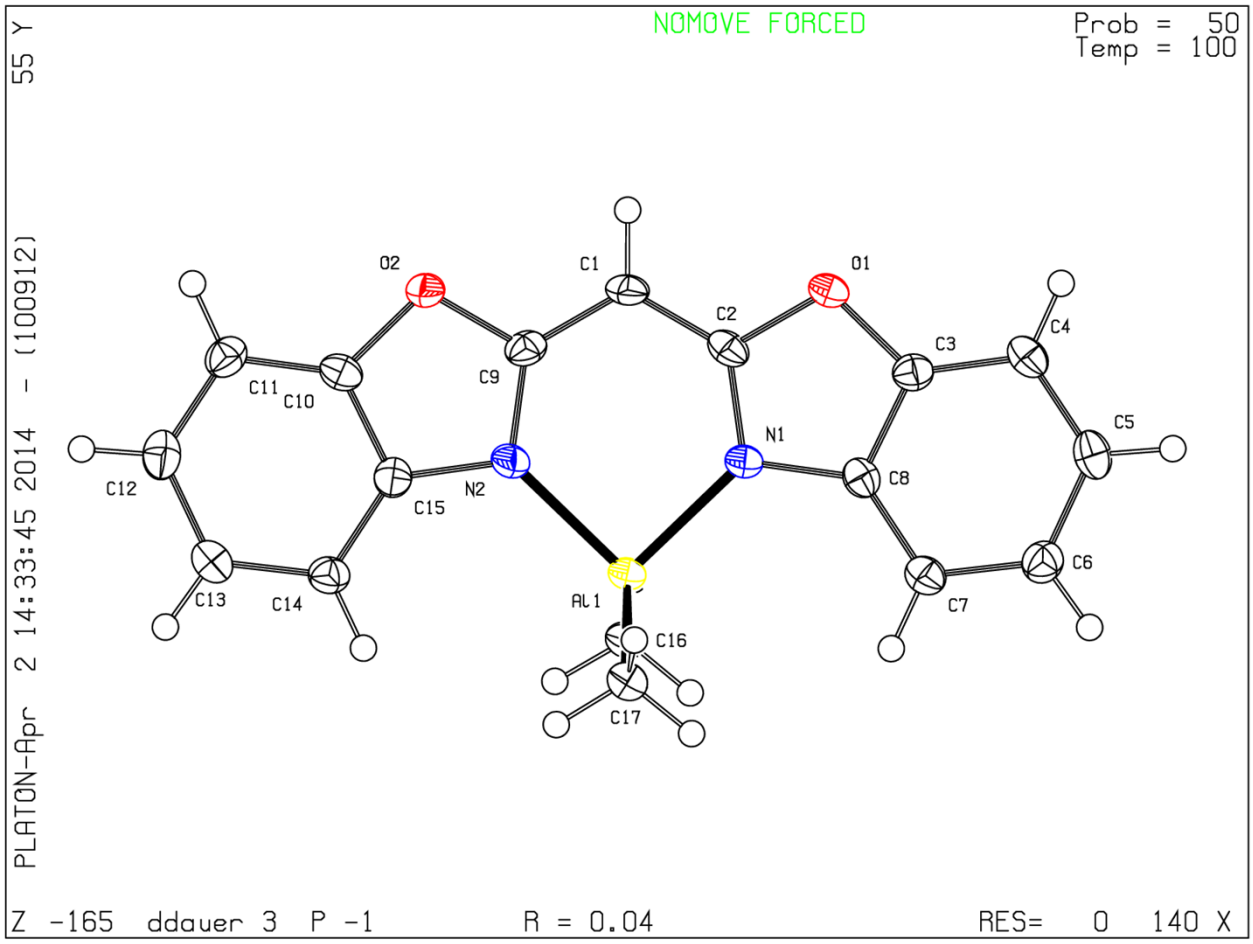
---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 05/02/2014; check.def file version of 05/02/2014

2.3 Bond lengths [Å] and angles [deg] for 3.



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

C(1)-C(2)	1.377(3)	C(4)-C(5)	1.386(3)
C(1)-C(9)	1.383(3)	C(4)-H(4)	0.9500
C(1)-H(1)	0.9500	C(5)-C(6)	1.394(3)
Al(1)-N(1)	1.9171(19)	C(5)-H(5)	0.9500
Al(1)-N(2)	1.918(2)	C(6)-C(7)	1.393(3)
Al(1)-C(17)	1.951(2)	C(6)-H(6)	0.9500
Al(1)-C(16)	1.959(2)	C(7)-C(8)	1.378(3)
C(2)-N(1)	1.348(3)	C(7)-H(7)	0.9500
C(2)-O(1)	1.368(3)	C(8)-N(1)	1.401(3)
O(1)-C(3)	1.390(3)	C(9)-N(2)	1.344(3)
C(3)-C(4)	1.369(3)	C(9)-O(2)	1.367(3)
C(3)-C(8)	1.383(3)	O(2)-C(10)	1.395(3)

C(10)-C(11)	1.368(3)
C(10)-C(15)	1.382(3)
C(11)-C(12)	1.388(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.390(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.388(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.380(3)
C(14)-H(14)	0.9500
C(15)-N(2)	1.406(3)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800

C(2)-C(1)-C(9)	119.5(2)
C(2)-C(1)-H(1)	120.3
C(9)-C(1)-H(1)	120.3
N(1)-Al(1)-N(2)	91.67(9)
N(1)-Al(1)-C(17)	111.92(10)
N(2)-Al(1)-C(17)	112.35(10)
N(1)-Al(1)-C(16)	111.56(10)
N(2)-Al(1)-C(16)	110.97(10)
C(17)-Al(1)-C(16)	115.89(11)
N(1)-C(2)-O(1)	111.75(19)
N(1)-C(2)-C(1)	128.2(2)
O(1)-C(2)-C(1)	120.1(2)
C(2)-O(1)-C(3)	106.06(17)
C(4)-C(3)-C(8)	123.7(2)
C(4)-C(3)-O(1)	128.3(2)
C(8)-C(3)-O(1)	108.03(19)
C(3)-C(4)-C(5)	115.9(2)
C(3)-C(4)-H(4)	122.0
C(5)-C(4)-H(4)	122.0
C(4)-C(5)-C(6)	121.4(2)
C(4)-C(5)-H(5)	119.3
C(6)-C(5)-H(5)	119.3
C(7)-C(6)-C(5)	121.5(2)
C(7)-C(6)-H(6)	119.2
C(5)-C(6)-H(6)	119.2
C(8)-C(7)-C(6)	116.9(2)
C(8)-C(7)-H(7)	121.6
C(6)-C(7)-H(7)	121.6
C(7)-C(8)-C(3)	120.6(2)
C(7)-C(8)-N(1)	131.3(2)
C(3)-C(8)-N(1)	108.09(19)
C(2)-N(1)-C(8)	106.07(18)
C(2)-N(1)-Al(1)	125.22(15)
C(8)-N(1)-Al(1)	128.54(15)
N(2)-C(9)-O(2)	112.05(19)
N(2)-C(9)-C(1)	127.8(2)
O(2)-C(9)-C(1)	120.1(2)
C(9)-O(2)-C(10)	105.89(17)
C(11)-C(10)-C(15)	123.6(2)
C(11)-C(10)-O(2)	128.4(2)
C(15)-C(10)-O(2)	108.01(19)
C(10)-C(11)-C(12)	116.0(2)
C(10)-C(11)-H(11)	122.0
C(12)-C(11)-H(11)	122.0
C(11)-C(12)-C(13)	121.3(2)
C(11)-C(12)-H(12)	119.4
C(13)-C(12)-H(12)	119.4
C(14)-C(13)-C(12)	121.8(2)
C(14)-C(13)-H(13)	119.1
C(12)-C(13)-H(13)	119.1
C(15)-C(14)-C(13)	116.7(2)
C(15)-C(14)-H(14)	121.6
C(13)-C(14)-H(14)	121.6
C(14)-C(15)-C(10)	120.6(2)
C(14)-C(15)-N(2)	131.4(2)
C(10)-C(15)-N(2)	108.01(19)

C(9)-N(2)-C(15)	106.02(18)	H(17A)-C(17)-H(17B)	109.5
C(9)-N(2)-Al(1)	125.50(15)	Al(1)-C(17)-H(17C)	109.5
C(15)-N(2)-Al(1)	128.32(15)	H(17A)-C(17)-H(17C)	109.5
Al(1)-C(16)-H(16A)	109.5	H(17B)-C(17)-H(17C)	109.5
Al(1)-C(16)-H(16B)	109.5		
H(16A)-C(16)-H(16B)	109.5		
Al(1)-C(16)-H(16C)	109.5		
H(16A)-C(16)-H(16C)	109.5		
H(16B)-C(16)-H(16C)	109.5		
Al(1)-C(17)-H(17A)	109.5		
Al(1)-C(17)-H(17B)	109.5		

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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_3

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_3

```
Bond precision:  C-C = 0.0030 A          Wavelength=0.71073

Cell:          a=7.998(2)        b=8.336(2)        c=13.294(3)
               alpha=93.54(2)    beta=103.31(2)    gamma=117.86(3)
Temperature:   100 K

                Calculated                Reported
Volume          747.6(4)                  747.6(4)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C17 H15 Al N2 O2          C17 H15 Al N2 O2
Sum formula     C17 H15 Al N2 O2          C17 H15 Al N2 O2
Mr              306.29                    306.29
Dx,g cm-3       1.361                     1.361
Z               2                         2
Mu (mm-1)       0.144                     0.144
F000            320.0                     320.0
F000'           320.24
```

h,k,lmax	9,10,16	9,10,16
Nref	2753	2745
Tmin,Tmax	0.986,0.989	0.816,0.970
Tmin'	0.983	

Correction method= MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.415

R(reflections)= 0.0447(2094) wR2(reflections)= 0.1181(2745)

S = 1.025 Npar= Npar = 201

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3 Why ?

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 22 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 24 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 6 Note

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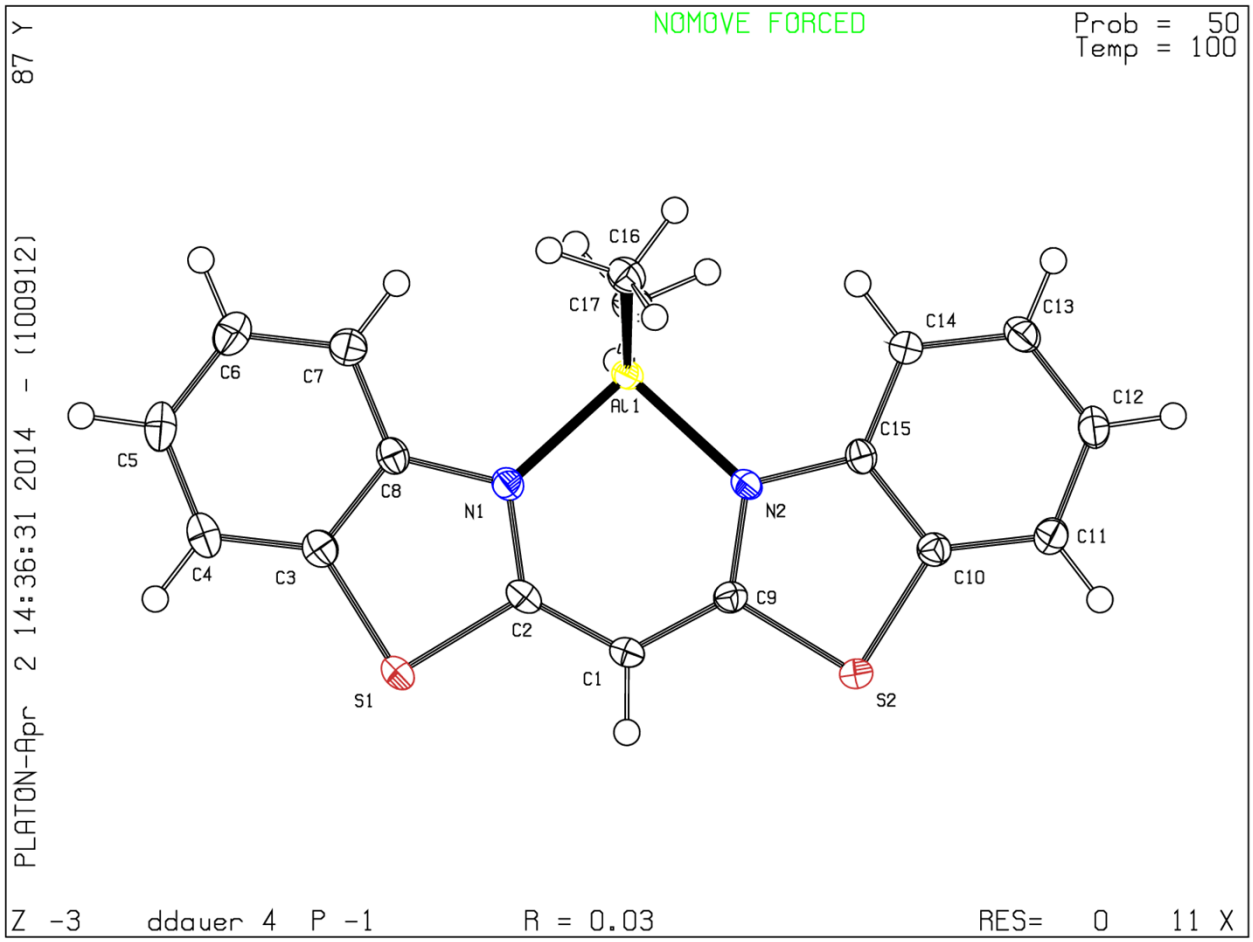
3 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 05/02/2014; check.def file version of 05/02/2014

2.4 Bond lengths [Å] and angles [deg] for 4.



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

C(1)-C(9)	1.389(2)	C(4)-C(5)	1.387(2)
C(1)-C(2)	1.391(2)	C(4)-H(4)	0.9500
C(1)-H(1)	0.9500	C(5)-C(6)	1.392(3)
Al(1)-N(2)	1.9231(13)	C(5)-H(5)	0.9500
Al(1)-N(1)	1.9235(14)	C(6)-C(7)	1.385(2)
Al(1)-C(16)	1.9602(16)	C(6)-H(6)	0.9500
Al(1)-C(17)	1.9625(16)	C(7)-C(8)	1.394(2)
C(2)-N(1)	1.3502(19)	C(7)-H(7)	0.9500
C(2)-S(1)	1.7471(16)	C(8)-N(1)	1.4027(19)
S(1)-C(3)	1.7384(16)	C(9)-N(2)	1.3533(19)
C(3)-C(4)	1.386(2)	C(9)-S(2)	1.7446(15)
C(3)-C(8)	1.398(2)	S(2)-C(10)	1.7387(16)

C(10)-C(11)	1.395(2)	C(4)-C(5)-C(6)	120.66(15)
C(10)-C(15)	1.403(2)	C(4)-C(5)-H(5)	119.7
C(11)-C(12)	1.388(2)	C(6)-C(5)-H(5)	119.7
C(11)-H(11)	0.9500	C(7)-C(6)-C(5)	120.98(15)
C(12)-C(13)	1.390(2)	C(7)-C(6)-H(6)	119.5
C(12)-H(12)	0.9500	C(5)-C(6)-H(6)	119.5
C(13)-C(14)	1.386(2)	C(6)-C(7)-C(8)	118.85(15)
C(13)-H(13)	0.9500	C(6)-C(7)-H(7)	120.6
C(14)-C(15)	1.396(2)	C(8)-C(7)-H(7)	120.6
C(14)-H(14)	0.9500	C(7)-C(8)-C(3)	119.70(14)
C(15)-N(2)	1.3966(19)	C(7)-C(8)-N(1)	126.02(14)
C(16)-H(16A)	0.9800	C(3)-C(8)-N(1)	114.28(13)
C(16)-H(16B)	0.9800	C(2)-N(1)-C(8)	111.86(12)
C(16)-H(16C)	0.9800	C(2)-N(1)-Al(1)	124.26(11)
C(17)-H(17A)	0.9800	C(8)-N(1)-Al(1)	123.84(10)
C(17)-H(17B)	0.9800	N(2)-C(9)-C(1)	126.23(14)
C(17)-H(17C)	0.9800	N(2)-C(9)-S(2)	113.19(11)
		C(1)-C(9)-S(2)	120.58(12)
C(9)-C(1)-C(2)	123.53(14)	C(10)-S(2)-C(9)	90.72(7)
C(9)-C(1)-H(1)	118.2	C(11)-C(10)-C(15)	121.51(14)
C(2)-C(1)-H(1)	118.2	C(11)-C(10)-S(2)	128.59(12)
N(2)-Al(1)-N(1)	94.79(6)	C(15)-C(10)-S(2)	109.90(11)
N(2)-Al(1)-C(16)	111.16(6)	C(12)-C(11)-C(10)	117.98(15)
N(1)-Al(1)-C(16)	111.26(7)	C(12)-C(11)-H(11)	121.0
N(2)-Al(1)-C(17)	108.76(6)	C(10)-C(11)-H(11)	121.0
N(1)-Al(1)-C(17)	110.46(7)	C(11)-C(12)-C(13)	120.89(15)
C(16)-Al(1)-C(17)	117.96(7)	C(11)-C(12)-H(12)	119.6
N(1)-C(2)-C(1)	126.48(14)	C(13)-C(12)-H(12)	119.6
N(1)-C(2)-S(1)	113.12(12)	C(14)-C(13)-C(12)	121.19(15)
C(1)-C(2)-S(1)	120.40(12)	C(14)-C(13)-H(13)	119.4
C(3)-S(1)-C(2)	90.72(7)	C(12)-C(13)-H(13)	119.4
C(4)-C(3)-C(8)	121.50(15)	C(13)-C(14)-C(15)	118.87(14)
C(4)-C(3)-S(1)	128.48(13)	C(13)-C(14)-H(14)	120.6
C(8)-C(3)-S(1)	110.02(11)	C(15)-C(14)-H(14)	120.6
C(3)-C(4)-C(5)	118.30(16)	C(14)-C(15)-N(2)	126.12(14)
C(3)-C(4)-H(4)	120.8	C(14)-C(15)-C(10)	119.55(14)
C(5)-C(4)-H(4)	120.8	N(2)-C(15)-C(10)	114.32(13)

C(9)-N(2)-C(15)	111.87(12)	Al(1)-C(17)-H(17C)	109.5
C(9)-N(2)-Al(1)	124.35(10)	H(17A)-C(17)-H(17C)	109.5
C(15)-N(2)-Al(1)	123.62(10)	H(17B)-C(17)-H(17C)	109.5
Al(1)-C(16)-H(16A)	109.5		
Al(1)-C(16)-H(16B)	109.5		
H(16A)-C(16)-H(16B)	109.5		
Al(1)-C(16)-H(16C)	109.5		
H(16A)-C(16)-H(16C)	109.5		
H(16B)-C(16)-H(16C)	109.5		
Al(1)-C(17)-H(17A)	109.5		
Al(1)-C(17)-H(17B)	109.5		
H(17A)-C(17)-H(17B)	109.5		

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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_4

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_4

```
Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:           a=7.126(1)        b=7.696(1)       c=14.730(2)
                alpha=90.50(1)    beta=93.12(1)    gamma=93.44(2)
Temperature:    100 K

                Calculated                Reported
Volume          805.11(19)                805.11(19)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C17 H15 Al N2 S2          C17 H15 Al N2 S2
Sum formula     C17 H15 Al N2 S2          C17 H15 Al N2 S2
Mr              338.43                    338.41
Dx,g cm-3       1.396                     1.396
Z               2                         2
Mu (mm-1)       0.382                     0.382
F000            352.0                     352.0
```

```
F000'           352.70
h,k,lmax        8,9,18                  8,9,18
Nref            3320                    3313
Tmin,Tmax       0.955,0.963             0.684,0.745
Tmin'           0.955

Correction method= MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.471

R(reflections)= 0.0320( 2997)     wR2(reflections)= 0.0897( 3313)

S = 1.034                 Npar= Npar = 201
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          2 Why ?
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         22          Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         22     Why      ?
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       231          Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         !          Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         6          Note
PLAT931_ALERT_5_G Found Twin Law (16-1 -2)[       ] Estimated BASF      0.49         Check
PLAT931_ALERT_5_G Found Twin Law (       )[ 0 4  1] Estimated BASF      0.61 Check
```

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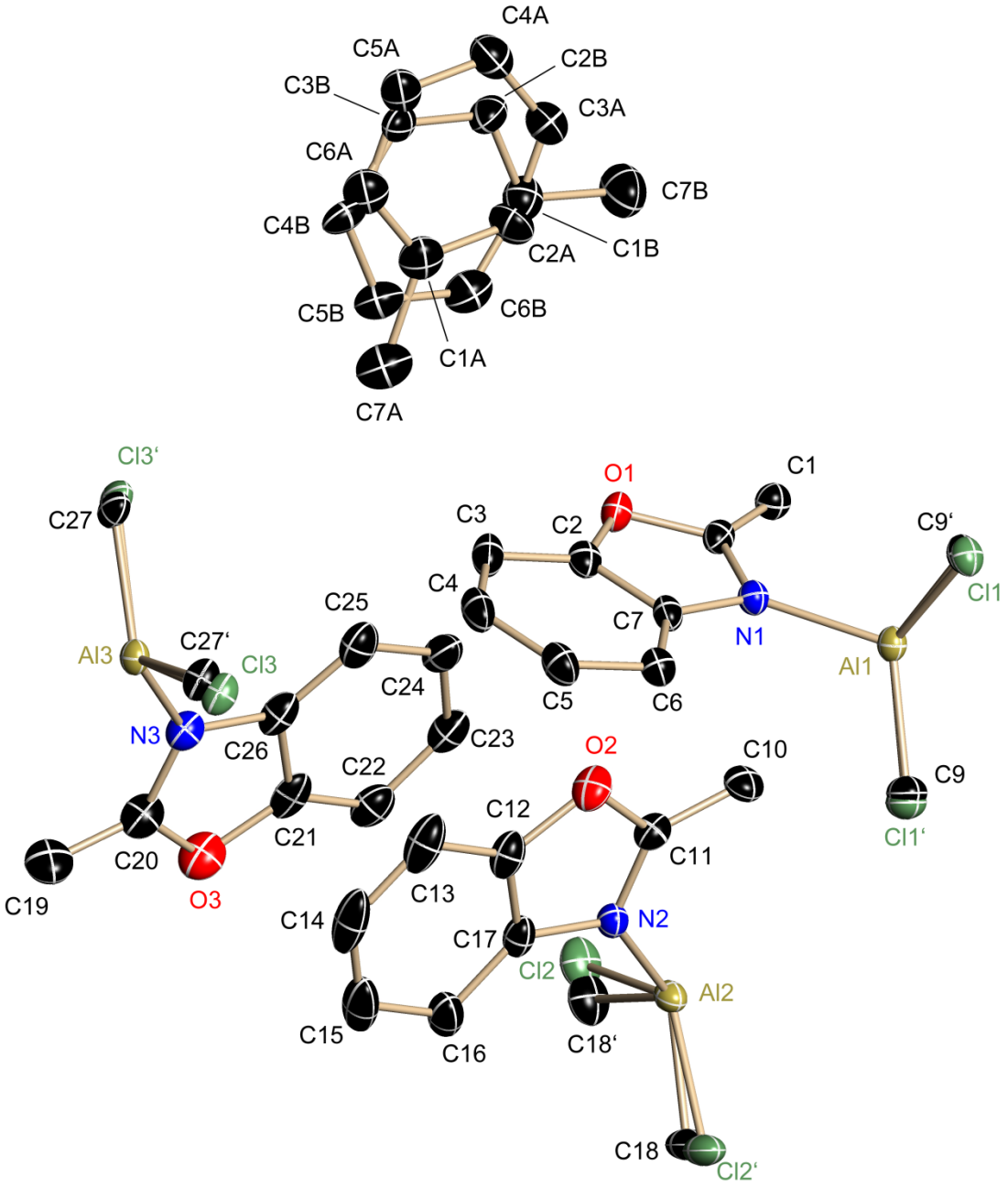
0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

PLATON version of 05/02/2014; check.def file version of 05/02/2014

2.5 Bond lengths [Å] and angles [deg] for 5.



Bond lengths [Å] and angles [deg] for **5**.

C(1)-C(2)	1.385(2)	C(3)-C(8)	1.386(3)
C(1)-C(2)#1	1.385(2)	C(3)-O(1)	1.388(2)
C(1)-H(1)	0.9500	C(4)-C(5)	1.394(3)
C(2)-N(1)	1.350(2)	C(4)-H(4)	0.9500
C(2)-O(1)	1.363(2)	C(5)-C(6)	1.391(3)
C(3)-C(4)	1.380(3)	C(5)-H(5)	0.9500

C(6)-C(7)	1.400(3)	Al(2)-C(18)	1.940(9)
C(6)-H(6)	0.9500	Al(2)-Cl(2')	2.120(9)
C(7)-C(8)	1.384(3)	Al(2)-Cl(2)	2.1522(15)
C(7)-H(7)	0.9500	C(18)-H(18A)	0.9800
C(8)-N(1)	1.410(2)	C(18)-H(18B)	0.9800
N(1)-Al(1)	1.8961(17)	C(18)-H(18C)	0.9800
Al(1)-N(1)#1	1.8961(17)	C(18')-H(18D)	0.9800
Al(1)-C(9)	1.942(12)	C(18')-H(18E)	0.9800
Al(1)-C(9')	1.99(6)	C(18')-H(18F)	0.9800
Al(1)-Cl(1')	2.061(14)	C(19)-C(20)	1.378(15)
Al(1)-Cl(1)	2.130(3)	C(19)-H(19A)	0.9603
C(9)-H(9A)	0.9800	C(20)-N(3)	1.348(10)
C(9)-H(9B)	0.9800	C(20)-O(3)	1.363(5)
C(9)-H(9C)	0.9800	C(21)-C(22)	1.381(10)
C(9')-H(9'A)	0.9800	C(21)-O(3)	1.388(11)
C(9')-H(9'B)	0.9800	C(21)-C(26)	1.390(12)
C(9')-H(9'C)	0.9800	C(22)-C(23)	1.379(8)
C(10)-C(11)#1	1.378(2)	C(22)-H(22)	0.9500
C(10)-C(11)	1.378(2)	C(23)-C(24)	1.384(9)
C(10)-H(10)	0.9500	C(23)-H(23)	0.9500
C(11)-N(2)	1.346(3)	C(24)-C(25)	1.401(10)
C(11)-O(2)	1.363(2)	C(24)-H(24)	0.9500
C(12)-C(17)	1.379(3)	C(25)-C(26)	1.372(11)
C(12)-C(13)	1.380(3)	C(25)-H(25)	0.9500
C(12)-O(2)	1.391(3)	C(26)-N(3)	1.419(5)
C(13)-C(14)	1.380(4)	N(3)-Al(3)	1.890(10)
C(13)-H(13)	0.9500	Al(3)-C(27)	1.935(12)
C(14)-C(15)	1.384(4)	Al(3)-C(27')	1.939(17)
C(14)-H(14)	0.9500	Al(3)-Cl(3')	2.105(13)
C(15)-C(16)	1.401(3)	Al(3)-Cl(3)	2.129(3)
C(15)-H(15)	0.9500	C(27)-H(27A)	0.9800
C(16)-C(17)	1.381(3)	C(27)-H(27B)	0.9800
C(16)-H(16)	0.9500	C(27)-H(27C)	0.9800
C(17)-N(2)	1.412(3)	C(27')-H(27D)	0.9800
N(2)-Al(2)	1.8899(17)	C(27')-H(27E)	0.9800
Al(2)-N(2)#1	1.8899(17)	C(27')-H(27F)	0.9800
Al(2)-C(18')	1.934(14)	C(1T)-C(2T)	1.3900

C(1T)-C(6T)	1.3900
C(1T)-C(7T)	1.525(9)
C(2T)-C(3T)	1.3900
C(2T)-H(2T)	0.9500
C(3T)-C(4T)	1.3900
C(3T)-H(3T)	0.9500
C(4T)-C(5T)	1.3900
C(4T)-H(4T)	0.9500
C(5T)-C(6T)	1.3900
C(5T)-H(5T)	0.9500
C(6T)-H(6T)	0.9500
C(7T)-H(7T1)	0.9800
C(7T)-H(7T2)	0.9800
C(7T)-H(7T3)	0.9800
C(1A)-C(2A)	1.3900
C(1A)-C(6A)	1.3900
C(1A)-C(7A)	1.498(11)
C(2A)-C(3A)	1.3900
C(2A)-H(2A)	0.9500
C(3A)-C(4A)	1.3900
C(3A)-H(3A)	0.9500
C(4A)-C(5A)	1.3900
C(4A)-H(4A)	0.9500
C(5A)-C(6A)	1.3900
C(5A)-H(5A)	0.9500
C(6A)-H(6A)	0.9500
C(7A)-H(7A1)	0.9800
C(7A)-H(7A2)	0.9800
C(7A)-H(7A3)	0.9800

C(2)-C(1)-C(2)#1	119.6(3)
C(2)-C(1)-H(1)	120.2
C(2)#1-C(1)-H(1)	120.2
N(1)-C(2)-O(1)	112.06(17)
N(1)-C(2)-C(1)	128.21(19)
O(1)-C(2)-C(1)	119.71(18)
C(4)-C(3)-C(8)	123.8(2)
C(4)-C(3)-O(1)	127.55(19)
C(8)-C(3)-O(1)	108.68(17)
C(3)-C(4)-C(5)	115.2(2)
C(3)-C(4)-H(4)	122.4
C(5)-C(4)-H(4)	122.4
C(6)-C(5)-C(4)	122.0(2)
C(6)-C(5)-H(5)	119.0
C(4)-C(5)-H(5)	119.0
C(5)-C(6)-C(7)	121.7(2)
C(5)-C(6)-H(6)	119.1
C(7)-C(6)-H(6)	119.1
C(8)-C(7)-C(6)	116.34(19)
C(8)-C(7)-H(7)	121.8
C(6)-C(7)-H(7)	121.8
C(7)-C(8)-C(3)	120.98(18)
C(7)-C(8)-N(1)	131.70(18)
C(3)-C(8)-N(1)	107.30(17)
C(2)-O(1)-C(3)	105.91(15)
C(2)-N(1)-C(8)	106.05(16)
C(2)-N(1)-Al(1)	124.64(13)
C(8)-N(1)-Al(1)	129.24(13)
N(1)#1-Al(1)-N(1)	93.90(10)
N(1)#1-Al(1)-C(9)	114.5(4)
N(1)-Al(1)-C(9)	114.5(4)
N(1)#1-Al(1)-C(9')	108.8(16)
N(1)-Al(1)-C(9')	108.8(16)
N(1)#1-Al(1)-Cl(1')	113.9(4)
N(1)-Al(1)-Cl(1')	113.9(4)
C(9')-Al(1)-Cl(1')	115(3)
N(1)#1-Al(1)-Cl(1)	109.44(9)
N(1)-Al(1)-Cl(1)	109.44(9)
C(9)-Al(1)-Cl(1)	113.3(6)
Al(1)-C(9)-H(9A)	109.5
Al(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
Al(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5

H(9B)-C(9)-H(9C)	109.5	N(2)#1-Al(2)-C(18')	115.5(4)
Al(1)-C(9')-H(9'A)	109.5	N(2)-Al(2)-C(18)	116.61(18)
Al(1)-C(9')-H(9'B)	109.5	N(2)#1-Al(2)-C(18)	116.61(18)
H(9'A)-C(9')-H(9'B)	109.5	N(2)-Al(2)-Cl(2')	110.32(19)
Al(1)-C(9')-H(9'C)	109.5	N(2)#1-Al(2)-Cl(2')	110.32(19)
H(9'A)-C(9')-H(9'C)	109.5	C(18')-Al(2)-Cl(2')	109.7(7)
H(9'B)-C(9')-H(9'C)	109.5	N(2)-Al(2)-Cl(2)	107.91(6)
C(11)#1-C(10)-C(11)	120.8(3)	N(2)#1-Al(2)-Cl(2)	107.91(6)
C(11)#1-C(10)-H(10)	119.6	C(18)-Al(2)-Cl(2)	111.6(3)
C(11)-C(10)-H(10)	119.6	Al(2)-C(18)-H(18A)	109.5
N(2)-C(11)-O(2)	112.40(17)	Al(2)-C(18)-H(18B)	109.5
N(2)-C(11)-C(10)	127.78(19)	H(18A)-C(18)-H(18B)	109.5
O(2)-C(11)-C(10)	119.81(18)	Al(2)-C(18)-H(18C)	109.5
C(17)-C(12)-C(13)	124.0(2)	H(18A)-C(18)-H(18C)	109.5
C(17)-C(12)-O(2)	108.82(18)	H(18B)-C(18)-H(18C)	109.5
C(13)-C(12)-O(2)	127.1(2)	Al(2)-C(18')-H(18D)	109.5
C(12)-C(13)-C(14)	115.3(2)	Al(2)-C(18')-H(18E)	109.5
C(12)-C(13)-H(13)	122.4	H(18D)-C(18')-H(18E)	109.5
C(14)-C(13)-H(13)	122.4	Al(2)-C(18')-H(18F)	109.5
C(13)-C(14)-C(15)	121.9(2)	H(18D)-C(18')-H(18F)	109.5
C(13)-C(14)-H(14)	119.1	H(18E)-C(18')-H(18F)	109.5
C(15)-C(14)-H(14)	119.1	C(20)-C(19)-H(19A)	120.3
C(14)-C(15)-C(16)	122.0(2)	N(3)-C(20)-O(3)	112.0(4)
C(14)-C(15)-H(15)	119.0	N(3)-C(20)-C(19)	128.3(6)
C(16)-C(15)-H(15)	119.0	O(3)-C(20)-C(19)	119.7(6)
C(17)-C(16)-C(15)	116.2(2)	C(22)-C(21)-O(3)	126.8(10)
C(17)-C(16)-H(16)	121.9	C(22)-C(21)-C(26)	124.6(9)
C(15)-C(16)-H(16)	121.9	O(3)-C(21)-C(26)	108.3(8)
C(12)-C(17)-C(16)	120.6(2)	C(23)-C(22)-C(21)	114.3(9)
C(12)-C(17)-N(2)	107.45(18)	C(23)-C(22)-H(22)	122.9
C(16)-C(17)-N(2)	131.9(2)	C(21)-C(22)-H(22)	122.9
C(11)-O(2)-C(12)	105.51(16)	C(22)-C(23)-C(24)	122.2(4)
C(11)-N(2)-C(17)	105.82(17)	C(22)-C(23)-H(23)	118.9
C(11)-N(2)-Al(2)	124.01(14)	C(24)-C(23)-H(23)	118.9
C(17)-N(2)-Al(2)	129.95(14)	C(23)-C(24)-C(25)	122.5(9)
N(2)-Al(2)-N(2)#1	94.75(11)	C(23)-C(24)-H(24)	118.8
N(2)-Al(2)-C(18')	115.5(4)	C(25)-C(24)-H(24)	118.8

C(26)-C(25)-C(24)	115.6(9)	C(3T)-C(2T)-H(2T)	120.0
C(26)-C(25)-H(25)	122.2	C(4T)-C(3T)-C(2T)	120.0
C(24)-C(25)-H(25)	122.2	C(4T)-C(3T)-H(3T)	120.0
C(25)-C(26)-C(21)	120.2(5)	C(2T)-C(3T)-H(3T)	120.0
C(25)-C(26)-N(3)	131.9(11)	C(3T)-C(4T)-C(5T)	120.0
C(21)-C(26)-N(3)	107.1(10)	C(3T)-C(4T)-H(4T)	120.0
C(20)-O(3)-C(21)	106.3(5)	C(5T)-C(4T)-H(4T)	120.0
C(20)-N(3)-C(26)	106.0(7)	C(6T)-C(5T)-C(4T)	120.0
C(20)-N(3)-Al(3)	124.9(4)	C(6T)-C(5T)-H(5T)	120.0
C(26)-N(3)-Al(3)	128.9(9)	C(4T)-C(5T)-H(5T)	120.0
N(3)-Al(3)-C(27)	115.7(15)	C(5T)-C(6T)-C(1T)	120.0
N(3)-Al(3)-C(27')	115.7(17)	C(5T)-C(6T)-H(6T)	120.0
C(27)-Al(3)-C(27')	108(2)	C(1T)-C(6T)-H(6T)	120.0
N(3)-Al(3)-Cl(3')	110.2(11)	C(1T)-C(7T)-H(7T1)	109.5
C(27)-Al(3)-Cl(3')	5.6(18)	C(1T)-C(7T)-H(7T2)	109.5
C(27')-Al(3)-Cl(3')	112.7(16)	H(7T1)-C(7T)-H(7T2)	109.5
N(3)-Al(3)-Cl(3)	108.9(8)	C(1T)-C(7T)-H(7T3)	109.5
C(27)-Al(3)-Cl(3)	112.8(8)	H(7T1)-C(7T)-H(7T3)	109.5
C(27')-Al(3)-Cl(3)	6.8(18)	H(7T2)-C(7T)-H(7T3)	109.5
Cl(3')-Al(3)-Cl(3)	116.7(8)	C(2A)-C(1A)-C(6A)	120.0
Al(3)-C(27)-H(27A)	109.5	C(2A)-C(1A)-C(7A)	119.0(9)
Al(3)-C(27)-H(27B)	109.5	C(6A)-C(1A)-C(7A)	121.0(9)
H(27A)-C(27)-H(27B)	109.5	C(3A)-C(2A)-C(1A)	120.0
Al(3)-C(27)-H(27C)	109.5	C(3A)-C(2A)-H(2A)	120.0
H(27A)-C(27)-H(27C)	109.5	C(1A)-C(2A)-H(2A)	120.0
H(27B)-C(27)-H(27C)	109.5	C(2A)-C(3A)-C(4A)	120.0
Al(3)-C(27')-H(27D)	109.5	C(2A)-C(3A)-H(3A)	120.0
Al(3)-C(27')-H(27E)	109.5	C(4A)-C(3A)-H(3A)	120.0
H(27D)-C(27')-H(27E)	109.5	C(5A)-C(4A)-C(3A)	120.0
Al(3)-C(27')-H(27F)	109.5	C(5A)-C(4A)-H(4A)	120.0
H(27D)-C(27')-H(27F)	109.5	C(3A)-C(4A)-H(4A)	120.0
H(27E)-C(27')-H(27F)	109.5	C(4A)-C(5A)-C(6A)	120.0
C(2T)-C(1T)-C(6T)	120.0	C(4A)-C(5A)-H(5A)	120.0
C(2T)-C(1T)-C(7T)	120.4(15)	C(6A)-C(5A)-H(5A)	120.0
C(6T)-C(1T)-C(7T)	119.6(15)	C(5A)-C(6A)-C(1A)	120.0
C(1T)-C(2T)-C(3T)	120.0	C(5A)-C(6A)-H(6A)	120.0
C(1T)-C(2T)-H(2T)	120.0	C(1A)-C(6A)-H(6A)	120.0

C(1A)-C(7A)-H(7A1)	109.5	C(1A)-C(7A)-H(7A3)	109.5
C(1A)-C(7A)-H(7A2)	109.5	H(7A1)-C(7A)-H(7A3)	109.5
H(7A1)-C(7A)-H(7A2)	109.5	H(7A2)-C(7A)-H(7A3)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1,z

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_5

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_5

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=21.226(3) b=15.558(2) c=14.163(2)
alpha=90 beta=112.76(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4312.9(12)	4312.9(12)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	2(C15 H9 Al N2 O2), 8(C16 H12 Al Cl N2 O2), 2(C14 H16), C2 H6,	C15.67 H12.67 Al0.83 Cl0.83 N1.67 O1.67
Sum formula	C188.02 H152.02 Al10 Cl10.02 N20 O20	C15.67 H12.67 Al0.83 Cl0.83 N1.67 O1.67

Mr	3636.38	302.97
Dx,g cm-3	1.400	1.400
Z	1	12
Mu (mm-1)	0.287	0.287
F000	1880.4	1880.0
F000'	1883.14	
h,k,lmax	26,19,17	26,19,17
Nref	4579	4564
Tmin,Tmax	0.936,0.976	0.707,0.745
Tmin'	0.933	

Correction method= MULTI-SCAN

Data completeness= 0.997 Theta(max)= 26.368

R(reflections)= 0.0414(4130) wR2(reflections)= 0.1025(4564)

S = 1.118 Npar= Npar = 449

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 4.791 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 10 Why ?

Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 12
From the CIF: _chemical_formula_sum C15.67 H12.67 Al0.83 Cl0.83 N1.6
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	188.04	188.00	0.04
H	152.04	152.00	0.04
Al	9.96	10.00	-0.04
Cl	9.96	10.00	-0.04
N	20.04	20.00	0.04
O	20.04	20.00	0.04

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 57 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 59 Why ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.08 Ratio
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 10.60 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al2 -- C18' .. 6.3 su
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 42 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 100 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 9 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 729 Note

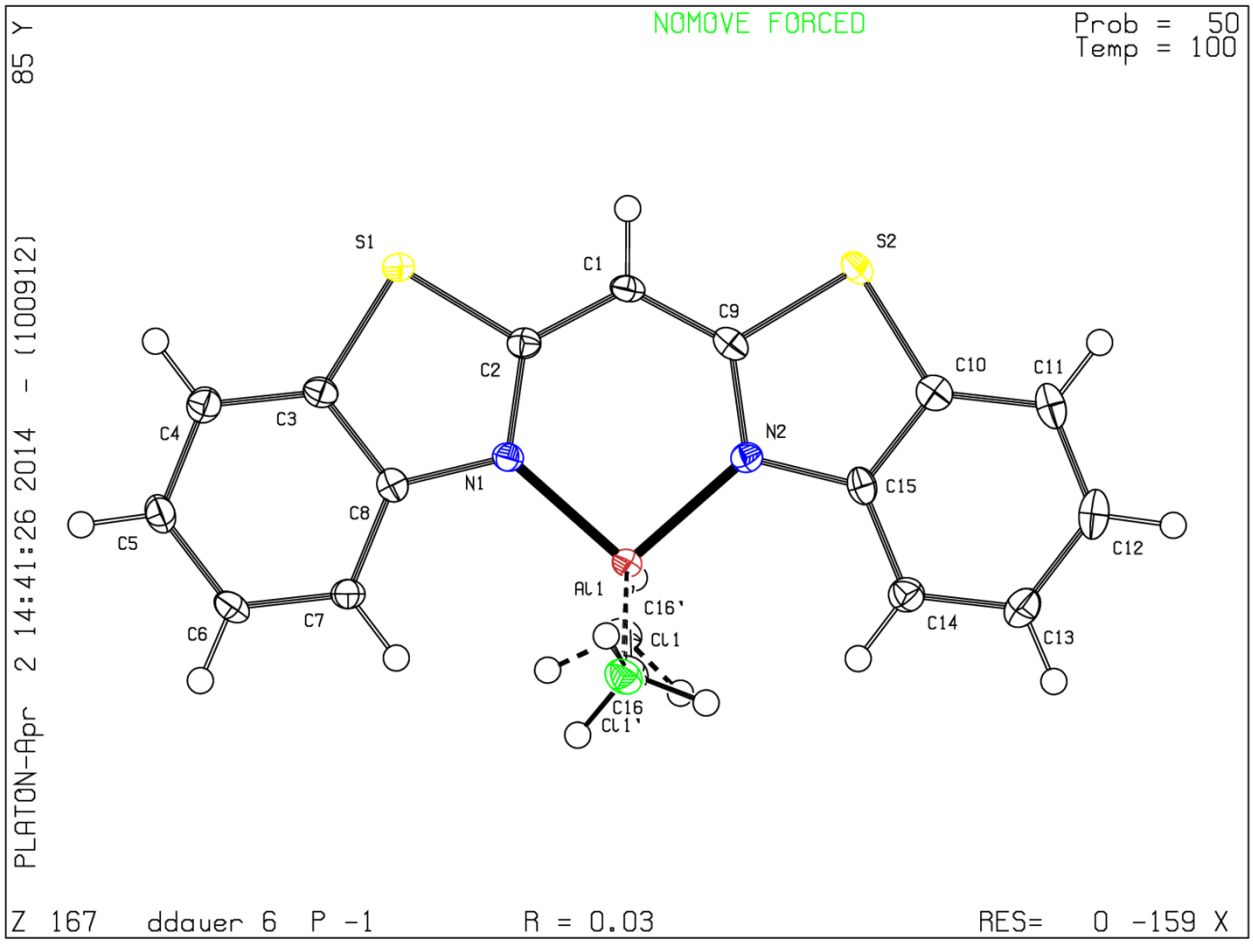
```
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          5   Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check

  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 15 ALERT level G = General information/check it is not something unexpected

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  4 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

PLATON version of 05/02/2014; check.def file version of 05/02/2014

2.6 Bond lengths [Å] and angles [deg] for 6.



Bond lengths [Å] and angles [deg] for **6**.

C(1)-C(2)	1.387(3)	C(6)-C(7)	1.388(3)
C(1)-C(9)	1.388(3)	C(6)-H(6)	0.9500
C(1)-H(1)	0.9500	C(7)-C(8)	1.395(3)
C(2)-N(1)	1.365(3)	C(7)-H(7)	0.9500
C(2)-S(1)	1.742(2)	C(8)-N(1)	1.409(3)
S(1)-C(3)	1.747(2)	N(1)-Al(1)	1.893(2)
C(3)-C(4)	1.392(3)	C(9)-N(2)	1.364(3)
C(3)-C(8)	1.394(3)	C(9)-S(2)	1.747(2)
C(4)-C(5)	1.392(3)	S(2)-C(10)	1.743(2)
C(4)-H(4)	0.9500	C(10)-C(11)	1.391(3)
C(5)-C(6)	1.393(3)	C(10)-C(15)	1.399(3)
C(5)-H(5)	0.9500	C(11)-C(12)	1.382(4)

C(11)-H(11)	0.9500	C(7)-C(6)-H(6)	119.4
C(12)-C(13)	1.397(4)	C(5)-C(6)-H(6)	119.4
C(12)-H(12)	0.9500	C(6)-C(7)-C(8)	118.6(2)
C(13)-C(14)	1.384(3)	C(6)-C(7)-H(7)	120.7
C(13)-H(13)	0.9500	C(8)-C(7)-H(7)	120.7
C(14)-C(15)	1.396(3)	C(3)-C(8)-C(7)	120.0(2)
C(14)-H(14)	0.9500	C(3)-C(8)-N(1)	114.15(19)
C(15)-N(2)	1.407(3)	C(7)-C(8)-N(1)	125.8(2)
N(2)-Al(1)	1.895(2)	C(2)-N(1)-C(8)	111.72(18)
Al(1)-C(16)	1.976(14)	C(2)-N(1)-Al(1)	123.45(15)
Al(1)-C(16')	2.01(2)	C(8)-N(1)-Al(1)	124.68(14)
Al(1)-Cl(1')	2.064(8)	N(2)-C(9)-C(1)	126.1(2)
Al(1)-Cl(1)	2.120(2)	N(2)-C(9)-S(2)	112.96(17)
C(16)-H(16A)	0.9800	C(1)-C(9)-S(2)	120.98(17)
C(16)-H(16B)	0.9800	C(10)-S(2)-C(9)	90.84(11)
C(16)-H(16C)	0.9800	C(11)-C(10)-C(15)	121.5(2)
C(16')-H(16D)	0.9800	C(11)-C(10)-S(2)	128.24(19)
C(16')-H(16E)	0.9800	C(15)-C(10)-S(2)	110.25(18)
C(16')-H(16F)	0.9800	C(12)-C(11)-C(10)	118.1(2)
		C(12)-C(11)-H(11)	121.0
C(2)-C(1)-C(9)	124.1(2)	C(10)-C(11)-H(11)	121.0
C(2)-C(1)-H(1)	118.0	C(11)-C(12)-C(13)	120.9(2)
C(9)-C(1)-H(1)	118.0	C(11)-C(12)-H(12)	119.5
N(1)-C(2)-C(1)	125.9(2)	C(13)-C(12)-H(12)	119.5
N(1)-C(2)-S(1)	113.05(16)	C(14)-C(13)-C(12)	121.0(2)
C(1)-C(2)-S(1)	121.02(17)	C(14)-C(13)-H(13)	119.5
C(2)-S(1)-C(3)	90.81(11)	C(12)-C(13)-H(13)	119.5
C(4)-C(3)-C(8)	121.6(2)	C(13)-C(14)-C(15)	118.6(2)
C(4)-C(3)-S(1)	128.10(18)	C(13)-C(14)-H(14)	120.7
C(8)-C(3)-S(1)	110.27(17)	C(15)-C(14)-H(14)	120.7
C(3)-C(4)-C(5)	118.0(2)	C(14)-C(15)-C(10)	119.8(2)
C(3)-C(4)-H(4)	121.0	C(14)-C(15)-N(2)	126.0(2)
C(5)-C(4)-H(4)	121.0	C(10)-C(15)-N(2)	114.1(2)
C(4)-C(5)-C(6)	120.7(2)	C(9)-N(2)-C(15)	111.80(19)
C(4)-C(5)-H(5)	119.6	C(9)-N(2)-Al(1)	123.29(16)
C(6)-C(5)-H(5)	119.6	C(15)-N(2)-Al(1)	124.80(15)
C(7)-C(6)-C(5)	121.1(2)	N(1)-Al(1)-N(2)	96.84(9)

N(1)-Al(1)-C(16)	113.9(6)	H(16A)-C(16)-H(16C)	109.5
N(2)-Al(1)-C(16)	113.1(6)	H(16B)-C(16)-H(16C)	109.5
N(1)-Al(1)-C(16')	108.3(11)	Al(1)-C(16')-H(16D)	109.5
N(2)-Al(1)-C(16')	110.1(12)	Al(1)-C(16')-H(16E)	109.5
N(1)-Al(1)-Cl(1')	111.9(3)	H(16D)-C(16')-H(16E)	109.5
N(2)-Al(1)-Cl(1')	114.4(3)	Al(1)-C(16')-H(16F)	109.5
C(16')-Al(1)-Cl(1')	113.9(10)	H(16D)-C(16')-H(16F)	109.5
N(1)-Al(1)-Cl(1)	108.57(12)	H(16E)-C(16')-H(16F)	109.5
N(2)-Al(1)-Cl(1)	109.98(13)		
C(16)-Al(1)-Cl(1)	113.2(5)		
Al(1)-C(16)-H(16A)	109.5		
Al(1)-C(16)-H(16B)	109.5		
H(16A)-C(16)-H(16B)	109.5		
Al(1)-C(16)-H(16C)	109.5		

---

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_6

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_6

```
Bond precision:  C-C = 0.0030 A          Wavelength=0.71073

Cell:           a=7.074(2)        b=7.694(2)       c=14.664(3)
                alpha=89.97(2)    beta=85.29(2)    gamma=85.89(2)
Temperature:    100 K

                Calculated                Reported
Volume          793.4(3)                  793.4(3)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C16 H12 Al Cl N2 S2       C16 H12 Al Cl N2 S2
Sum formula     C16 H12 Al Cl N2 S2       C16 H12 Al Cl N2 S2
Mr              358.85                    358.83
Dx,g cm-3       1.502                     1.502
```

Z	2	2
Mu (mm-1)	0.555	0.555
F000	368.0	368.0
F000'	368.99	
h,k,lmax	8,9,17	8,9,17
Nref	2908	2882
Tmin,Tmax	0.941,0.957	0.754,0.914
Tmin'	0.941	

Correction method= MULTI-SCAN

Data completeness= 0.991 Theta(max)= 25.376

R(reflections)= 0.0348(2502) wR2(reflections)= 0.0801(2882)

S = 1.054 Npar= Npar = 209

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 38 Why ?

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	24	Note
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal	0.02000	Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cl1 -- Al1 ..	6.0	su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Al1 -- C16' ..	6.0	su
PLAT301_ALERT_3_G	Main Residue Disorder ..... Percentage =	9	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	32	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	8	Note

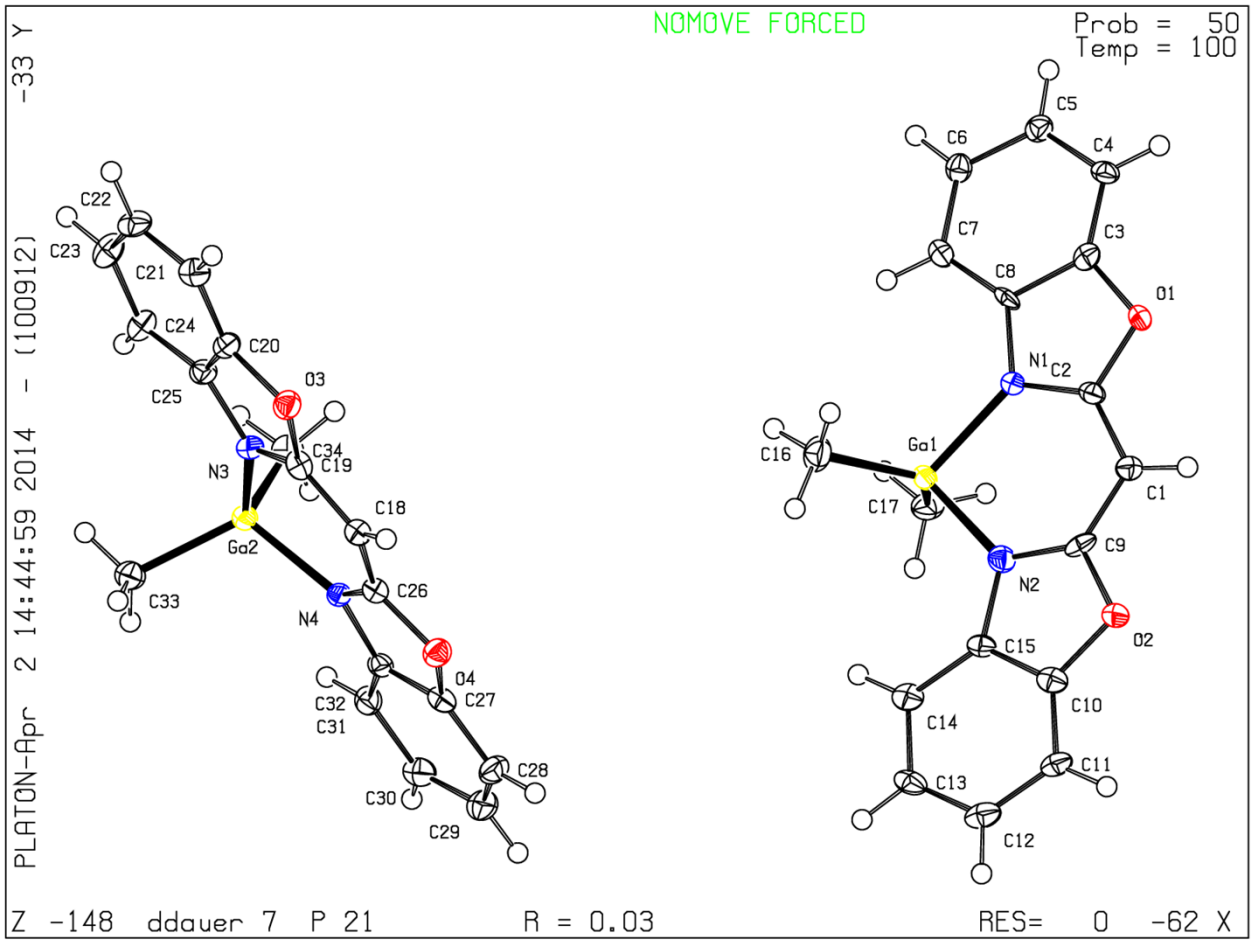
---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 05/02/2014; check.def file version of 05/02/2014

2.7 Bond lengths [Å] and angles [deg] for 7.



Bond lengths [Å] and angles [deg] for **7**.

C(1)-C(9)	1.393(8)	C(6)-C(7)	1.386(9)
C(1)-C(2)	1.399(9)	C(6)-H(6)	0.9500
C(1)-H(1)	0.9500	C(7)-C(8)	1.396(9)
C(2)-N(1)	1.331(9)	C(7)-H(7)	0.9500
C(2)-O(1)	1.369(8)	C(8)-N(1)	1.379(8)
O(1)-C(3)	1.394(8)	N(1)-Ga(1)	1.998(5)
C(3)-C(4)	1.368(9)	C(9)-N(2)	1.310(7)
C(3)-C(8)	1.406(9)	C(9)-O(2)	1.363(7)
C(4)-C(5)	1.396(8)	O(2)-C(10)	1.389(8)
C(4)-H(4)	0.9500	C(10)-C(11)	1.372(9)
C(5)-C(6)	1.401(9)	C(10)-C(15)	1.378(10)
C(5)-H(5)	0.9500	C(11)-C(12)	1.391(10)

C(11)-H(11)	0.9500	O(4)-C(27)	1.400(8)
C(12)-C(13)	1.398(11)	C(27)-C(28)	1.375(10)
C(12)-H(12)	0.9500	C(27)-C(32)	1.383(9)
C(13)-C(14)	1.388(9)	C(28)-C(29)	1.399(10)
C(13)-H(13)	0.9500	C(28)-H(28)	0.9500
C(14)-C(15)	1.395(9)	C(29)-C(30)	1.403(11)
C(14)-H(14)	0.9500	C(29)-H(29)	0.9500
C(15)-N(2)	1.411(8)	C(30)-C(31)	1.390(9)
N(2)-Ga(1)	1.994(5)	C(30)-H(30)	0.9500
Ga(1)-C(16)	1.965(7)	C(31)-C(32)	1.384(9)
Ga(1)-C(17)	1.972(7)	C(31)-H(31)	0.9500
C(16)-H(16A)	0.9800	C(32)-N(4)	1.413(8)
C(16)-H(16B)	0.9800	N(4)-Ga(2)	1.990(5)
C(16)-H(16C)	0.9800	Ga(2)-C(33)	1.968(7)
C(17)-H(17A)	0.9800	Ga(2)-C(34)	1.969(6)
C(17)-H(17B)	0.9800	C(33)-H(33A)	0.9800
C(17)-H(17C)	0.9800	C(33)-H(33B)	0.9800
C(18)-C(19)	1.386(9)	C(33)-H(33C)	0.9800
C(18)-C(26)	1.397(8)	C(34)-H(34A)	0.9800
C(18)-H(18)	0.9500	C(34)-H(34B)	0.9800
C(19)-N(3)	1.322(9)	C(34)-H(34C)	0.9800
C(19)-O(3)	1.386(8)		
O(3)-C(20)	1.395(8)	C(9)-C(1)-C(2)	120.1(6)
C(20)-C(21)	1.368(9)	C(9)-C(1)-H(1)	120.0
C(20)-C(25)	1.382(9)	C(2)-C(1)-H(1)	120.0
C(21)-C(22)	1.396(9)	N(1)-C(2)-O(1)	112.5(6)
C(21)-H(21)	0.9500	N(1)-C(2)-C(1)	128.2(6)
C(22)-C(23)	1.402(9)	O(1)-C(2)-C(1)	119.3(6)
C(22)-H(22)	0.9500	C(2)-O(1)-C(3)	105.4(5)
C(23)-C(24)	1.392(9)	C(4)-C(3)-O(1)	128.8(6)
C(23)-H(23)	0.9500	C(4)-C(3)-C(8)	124.0(7)
C(24)-C(25)	1.391(9)	O(1)-C(3)-C(8)	107.2(6)
C(24)-H(24)	0.9500	C(3)-C(4)-C(5)	115.3(7)
C(25)-N(3)	1.396(9)	C(3)-C(4)-H(4)	122.4
N(3)-Ga(2)	2.001(6)	C(5)-C(4)-H(4)	122.4
C(26)-N(4)	1.328(7)	C(4)-C(5)-C(6)	122.2(6)
C(26)-O(4)	1.362(7)	C(4)-C(5)-H(5)	118.9

C(6)-C(5)-H(5)	118.9	C(15)-N(2)-Ga(1)	126.1(5)
C(7)-C(6)-C(5)	121.6(6)	C(16)-Ga(1)-C(17)	123.8(3)
C(7)-C(6)-H(6)	119.2	C(16)-Ga(1)-N(2)	110.5(3)
C(5)-C(6)-H(6)	119.2	C(17)-Ga(1)-N(2)	110.3(3)
C(6)-C(7)-C(8)	116.9(6)	C(16)-Ga(1)-N(1)	110.6(3)
C(6)-C(7)-H(7)	121.5	C(17)-Ga(1)-N(1)	107.4(3)
C(8)-C(7)-H(7)	121.5	N(2)-Ga(1)-N(1)	88.6(2)
N(1)-C(8)-C(7)	131.9(6)	Ga(1)-C(16)-H(16A)	109.5
N(1)-C(8)-C(3)	108.0(6)	Ga(1)-C(16)-H(16B)	109.5
C(7)-C(8)-C(3)	120.0(6)	H(16A)-C(16)-H(16B)	109.5
C(2)-N(1)-C(8)	106.8(5)	Ga(1)-C(16)-H(16C)	109.5
C(2)-N(1)-Ga(1)	126.5(4)	H(16A)-C(16)-H(16C)	109.5
C(8)-N(1)-Ga(1)	126.2(4)	H(16B)-C(16)-H(16C)	109.5
N(2)-C(9)-O(2)	113.1(5)	Ga(1)-C(17)-H(17A)	109.5
N(2)-C(9)-C(1)	127.8(6)	Ga(1)-C(17)-H(17B)	109.5
O(2)-C(9)-C(1)	119.2(6)	H(17A)-C(17)-H(17B)	109.5
C(9)-O(2)-C(10)	105.7(5)	Ga(1)-C(17)-H(17C)	109.5
C(11)-C(10)-C(15)	124.0(7)	H(17A)-C(17)-H(17C)	109.5
C(11)-C(10)-O(2)	128.5(7)	H(17B)-C(17)-H(17C)	109.5
C(15)-C(10)-O(2)	107.4(6)	C(19)-C(18)-C(26)	119.3(6)
C(10)-C(11)-C(12)	115.9(7)	C(19)-C(18)-H(18)	120.3
C(10)-C(11)-H(11)	122.0	C(26)-C(18)-H(18)	120.3
C(12)-C(11)-H(11)	122.0	N(3)-C(19)-O(3)	112.2(6)
C(11)-C(12)-C(13)	121.2(7)	N(3)-C(19)-C(18)	129.5(6)
C(11)-C(12)-H(12)	119.4	O(3)-C(19)-C(18)	118.3(6)
C(13)-C(12)-H(12)	119.4	C(19)-O(3)-C(20)	104.7(5)
C(14)-C(13)-C(12)	121.8(7)	C(21)-C(20)-C(25)	123.8(7)
C(14)-C(13)-H(13)	119.1	C(21)-C(20)-O(3)	127.8(7)
C(12)-C(13)-H(13)	119.1	C(25)-C(20)-O(3)	108.5(6)
C(13)-C(14)-C(15)	116.8(7)	C(20)-C(21)-C(22)	115.9(7)
C(13)-C(14)-H(14)	121.6	C(20)-C(21)-H(21)	122.1
C(15)-C(14)-H(14)	121.6	C(22)-C(21)-H(21)	122.1
C(10)-C(15)-C(14)	120.2(7)	C(21)-C(22)-C(23)	121.2(7)
C(10)-C(15)-N(2)	108.0(6)	C(21)-C(22)-H(22)	119.4
C(14)-C(15)-N(2)	131.8(7)	C(23)-C(22)-H(22)	119.4
C(9)-N(2)-C(15)	105.8(5)	C(24)-C(23)-C(22)	121.9(7)
C(9)-N(2)-Ga(1)	128.1(5)	C(24)-C(23)-H(23)	119.1

C(22)-C(23)-H(23)	119.1	C(27)-C(32)-C(31)	120.9(7)
C(25)-C(24)-C(23)	116.2(7)	C(27)-C(32)-N(4)	107.9(6)
C(25)-C(24)-H(24)	121.9	C(31)-C(32)-N(4)	131.2(7)
C(23)-C(24)-H(24)	121.9	C(26)-N(4)-C(32)	105.6(5)
C(20)-C(25)-C(24)	121.0(7)	C(26)-N(4)-Ga(2)	126.2(5)
C(20)-C(25)-N(3)	107.7(6)	C(32)-N(4)-Ga(2)	128.2(5)
C(24)-C(25)-N(3)	131.3(7)	C(33)-Ga(2)-C(34)	121.3(3)
C(19)-N(3)-C(25)	107.0(6)	C(33)-Ga(2)-N(4)	112.8(3)
C(19)-N(3)-Ga(2)	125.9(5)	C(34)-Ga(2)-N(4)	110.1(3)
C(25)-N(3)-Ga(2)	127.2(5)	C(33)-Ga(2)-N(3)	107.0(3)
N(4)-C(26)-O(4)	113.3(5)	C(34)-Ga(2)-N(3)	111.3(3)
N(4)-C(26)-C(18)	129.0(6)	N(4)-Ga(2)-N(3)	89.8(2)
O(4)-C(26)-C(18)	117.7(5)	Ga(2)-C(33)-H(33A)	109.5
C(26)-O(4)-C(27)	105.3(5)	Ga(2)-C(33)-H(33B)	109.5
C(28)-C(27)-C(32)	123.7(7)	H(33A)-C(33)-H(33B)	109.5
C(28)-C(27)-O(4)	128.4(7)	Ga(2)-C(33)-H(33C)	109.5
C(32)-C(27)-O(4)	107.8(6)	H(33A)-C(33)-H(33C)	109.5
C(27)-C(28)-C(29)	115.5(7)	H(33B)-C(33)-H(33C)	109.5
C(27)-C(28)-H(28)	122.2	Ga(2)-C(34)-H(34A)	109.5
C(29)-C(28)-H(28)	122.2	Ga(2)-C(34)-H(34B)	109.5
C(28)-C(29)-C(30)	121.5(7)	H(34A)-C(34)-H(34B)	109.5
C(28)-C(29)-H(29)	119.3	Ga(2)-C(34)-H(34C)	109.5
C(30)-C(29)-H(29)	119.3	H(34A)-C(34)-H(34C)	109.5
C(31)-C(30)-C(29)	121.4(7)	H(34B)-C(34)-H(34C)	109.5
C(31)-C(30)-H(30)	119.3		
C(29)-C(30)-H(30)	119.3		
C(32)-C(31)-C(30)	116.9(7)		
C(32)-C(31)-H(31)	121.5		
C(30)-C(31)-H(31)	121.5		

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_7

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_7

```
Bond precision:  C-C = 0.0104 A          Wavelength=0.71073

Cell:             a=8.386(2)     b=13.944(3)          c=13.838(3)
                  alpha=90       beta=107.60(2)       gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	1542.4(6)	1542.4(6)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C17 H15 Ga N2 O2	C17 H15 Ga N2 O2
Sum formula	C17 H15 Ga N2 O2	C17 H15 Ga N2 O2
Mr	349.03	349.03
Dx,g cm-3	1.503	1.503
Z	4	4
Mu (mm-1)	1.792	1.792
F000	712.0	712.0
F000’	713.11	
h,k,lmax	11,18,18	11,18,18
Nref	7694[4002]	7674
Tmin,Tmax	0.855,0.882	0.703,0.746
Tmin’	0.853	

```
Correction method= MULTI-SCAN

Data completeness= 1.92/1.00      Theta(max)= 28.321

R(reflections)= 0.0339( 7502)     wR2(reflections)= 0.0798( 7674)

S = 1.026                 Npar= Npar = 402
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.551
          From the CIF: _refine_ls_abs_structure_Flack_su    0.006
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       9.94   Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.51  Why ?
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0104   Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          3 Why ?
```

Alert level G

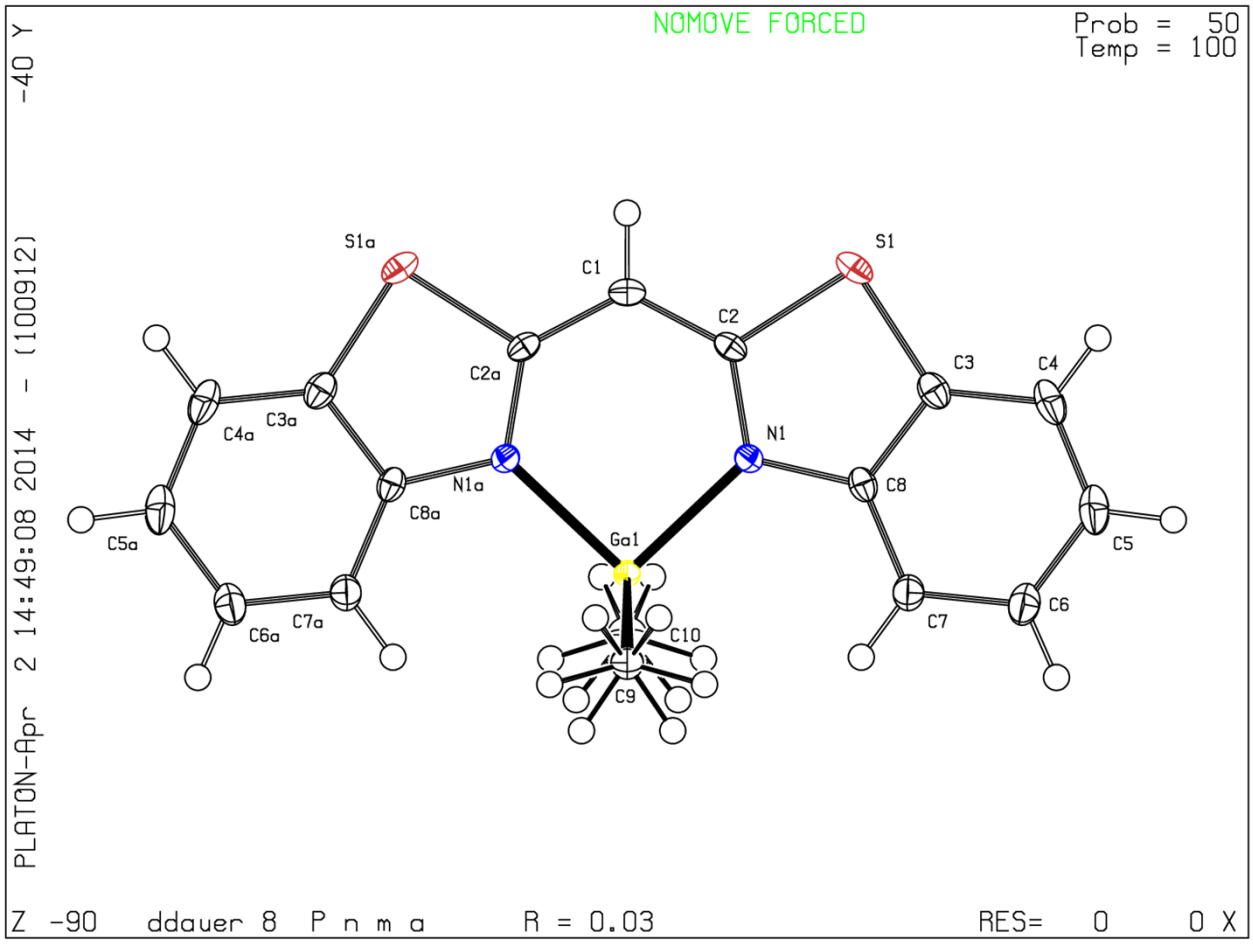
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         44 Note
PLAT033_ALERT_4_G Flack x Value Deviates > 2*sigma from Zero .....      0.551
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        176   Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          !   Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          4   Note
PLAT931_ALERT_5_G Found Twin Law ( 0 0  1)[       ] Estimated BASF       0.45 Check
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 05/02/2014; check.def file version of 05/02/2014

2.8 Bond lengths [Å] and angles [deg] for 8.



Bond lengths [Å] and angles [deg] for **8**.

Ga(1)-C(10)	1.964(2)	C(3)-C(8)	1.401(2)
Ga(1)-C(9)	1.969(2)	C(4)-C(5)	1.384(3)
Ga(1)-N(1)#1	1.9945(13)	C(4)-H(4)	0.9500
Ga(1)-N(1)	1.9945(13)	C(5)-C(6)	1.397(3)
C(1)-C(2)	1.3909(19)	C(5)-H(5)	0.9500
C(1)-C(2)#1	1.3909(19)	C(9)-H(9A)	0.9800
C(1)-H(1)	0.9500	C(9)-H(9B)	0.9800
S(1)-C(3)	1.7404(18)	C(9)-H(9C)	0.9800
S(1)-C(2)	1.7514(16)	C(8)-C(7)	1.396(2)
N(1)-C(2)	1.3436(19)	C(7)-C(6)	1.388(2)
N(1)-C(8)	1.3938(19)	C(7)-H(7)	0.9500
C(3)-C(4)	1.391(2)	C(6)-H(6)	0.9500

C(10)-H(10A)	0.9800	C(6)-C(5)-H(5)	119.5
C(10)-H(10B)	0.9800	Ga(1)-C(9)-H(9A)	109.5
C(10)-H(10C)	0.9800	Ga(1)-C(9)-H(9B)	109.5
		H(9A)-C(9)-H(9B)	109.5
C(10)-Ga(1)-C(9)	125.57(10)	Ga(1)-C(9)-H(9C)	109.5
C(10)-Ga(1)-N(1)#1	108.52(6)	H(9A)-C(9)-H(9C)	109.5
C(9)-Ga(1)-N(1)#1	108.18(6)	H(9B)-C(9)-H(9C)	109.5
C(10)-Ga(1)-N(1)	108.52(6)	N(1)-C(8)-C(7)	125.84(14)
C(9)-Ga(1)-N(1)	108.18(6)	N(1)-C(8)-C(3)	114.38(14)
N(1)#1-Ga(1)-N(1)	92.99(8)	C(7)-C(8)-C(3)	119.79(15)
C(2)-C(1)-C(2)#1	124.0(2)	C(6)-C(7)-C(8)	118.69(16)
C(2)-C(1)-H(1)	118.0	C(6)-C(7)-H(7)	120.7
C(2)#1-C(1)-H(1)	118.0	C(8)-C(7)-H(7)	120.7
C(3)-S(1)-C(2)	90.60(8)	C(7)-C(6)-C(5)	120.90(17)
C(2)-N(1)-C(8)	112.29(13)	C(7)-C(6)-H(6)	119.5
C(2)-N(1)-Ga(1)	123.78(11)	C(5)-C(6)-H(6)	119.5
C(8)-N(1)-Ga(1)	123.92(10)	Ga(1)-C(10)-H(10A)	109.5
N(1)-C(2)-C(1)	127.20(15)	Ga(1)-C(10)-H(10B)	109.5
N(1)-C(2)-S(1)	112.99(11)	H(10A)-C(10)-H(10B)	109.5
C(1)-C(2)-S(1)	119.78(12)	Ga(1)-C(10)-H(10C)	109.5
C(4)-C(3)-C(8)	121.55(16)	H(10A)-C(10)-H(10C)	109.5
C(4)-C(3)-S(1)	128.70(14)	H(10B)-C(10)-H(10C)	109.5
C(8)-C(3)-S(1)	109.75(12)		
C(5)-C(4)-C(3)	118.08(16)		
C(5)-C(4)-H(4)	121.0		
C(3)-C(4)-H(4)	121.0		
C(4)-C(5)-C(6)	120.98(16)		
C(4)-C(5)-H(5)	119.5		

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_8

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_8

Bond precision: C-C = 0.0022 A Wavelength=0.56086

Cell: a=15.446(3) b=15.177(3) c=6.929(2)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1624.3(6)	1624.3(6)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C17 H15 Ga N2 S2	C17 H15 Ga N2 S2
Sum formula	C17 H15 Ga N2 S2	C17 H15 Ga N2 S2
Mr	381.17	381.15
Dx,g cm-3	1.559	1.559
Z	4	4
Mu (mm-1)	1.023	1.023
F000	776.0	776.0
F000'	777.88	
h,k,lmax	22,21,9	22,21,9
Nref	2582	2580
Tmin,Tmax	0.721,0.766	0.677,0.745
Tmin'	0.651	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 23.681

R(reflections)= 0.0251(2463) wR2(reflections)= 0.0602(2580)

S = 1.268 Npar= Npar = 108

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

RADNW01_ALERT_1_C The radiation wavelength lies outside the expected range for the supplied radiation type. Expected range 0.56080-0.56085
Wavelength given = 0.56086
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.173 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Why ?

Alert level G

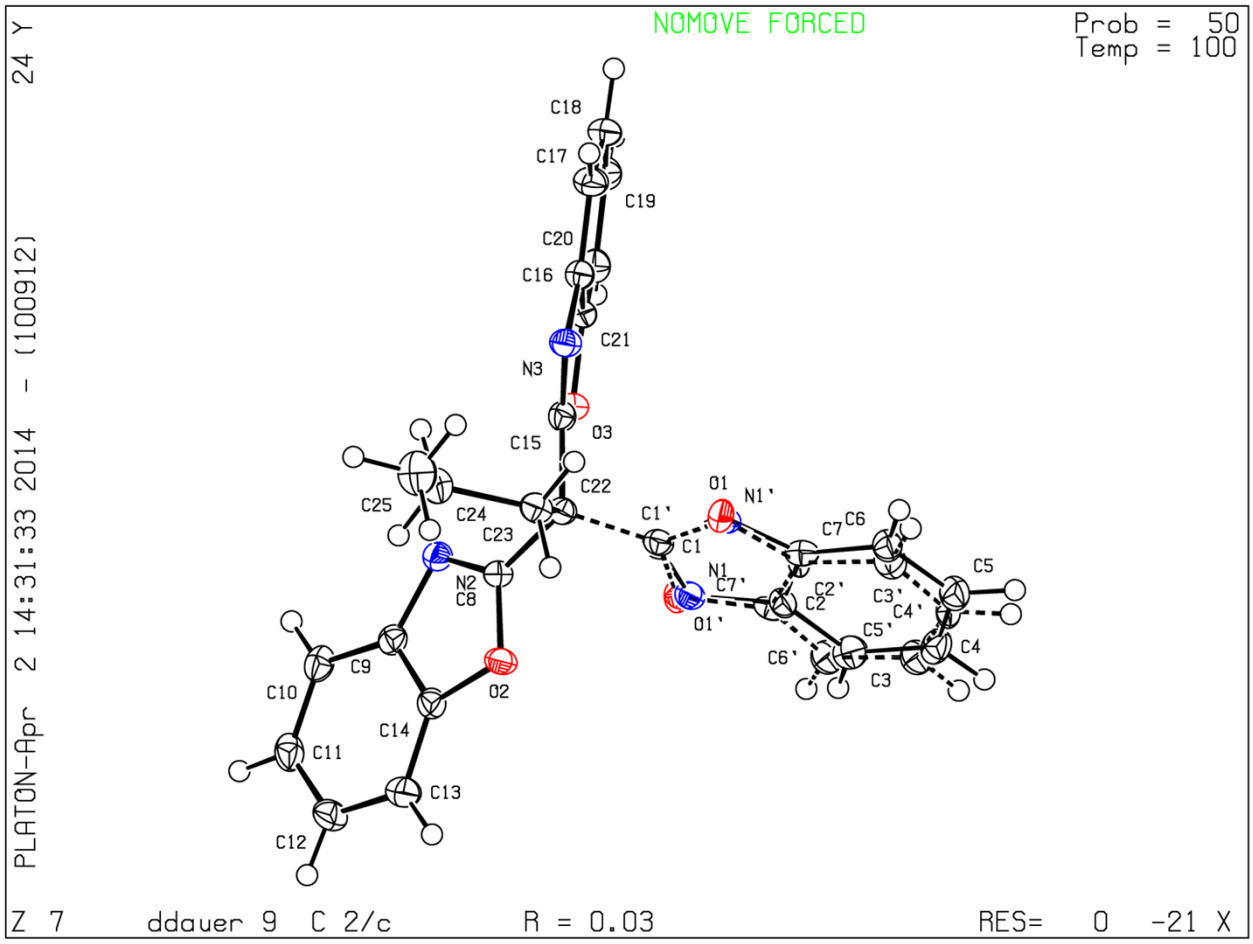
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3          Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         13     Why      ?
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        103 Note
```

```
 0 ALERT level A = Most likely a serious problem - resolve or explain
 0 ALERT level B = A potentially serious problem, consider carefully
 3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 3 ALERT level G = General information/check it is not something unexpected

 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 2 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
 0 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check
```

PLATON version of 05/02/2014; check.def file version of 05/02/2014

2.9 Bond lengths [Å] and angles [deg] for 9.



Bond lengths [Å] and angles [deg] for **9**.

C(22)-C(1')	1.501(10)	C(3)-H(3)	0.9500
C(22)-C(8)	1.5051(16)	C(4)-C(5)	1.400(4)
C(22)-C(15)	1.5120(16)	C(4)-H(4)	0.9500
C(22)-C(1)	1.521(6)	C(5)-C(6)	1.382(5)
C(22)-C(23)	1.5504(17)	C(5)-H(5)	0.9500
O(1)-C(1)	1.375(8)	C(6)-C(7)	1.378(6)
O(1)-C(7)	1.391(7)	C(6)-H(6)	0.9500
N(1)-C(1)	1.285(8)	O(1')-C(1')	1.368(13)
N(1)-C(2)	1.405(8)	O(1')-C(7')	1.382(11)
C(2)-C(7)	1.381(6)	N(1')-C(1')	1.289(13)
C(2)-C(3)	1.398(6)	N(1')-C(2')	1.394(12)
C(3)-C(4)	1.385(4)	C(2')-C(7')	1.371(9)

C(2')-C(3')	1.407(10)	C(23)-C(24)	1.5276(18)
C(3')-C(4')	1.381(8)	C(23)-H(23A)	0.9900
C(3')-H(3')	0.9500	C(23)-H(23B)	0.9900
C(4')-C(5')	1.391(7)	C(24)-C(25)	1.5199(19)
C(4')-H(4')	0.9500	C(24)-H(24A)	0.9900
C(5')-C(6')	1.380(7)	C(24)-H(24B)	0.9900
C(5')-H(5')	0.9500	C(25)-H(25A)	0.9800
C(6')-C(7')	1.372(10)	C(25)-H(25B)	0.9800
C(6')-H(6')	0.9500	C(25)-H(25C)	0.9800
O(2)-C(8)	1.3732(14)		
O(2)-C(14)	1.3830(14)	C(1')-C(22)-C(8)	111.9(8)
N(2)-C(8)	1.2824(16)	C(1')-C(22)-C(15)	105.3(14)
N(2)-C(9)	1.4112(15)	C(8)-C(22)-C(15)	113.07(10)
O(3)-C(15)	1.3674(15)	C(8)-C(22)-C(1)	108.0(5)
O(3)-C(21)	1.3872(14)	C(15)-C(22)-C(1)	105.3(8)
N(3)-C(15)	1.2886(16)	C(1')-C(22)-C(23)	107.8(9)
N(3)-C(16)	1.4039(16)	C(8)-C(22)-C(23)	108.69(10)
C(9)-C(14)	1.3845(18)	C(15)-C(22)-C(23)	109.91(10)
C(9)-C(10)	1.3962(17)	C(1)-C(22)-C(23)	111.9(5)
C(13)-C(14)	1.3781(18)	C(1)-O(1)-C(7)	103.8(6)
C(13)-C(12)	1.3865(19)	C(1)-N(1)-C(2)	104.9(6)
C(13)-H(13)	0.9500	N(1)-C(1)-O(1)	115.2(6)
C(10)-C(11)	1.3855(19)	N(1)-C(1)-C(22)	129.4(7)
C(10)-H(10)	0.9500	O(1)-C(1)-C(22)	115.2(6)
C(12)-C(11)	1.399(2)	C(7)-C(2)-C(3)	121.1(5)
C(12)-H(12)	0.9500	C(7)-C(2)-N(1)	108.6(6)
C(11)-H(11)	0.9500	C(3)-C(2)-N(1)	130.3(6)
C(16)-C(21)	1.3842(17)	C(4)-C(3)-C(2)	115.8(4)
C(16)-C(17)	1.3935(17)	C(4)-C(3)-H(3)	122.1
C(20)-C(21)	1.3822(17)	C(2)-C(3)-H(3)	122.1
C(20)-C(19)	1.3857(18)	C(3)-C(4)-C(5)	122.0(3)
C(20)-H(20)	0.9500	C(3)-C(4)-H(4)	119.0
C(17)-C(18)	1.3839(19)	C(5)-C(4)-H(4)	119.0
C(17)-H(17)	0.9500	C(6)-C(5)-C(4)	122.0(3)
C(19)-C(18)	1.4025(19)	C(6)-C(5)-H(5)	119.0
C(19)-H(19)	0.9500	C(4)-C(5)-H(5)	119.0
C(18)-H(18)	0.9500	C(7)-C(6)-C(5)	115.4(4)

C(7)-C(6)-H(6)	122.3	C(10)-C(9)-N(2)	131.14(12)
C(5)-C(6)-H(6)	122.3	C(14)-C(13)-C(12)	115.12(13)
C(6)-C(7)-C(2)	123.6(5)	C(14)-C(13)-H(13)	122.4
C(6)-C(7)-O(1)	129.0(5)	C(12)-C(13)-H(13)	122.4
C(2)-C(7)-O(1)	107.5(6)	C(11)-C(10)-C(9)	116.57(12)
C(1')-O(1')-C(7')	101.2(9)	C(11)-C(10)-H(10)	121.7
C(1')-N(1')-C(2')	102.7(11)	C(9)-C(10)-H(10)	121.7
N(1')-C(1')-O(1')	117.9(10)	C(13)-C(12)-C(11)	121.86(13)
N(1')-C(1')-C(22)	127.3(12)	C(13)-C(12)-H(12)	119.1
O(1')-C(1')-C(22)	114.7(11)	C(11)-C(12)-H(12)	119.1
C(7')-C(2')-N(1')	109.1(10)	C(10)-C(11)-C(12)	121.95(12)
C(7')-C(2')-C(3')	122.7(9)	C(10)-C(11)-H(11)	119.0
N(1')-C(2')-C(3')	128.3(9)	C(12)-C(11)-H(11)	119.0
C(4')-C(3')-C(2')	115.3(7)	N(3)-C(15)-O(3)	116.26(11)
C(4')-C(3')-H(3')	122.3	N(3)-C(15)-C(22)	124.95(11)
C(2')-C(3')-H(3')	122.3	O(3)-C(15)-C(22)	118.07(10)
C(3')-C(4')-C(5')	120.9(6)	C(13)-C(14)-O(2)	127.88(12)
C(3')-C(4')-H(4')	119.6	C(13)-C(14)-C(9)	124.38(12)
C(5')-C(4')-H(4')	119.6	O(2)-C(14)-C(9)	107.73(10)
C(6')-C(5')-C(4')	123.5(6)	C(21)-C(16)-C(17)	120.52(12)
C(6')-C(5')-H(5')	118.3	C(21)-C(16)-N(3)	108.71(10)
C(4')-C(5')-H(5')	118.3	C(17)-C(16)-N(3)	130.76(12)
C(7')-C(6')-C(5')	115.5(7)	C(21)-C(20)-C(19)	115.51(12)
C(7')-C(6')-H(6')	122.2	C(21)-C(20)-H(20)	122.2
C(5')-C(6')-H(6')	122.2	C(19)-C(20)-H(20)	122.2
C(2')-C(7')-C(6')	122.2(9)	C(18)-C(17)-C(16)	116.68(12)
C(2')-C(7')-O(1')	109.0(9)	C(18)-C(17)-H(17)	121.7
C(6')-C(7')-O(1')	128.8(9)	C(16)-C(17)-H(17)	121.7
C(8)-O(2)-C(14)	103.29(9)	C(20)-C(19)-C(18)	121.69(12)
C(8)-N(2)-C(9)	103.75(10)	C(20)-C(19)-H(19)	119.2
C(15)-O(3)-C(21)	103.33(9)	C(18)-C(19)-H(19)	119.2
C(15)-N(3)-C(16)	104.01(10)	C(17)-C(18)-C(19)	121.82(12)
N(2)-C(8)-O(2)	116.51(11)	C(17)-C(18)-H(18)	119.1
N(2)-C(8)-C(22)	129.61(11)	C(19)-C(18)-H(18)	119.1
O(2)-C(8)-C(22)	113.57(10)	C(20)-C(21)-C(16)	123.75(11)
C(14)-C(9)-C(10)	120.11(12)	C(20)-C(21)-O(3)	128.57(11)
C(14)-C(9)-N(2)	108.72(10)	C(16)-C(21)-O(3)	107.69(10)

C(24)-C(23)-C(22)	113.34(10)	C(24)-C(25)-H(25A)	109.5
C(24)-C(23)-H(23A)	108.9	C(24)-C(25)-H(25B)	109.5
C(22)-C(23)-H(23A)	108.9	H(25A)-C(25)-H(25B)	109.5
C(24)-C(23)-H(23B)	108.9	C(24)-C(25)-H(25C)	109.5
C(22)-C(23)-H(23B)	108.9	H(25A)-C(25)-H(25C)	109.5
H(23A)-C(23)-H(23B)	107.7	H(25B)-C(25)-H(25C)	109.5
C(25)-C(24)-C(23)	111.22(11)		
C(25)-C(24)-H(24A)	109.4		
C(23)-C(24)-H(24A)	109.4		
C(25)-C(24)-H(24B)	109.4		
C(23)-C(24)-H(24B)	109.4		
H(24A)-C(24)-H(24B)	108.0		

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddauer_9

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ddauer_9

```
Bond precision:  C-C = 0.0019 A          Wavelength=0.71073

Cell:            a=31.997(3)     b=8.907(1)          c=15.673(2)
                 alpha=90        beta=117.53(1)      gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           3961.0(8)                 3961.0(8)
Space group      C 2/c                     C 2/c
Hall group       -C 2yc                    -C 2yc
Moiety formula   C25 H19 N3 O3             C25 H19 N3 O3
Sum formula      C25 H19 N3 O3             C25 H19 N3 O3
Mr               409.43                    409.43
Dx,g cm-3        1.373                     1.373
Z                8                         8
Mu (mm-1)        0.092                     0.092
F000             1712.0                    1712.0
F000'            1712.75
h,k,lmax         40,11,20                  40,11,20
Nref             4382                      4360
Tmin,Tmax        0.982,0.982               0.922,0.970
Tmin'            0.982

Correction method= MULTI-SCAN

Data completeness= 0.995          Theta(max)= 27.122

R(reflections)= 0.0347( 3662)     wR2(reflections)= 0.0891( 4360)  S =

1.043                      Npar= Npar = 358
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 19 Why ?

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         37         Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         18     Why     ?
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =                29         Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          !         Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        594         Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          3 Note
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 05/02/2014; check.def file version of 05/02/2014