checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: compound_1_

Bond precision: C-C = 0.0022 A Wavelength=0.71073

Cell: **a=38.802(16)** **b=9.746(4)** **c=18.301(8)**
alpha=90 **beta=117.007(9)** **gamma=90**
Temperature: **100 K**

	Calculated	Reported
Volume	6166(5)	6166(5)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C34 H47 Al	C34 H47 Al
Sum formula	C34 H47 Al	C34 H47 Al
Mr	482.70	482.70
Dx,g cm-3	1.040	1.040
Z	8	8
Mu (mm-1)	0.084	0.084
F000	2112.0	2112.0
F000’	2113.13	
h,k,lmax	47,12,22	47,12,22
Nref	6056	6056
Tmin,Tmax	0.976,0.992	0.954,0.995
Tmin’	0.957	

Correction method= MULTI-SCAN

Data completeness= 1.000 **Theta(max)= 26.000**

R(reflections)= 0.0417(4901) **wR2(reflections)= 0.1271(6056)**

S = 1.020 **Npar= 316**

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
PLAT230_ALERT_2_C Hirshfeld Test Diff for C31 -- C32 .. 5.99 su

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0 **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
0 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

Datablock: compound_2_

Bond precision: C-C = 0.0084 A Wavelength=0.71073

Cell: a=10.119(2) b=7.5504(14) c=27.389(6)
alpha=90 beta=92.576(8) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2090.5(7)	2090.5(7)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H19 Al Cl4	C22 H19 Al Cl4
Sum formula	C22 H19 Al Cl4	C22 H19 Al Cl4
Mr	452.15	452.15
Dx,g cm-3	1.437	1.437
Z	4	4
Mu (mm-1)	0.613	0.613
F000	928.0	928.0
F000’	930.84	
h,k,lmax	12,8,32	11,8,32
Nref	3656	3556
Tmin,Tmax	0.957,0.976	0.804,0.979
Tmin’	0.802	

Correction method= MULTI-SCAN

Data completeness= 0.973 Theta(max)= 24.990

R(reflections)= 0.0806(2882) wR2(reflections)= 0.1756(3556)

S = 1.201 Npar= 244

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.97
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.75 Ratio

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ..   8

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.   10.00
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c P21/n

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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
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: compound_3_

Bond precision: C-C = 0.0033 A   Wavelength=1.54178

Cell: a=13.4689(2) b=17.0328(2) c=23.6118(3)
alpha=90 beta=119.949(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4693.54(12)	4693.54(11)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P2 ybc
Moiety formula	C33 H47.80 Al B11 Cl6.20, C6 H6	C33 H47.80 Al B11 Cl6.20, C6 H6
Sum formula	C39 H53.80 Al B11 Cl6.20	C39 H53.80 Al B11 Cl6.20
Mr	888.30	888.30
Dx,g cm-3	1.257	1.257
Z	4	4
Mu (mm-1)	3.827	3.827
F000	1844.8	1844.8
F000’	1857.79	
h,k,lmax	16,20,28	16,20,28
Nref	8431	8326
Tmin,Tmax	0.488,0.563	0.515,0.598
Tmin’	0.443	

Correction method= MULTI-SCAN

Data completeness= 0.988   Theta(max)= 67.400

R(reflections)= 0.0343(7224) wR2(reflections)= 0.0914(8326)

S = 1.023 Npar= 575

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 G
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 0.00 Perc.
PLAT343_ALERT_2_G Check sp? Angle Range in Main Residue for .. C4B

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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
1 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

Datablock: compound_4.C6H6_

Bond precision: C-C = 0.0029 A Wavelength=0.71073

Cell: **a=12.1316(14)** **b=12.1249(14)** **c=25.840(3)**
alpha=90 **beta=96.978(2)** **gamma=90**
Temperature: **100 K**

	Calculated	Reported
Volume	3772.8(8)	3772.8(7)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C21 H20 Al B11 Cl10, C6 H6	C21 H20 Al B11 Cl10, C6 H6
Sum formula	C27 H26 Al B11 Cl10	C27 H26 Al B11 Cl10
Mr	850.87	850.87
Dx,g cm-3	1.498	1.498
Z	4	4
Mu (mm-1)	0.785	0.785
F000	1704.0	1704.0
F000’	1710.46	
h,k,lmax	16,16,34	16,16,34
Nref	9386	9361
Tmin,Tmax	0.784,0.917	0.790,0.921
Tmin’	0.784	

Correction method= MULTI-SCAN

Data completeness= 0.997 Theta(max)= 28.310

R(reflections)= 0.0341(7840) wR2(reflections)= 0.0874(9361)

S = 1.003 Npar= 452

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

```
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       3.19 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cl7    --  Al1     ..       8.83 su
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C1A    -   H1A    ...       1.12 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C19    --  C20'    ..       0.20 Ang.
```

Alert level G

```
PLAT301_ALERT_3_G Note: Main Residue  Disorder ..................       2.00 Perc.
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C1A
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          1
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
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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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: compound_5_

Bond precision: C-C = 0.0108 A Wavelength=0.71073

Cell: a=13.736(10) b=20.352(15) c=17.040(12)
alpha=90 beta=107.880(16) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4534(6)	4534(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C33 H48 Al B11 I6	C33 H48 Al B11 I6
Sum formula	C33 H48 Al B11 I6	C33 H48 Al B11 I6
Mr	1352.01	1352.00
Dx,g cm-3	1.981	1.981
Z	4	4
Mu (mm-1)	4.154	4.155
F000	2528.0	2528.0
F000’	2517.57	
h,k,lmax	18,26,22	17,26,21
Nref	11061	9945
Tmin,Tmax	0.175,0.436	0.262,0.490
Tmin’	0.147	

Correction method= MULTI-SCAN

Data completeness= 0.899 **Theta(max)= 28.100**

R(reflections)= 0.0510(5984) **wR2(reflections)= 0.0986(9945)**

S = 0.975 **Npar= 469**

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

PLAT213_ALERT_2_C Atom C7 has ADP max/min Ratio ..... 3.80 oblat
PLAT213_ALERT_2_C Atom C19 has ADP max/min Ratio ..... 3.20 oblat
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.64 Ratio
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 11
PLAT351_ALERT_3_C Long C-H Bond (0.96A) C1B - H1B ... 1.12 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference B2 -- B3 .. 0.15 Ang.

Alert level G

PLAT343_ALERT_2_G Check sp? Angle Range in Main Residue for .. C1B
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 103
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c P21/n

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6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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0 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
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: compound_7.4C6H6_

Bond precision: C-C = 0.0059 A Wavelength=0.71073

Cell: a=13.723(4) b=19.109(6) c=15.786(5)
alpha=90 beta=115.330(12) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3742(2)	3742(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2yc
Moiety formula	C64 H86 Al2 O2, 4(C6 H6)	C64 H86 O2 Al2, 4(C6 H6)
Sum formula	C88 H110 Al2 O2	C88 H110 Al2 O2
Mr	1253.72	1253.72
Dx,g cm-3	1.113	1.113
Z	2	2
Mu (mm-1)	0.086	0.086
F000	1360.0	1360.0
F000’	1360.70	
h,k,lmax	14,20,17	14,20,17
Nref	5024	5021
Tmin,Tmax	0.979,0.991	0.962,0.994
Tmin’	0.964	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 22.720

R(reflections)= 0.0603(3195) wR2(reflections)= 0.1514(5021)

S = 1.001 Npar= 424

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 A
THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5434

Alert level B

PLAT420_ALERT_2_B D-H Without Acceptor O1 - H1 ... ?

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.133
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.53
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 6
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ ?
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P 2yc

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0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: compound_8_

Bond precision: C-C = 0.0151 A Wavelength=0.71073

Cell: **a=9.967(4) b=31.025(12) c=15.405(6)**
alpha=90 beta=94.07(6) gamma=90
Temperature: **100 K**

	Calculated	Reported
Volume	4752(3)	4752(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2yc
Moiety formula	C28 H36 Al Cl4 N2, C H6 B11 I6	C28 H34 Al Cl4 N2, C H6 B11 I6
Sum formula	C29 H42 Al B11 Cl4 I6 N2	C29 H42 Al B11 Cl4 I6 N2
Mr	1467.74	1467.74
Dx,g cm-3	2.052	2.052
Z	4	4
Mu (mm-1)	4.191	4.192
F000	2736.0	2736.0
F000’	2727.93	
h,k,lmax	12,38,19	12,38,19
Nref	9732	9582
Tmin,Tmax	0.421,0.605	0.330,0.633
Tmin’	0.231	

Correction method= MULTI-SCAN

Data completeness= 0.985 **Theta(max)= 26.370**

R(reflections)= 0.0718(6303) **wR2(reflections)= 0.1339(9582)**

S = 1.000 **Npar= 485**

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 B

PLAT149_ALERT_3_B su on the beta Angle is Too Large (x 100) .. 6 Deg.

Alert level C

PLAT213_ALERT_2_C Atom C29 has ADP max/min Ratio ..... 3.30 prola
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 15
PLAT351_ALERT_3_C Long C-H Bond (0.96A) C1A - H1A ... 1.12 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N24 - H24A ... ?
PLAT420_ALERT_2_C D-H Without Acceptor N24 - H24B ... ?
PLAT431_ALERT_2_C Short Inter HL..A Contact I5 .. Cl4 .. 3.59 Ang.
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ ?
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P 2yc

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Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C29 H42 Al1 B11 Cl4 I6 N2
Atom count from _chemical_formula_moiety:C29 H40 Al1 B11 Cl4 I6 N2
PLAT343_ALERT_2_G Check sp? Angle Range in Main Residue for .. C1A
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 352

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0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF in IUCr journals

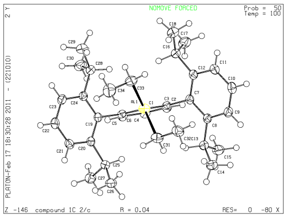
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

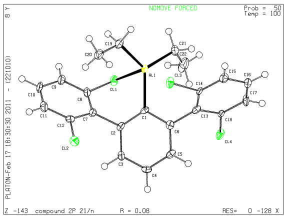
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/10/2010; check.def file version of 11/10/2010

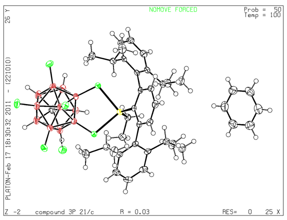
Datablock compound_1_ - ellipsoid plot



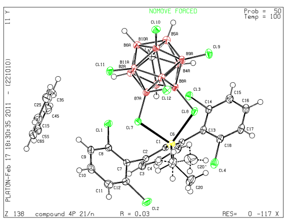
Datablock compound_2_ - ellipsoid plot



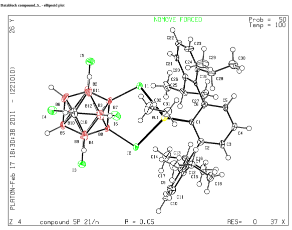
Datablock compound_3_ - ellipsoid plot



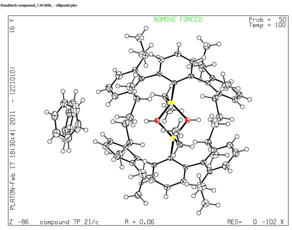
Datablock compound_4.C6H6_ - ellipsoid plot



Datablock compound_5_ - ellipsoid plot



Datablock compound_7.4C6H6_ - ellipsoid plot



Datablock compound_8_ - ellipsoid plot