checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

Bond precision: N- B = 0.0045 A Wavelength=1.54178

Cell: a=9.6860(2) b=11.3287(2) c=16.4121(2)
alpha=90 beta=90 gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	1800.90(5)	1800.90(5)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C6 H24 As B2 N2, Al Cl4	C6 H24 As B2 N2, Al Cl4
Sum formula	C6 H24 Al As B2 Cl4 N2	C6 H24 Al As B2 Cl4 N2
Mr	389.59	389.59
Dx,g cm-3	1.437	1.437
Z	4	4
Mu (mm-1)	8.319	8.319
F000	792.0	792.0
F000'	795.72	
h,k,lmax	12,14,20	11,13,20
Nref	2077[3626]	3485
Tmin,Tmax	0.211,0.316	0.258,0.438
Tmin'	0.094	

Correction method= ANALYTICAL

Data completeness= 1.68/0.96 Theta(max)= 73.450

R(reflections)= 0.0301(3438) wR2(reflections)= 0.0788(3485)

S = 1.037 Npar= 175

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

PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 5.1 Ratio
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for N2
PLAT420_ALERT_2_C D-H Without Acceptor As1 - H1 ... ?
PLAT420_ALERT_2_C D-H Without Acceptor As1 - H2 ... ?

Alert level G

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REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max           73.45
          From the CIF: _reflns_number_total               3485
          Count of symmetry unique reflns         2077
          Completeness (_total/calc)           167.79%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      1408
          Fraction of Friedel pairs measured     0.678
          Are heavy atom types Z>Si present        yes
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT153_ALERT_1_G The su's on the Cell Axes   are Equal .........    0.00020 Ang.
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Al1     (III)         3.02
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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
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 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
   1 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
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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 21/12/2011; check.def file version of 16/12/2011

Datablock 1 - ellipsoid plot