checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 11913sadabs

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: 11913sadabs

```
Bond precision:  N- C = 0.0085 A         Wavelength=0.71073

Cell:            a=8.5770(17)     b=6.4756(13)     c=7.2306(14)
                 alpha=90         beta=90          gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	401.60(14)	401.60(14)
Space group	P b c m	P b c m
Hall group	-P 2c 2b	-P 2c 2b
Moiety formula	C2 N3 Tl	C2 N3 Tl
Sum formula	C2 N3 Tl	C2 N3 Tl
Mr	270.43	270.42
Dx,g cm-3	4.473	4.473
Z	4	4
Mu (mm-1)	40.022	40.022
F000	456.0	456.0
F000’	446.14	
h,k,lmax	13,9,11	13,9,11
Nref	818	816
Tmin,Tmax	0.160,0.449	0.152,0.463
Tmin’	0.124	

```
Correction method= # Reported T Limits: Tmin=0.152 Tmax=0.463
AbsCorr = GAUSSIAN

Data completeness= 0.998          Theta(max)= 33.088

R(reflections)= 0.0187( 549)      wR2(reflections)= 0.0445( 816)

S = 1.088                 Npar= 36
```

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

```
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.7 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     19.548 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.081 Check
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.58A   From Tl1           -1.53 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.04A   From N1             0.44 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.04A   From N1             0.44 eA-3
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
```

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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
   6 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

   2 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
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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* or *IUCrData*, 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 19/10/2018; check.def file version of 15/10/2018

Datablock 11913sadabs - ellipsoid plot