checkCIF/PLATON report

Structure factors have been supplied for datablock(s) NA01a

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: NA01a

Bond precision: C-C = 0.0078 A   Wavelength=0.71073

Cell: a=9.0608(19)   b=37.640(8)   c=11.263(2)
               alpha=90   beta=103.230(2)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3739.3(13)	3739.3(14)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C25 H64 Si8	?
Sum formula	C25 H64 Si8	C25 H64 Si8
Mr	589.48	589.48
Dx,g cm-3	1.047	1.047
Z	4	4
Mu (mm-1)	0.300	0.300
F000	1304.0	1304.0
F000'	1306.78	
h,k,lmax	10,44,13	10,44,13
Nref	6588	6539
Tmin,Tmax	0.965,0.970	0.889,0.971
Tmin'	0.887	

Correction method= # Reported T Limits: Tmin=0.889 Tmax=0.971
AbsCorr = EMPIRICAL

Data completeness= 0.993   Theta(max)= 25.000

R(reflections)= 0.0729(5971)   wR2(reflections)= 0.1806(6539)

S = 1.335   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

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.00783 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      10.700 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......       2.550 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         48 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....          1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H15            -0.32 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
```

Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      18.54 Why ?
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       84% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...          2 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 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
   8 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
```

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 09/11/2017; check.def file version of 08/11/2017