

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) NA152a_a

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: NA152a_a

Bond precision: C-C = 0.0030 A

Wavelength=0.71073

Cell: a=11.9302(9) b=12.8081(10) c=15.7049(13)
 alpha=95.628(2) beta=98.481(2) gamma=90.755(2)
Temperature: 100 K

| | Calculated | Reported |
|----------------|--------------------|--------------------|
| Volume | 2361.1(3) | 2361.1(3) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C44 H58 Si6, C7 H8 | C44 H58 Si6, C7 H8 |
| Sum formula | C51 H66 Si6 | C51 H66 Si6 |
| Mr | 847.58 | 847.57 |
| Dx,g cm-3 | 1.192 | 1.192 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.211 | 0.211 |
| F000 | 912.0 | 912.0 |
| F000' | 913.20 | |
| h,k,lmax | 14,15,19 | 14,15,19 |
| Nref | 8802 | 8802 |
| Tmin,Tmax | 0.992,0.996 | 0.664,0.746 |
| Tmin' | 0.983 | |

Correction method= # Reported T Limits: Tmin=0.664 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 1.000

Theta(max)= 25.500

R(reflections)= 0.0350(7374)

wR2(reflections)= 0.0954(8802)

S = 1.028

Npar= 568

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 | Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range | 3.1 | Ratio |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for Average U(i,j) Tensor | 3.2 | Note |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for Average U(i,j) Tensor | 2.3 | Note |

● **Alert level G**

| | | | |
|-------------------|--|-------|--------|
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 14 | Report |
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal ..(Note) | 0.002 | Degree |
| PLAT178_ALERT_4_G | The CIF-Embedded .res File Contains SIMU Records | 1 | Report |
| PLAT187_ALERT_4_G | The CIF-Embedded .res File Contains RIGU Records | 2 | Report |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 2) | 100% | Note |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 3) | 100% | Note |
| PLAT304_ALERT_4_G | Non-Integer Number of Atoms in Resd 2 | 9.72 | Check |
| PLAT304_ALERT_4_G | Non-Integer Number of Atoms in Resd 3 | 5.28 | Check |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 126 | Note |
| PLAT960_ALERT_3_G | Number of Intensities with I < - 2*sig(I) ... | 13 | Check |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 5 | Info |

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
6 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

