

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tg199

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: tg199

| | | |
|-----------------|------------------|--------------------------------|
| Bond precision: | C-C = 0.0021 A | Wavelength=1.39222 |
| Cell: | a=10.6741(2) | b=14.2858(2) c=17.5012(3) |
| | alpha=90 | beta=99.597(2) gamma=90 |
| Temperature: | 123 K | |
| | Calculated | Reported |
| Volume | 2631.38(8) | 2631.37(8) |
| Space group | P 21/n | P 21/n |
| Hall group | -P 2yn | -P 2yn |
| Moiety formula | C30 H25 Cl O Si2 | C30 H25 Cl O Si2 |
| Sum formula | C30 H25 Cl O Si2 | C30 H25 Cl O Si2 |
| Mr | 493.13 | 493.13 |
| Dx,g cm-3 | 1.245 | 1.245 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.688 | 1.690 |
| F000 | 1032.0 | 1032.0 |
| F000' | 1036.98 | |
| h,k,lmax | 14,19,23 | 14,19,23 |
| Nref | 6736 | 6570 |
| Tmin,Tmax | 0.816,0.868 | 0.795,1.000 |
| Tmin' | 0.762 | |

Correction method= # Reported T Limits: Tmin=0.795 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.975 Theta(max)= 69.661

R(reflections)= 0.0347(5823) wR2(reflections)= 0.0994(6570)

S = 1.045 Npar= 407

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

| | | |
|-------------------|--|--------------|
| PLAT092_ALERT_4_G | Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka | 1.39222 Ang. |
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for Cl --Si2 | 9.3 s.u. |
| PLAT396_ALERT_2_G | Deviating Si-O-Si Angle From 150 for O | 165.1 Degree |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 162 Note |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity | 3.4 Low |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 17 Info |
| PLAT984_ALERT_1_G | The C-f'= 0.0159 Deviates from the B&C-Value | 0.0147 Check |
| PLAT984_ALERT_1_G | The Cl-f'= 0.3404 Deviates from the B&C-Value | 0.3386 Check |
| PLAT984_ALERT_1_G | The O-f'= 0.0440 Deviates from the B&C-Value | 0.0415 Check |
| PLAT985_ALERT_1_G | The Cl-f"= 0.5791 Deviates from the B&C-Value | 0.5824 Check |
| PLAT985_ALERT_1_G | The O-f"= 0.0271 Deviates from the B&C-Value | 0.0260 Check |
| PLAT985_ALERT_1_G | The Si-f"= 0.2674 Deviates from the B&C-Value | 0.2717 Check |

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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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected
- 7 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
2 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
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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* 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.

