

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tps213mono

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: tps213mono

Bond precision: C-C = 0.0067 Å Wavelength=0.71073

Cell: a=8.1123(16) b=14.126(3) c=24.766(5)
 alpha=90 beta=99.36(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2800.3(10)	2800.4(10)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H45 Na O3 Si	C26 H45 Na O3 Si
Sum formula	C26 H45 Na O3 Si	C26 H45 Na O3 Si
Mr	456.70	456.70
Dx,g cm-3	1.083	1.083
Z	4	4
Mu (mm-1)	0.121	0.121
F000	1000.0	1000.0
F000'	1000.80	
h,k,lmax	10,17,30	10,17,30
Nref	5551	5468
Tmin,Tmax	0.977,0.992	0.982,0.992
Tmin'	0.964	

Correction method= # Reported T Limits: Tmin=0.982 Tmax=0.992
AbsCorr = INTEGRATION

Data completeness= 0.985 Theta(max)= 26.088

R(reflections)= 0.0931(2890) wR2(reflections)= 0.2846(5468)

S = 1.003 Npar= 287

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

REFLE01_ALERT_3_C The _reflns_threshold_multiplier given is >= 4
Premultiplier = 4.00
REFLE01_ALERT_3_C The _reflns_threshold_multiplier given is >= 4
Premultiplier = 4.00
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0067 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C19 - C20 .. 1.41 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.997 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 41 Report

● Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 5 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.17 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints 40 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 42 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
3 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.

