

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tps120-3h

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: tps120-3h

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Bond precision:	C-C = 0.0075 A	Wavelength=0.71073
Cell:	a=9.4746(4)	b=14.9924(8)      c=21.7467(8)
	alpha=90	beta=101.490(3)      gamma=90
Temperature:	220 K	
	Calculated	Reported
Volume	3027.2(2)	3027.1(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C44 H74 Ca2 I2 O4 Si2 [+ solvent]	C44 H74 Ca2 I2 O4 Si2
Sum formula	C44 H74 Ca2 I2 O4 Si2 [+ solvent]	C44 H74 Ca2 I2 O4 Si2
Mr	1057.17	1057.17
Dx, g cm-3	1.160	1.160
Z	2	2
Mu (mm-1)	1.278	1.278
F000	1088.0	1088.0
F000'	1087.66	
h,k,lmax	11,18,26	11,18,26
Nref	6016	5910
Tmin,Tmax	0.663,0.703	0.648,0.728
Tmin'	0.650	

Correction method= # Reported T Limits: Tmin=0.648 Tmax=0.728  
AbsCorr = INTEGRATION

Data completeness= 0.982      Theta(max)= 26.125

R(reflections)= 0.0392( 3630)      wR2(reflections)= 0.1181( 5910)

S = 0.975      Npar= 251

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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 B

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C7	--	C11	..	8.3 s.u.
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of			Si1 Check



#### Alert level C

ABSTY02\_ALERT\_1\_C An \_exptl\_absorpt\_correction\_type has been given without  
a literature citation. This should be contained in the  
\_exptl\_absorpt\_process\_details field.  
Absorption correction given as integration

PLAT234_ALERT_4_C	Large Hirshfeld Difference	C16	--	C17	..	0.20 Ang.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of			C16 Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of			C21 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of			Ca1 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of			O2 Check
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond	C17	-	C18	.. 1.43 Ang.
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance	...				-1.217 Report
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600				48 Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	...				1 Check
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.					0 Note



#### Alert level G

PLAT371_ALERT_2_G	Long	C(sp2)-C(sp1) Bond	C5	-	C6	.. 1.44 Ang.
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	....				C11 Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in Structure	...				197 A**3
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed					! Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)					1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600				57 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	....				1 Note

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 ALERT type 3 Indicator that the structure quality may be low  
5 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.

