

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) V2PS10

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: V2PS10

Bond precision:	S- P = 0.0005 A	Wavelength=0.68890	
Cell:	a=12.69038 (14)	b=7.33484 (7)	c=23.6081 (2)
	alpha=90	beta=95.8478 (9)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2186.05 (4)	2186.05 (4)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	P2 S20 V4	P S10 V2	
Sum formula	P2 S20 V4	P S10 V2	
Mr	906.90	453.45	
Dx, g cm ⁻³	2.756	2.756	
Z	4	8	
Mu (mm ⁻¹)	3.354	3.354	
F000	1768.0	1768.0	
F000'	1782.98		
h, k, lmax	19, 11, 36	19, 11, 36	
Nref	8343	8302	
Tmin, Tmax	0.961, 0.967	0.768, 1.000	
Tmin'	0.935		

Correction method= # Reported T Limits: Tmin=0.768 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.995 Theta(max)= 31.999

R(reflections)= 0.0203 (7288)	wR2(reflections)=
S = 1.017	0.0496 (8302)
Npar= 235	

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

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: P2 S20 V4
Rep.: P S10 V2
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
-13 1 6, -11 0 6, -12 0 8, -10 0 20, -10 1 20, 7 0 20,
-7 0 24,



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.68890 Ang.
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing 0.00007 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00020 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for V1 (V) . 4.69 Info
PLAT794_ALERT_5_G Tentative Bond Valency for V2 (V) . 4.67 Info
PLAT794_ALERT_5_G Tentative Bond Valency for V3 (V) . 4.65 Info
PLAT794_ALERT_5_G Tentative Bond Valency for V4 (V) . 4.71 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 34 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
-13 1 6, -11 0 6, -12 0 8,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 1.35 Note
Predicted wR2: Based on SigI**2 3.69 or SHELX Weight 4.95

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
6 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.

