

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) msw22_1a

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: msw22_1a

Bond precision:	C-C = 0.0030 A	Wavelength=0.71073	
Cell:	a=10.0420(1)	b=10.0420(1)	c=29.2155(2)
	alpha=90	beta=90	gamma=120
Temperature:	100 K		
	Calculated	Reported	
Volume	2551.43(5)	2551.43(5)	
Space group	R 3 c	R 3 c	
Hall group	R 3 -2" c	R 3 -2" c	
Moiety formula	C9 H21 F3 N3 Sn, C F3 O3 S	C9 H21 F3 N3 Sn1, C1 F3 O3 S1	
Sum formula	C10 H21 F6 N3 O3 S Sn	C10 H21 F6 N3 O3 S Sn	
Mr	496.07	496.05	
Dx, g cm-3	1.937	1.937	
Z	6	6	
Mu (mm-1)	1.701	1.701	
F000	1476.0	1476.0	
F000'	1473.76		
h,k,lmax	13,13,39	13,13,39	
Nref	1482[744]	1475	
Tmin,Tmax	0.783,0.903	0.888,1.000	
Tmin'	0.600		

Correction method= # Reported T Limits: Tmin=0.888 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.98/1.00 Theta(max)= 28.673

R(reflections)= 0.0125(1469) wR2(reflections)= 0.0349(1475)

S = 1.144 Npar= 74

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 G

PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0	0.997	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub	100 %Fit
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	0.00020	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		12 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Sn01 (IV)		4.14 Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		3 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0 Info

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
2 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 05/12/2020; check.def file version of 05/12/2020

Datablock msw22_1a - ellipsoid plot

