

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) li274

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: li274

Bond precision: C-C = 0.0157 Å Wavelength=0.71073

Cell: a=20.5260(16) b=10.3670(6) c=17.0858(10)
 alpha=90 beta=90 gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	3635.7(4)	3635.7(4)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C41 H39 I Ni P3	C41 H39 I Ni P3
Sum formula	C41 H39 I Ni P3	C41 H39 I Ni P3
Mr	810.22	810.24
Dx,g cm-3	1.480	1.480
Z	4	4
Mu (mm-1)	1.543	1.543
F000	1644.0	1644.0
F000'	1645.09	
h,k,lmax	34,17,28	30,16,28
Nref	18027[9249]	14073
Tmin,Tmax		0.774,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.774 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.52/0.78 Theta(max)= 36.624

R(reflections)= 0.0787(6136) wR2(reflections)= 0.2167(14073)

S = 0.941 Npar= 417

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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.181
PLAT020_ALERT_3_B The value of Rint is greater than 0.12 0.181 Report
PLAT973_ALERT_2_B Check Calcd Positive Residual Density on Ni05 1.87 eA-3

Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 44 %
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01575 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 10.563 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.490 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.789 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.082 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.045 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 72 %
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum found in CIF Please Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I001 -- Ni05 .. 16.7 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 85 Note
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 1301 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 4 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 4 Units

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
13 **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
- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

