

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) LaNiSi

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: LaNiSi

Bond precision:	Ni-Si = 0.0070 Å	Wavelength=0.71073		
Cell:	a=7.435 (5)	b=14.227 (9)	c=6.069 (4)	
	alpha=90	beta=90	gamma=90	
Temperature:	300 K			

	Calculated	Reported
Volume	642.0 (7)	641.9 (7)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	La3 Ni3 Si2	?
Sum formula	La3 Ni3 Si2	La1.50 Ni1.50 Si
Mr	648.98	324.52
Dx, g cm-3	6.714	6.716
Z	4	8
Mu (mm-1)	28.368	28.370
F000	1132.0	1132.0
F000'	1133.74	
h, k, lmax	8, 16, 7	8, 16, 7
Nref	594	581
Tmin, Tmax	0.266, 0.427	0.299, 0.746
Tmin'	0.099	

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Correction method= # Reported T Limits: Tmin=0.299 Tmax=0.746
AbsCorr = MULTI-SCAN
```

Data completeness= 0.978 Theta(max)= 24.951

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R(reflections)= 0.0543( 362)      wR2(reflections)=
S = 1.048                        0.1150( 581)
Npar= 40
```

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 0.227

Author Response: Because the diffraction data signal is very weak, low Rint values cannot be obtained during absorption correction.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.28Ang From Ni1 2.88 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.36Ang From La2 2.57 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.98Ang From La1 -2.54 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.



Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard
identifier.
gray

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.978 Why?

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 10.722 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.594 13 Report

4 0 1, 7 5 1, 3 10 1, 5 10 1, 5 11 1, 3 4 2,

2 6 2, 6 6 3, 2 8 3, 5 2 4, 4 8 5, 1 2 6,

0 8 6,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.07Ang From La1 2.23 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.77Ang From Ni2 2.22 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.95Ang From Ni2 2.21 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.08Ang From La1 1.95 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.83Ang From La2 1.88 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.05Ang From Ni1 1.86 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.39Ang From La1 1.84 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.15Ang From La2 1.84 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.28Ang From La1 1.77 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.24Ang From La2 1.77 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.43Ang From Si1 1.77 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.46Ang From La1 1.76 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.35Ang From La1 1.75 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.45Ang From La1 1.66 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.03Ang From La1 1.64 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.05Ang From Ni1 1.63 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.72Ang From La1 1.62 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.44Ang From Ni1 1.61 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.69Ang From La1 1.51 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 2.05Ang From La2 -2.46 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.37Ang From Ni2 -2.13 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.67Ang From Si1 -2.09 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.98Ang From La1 -2.06 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.29Ang From La1 -1.98 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.86Ang From Ni2 -1.96 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From La1 -1.91 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.06Ang From Ni1 -1.90 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From Si1 -1.86 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.72Ang From Si1 -1.86 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.45Ang From La2 -1.82 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.16Ang From La1 -1.78 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From La1 -1.78 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.50Ang From La1 -1.76 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.70Ang From Ni1 -1.73 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.59Ang From Ni2 -1.70 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From La1 -1.69 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.86Ang From Ni1 -1.67 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.93Ang From La1 -1.63 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.24Ang From La2 -1.59 eA-3

Author Response: The diffraction data are not very good, so leads to this alert.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	3 Info
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12	0.227 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	18.67 Why ?
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	34% Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	1.151 Note

Predicted wR2: Based on SigI**2 9.99 or SHELX Weight 10.98

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
44 **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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
44 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
0 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.

