

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0018 Å Wavelength=0.70000

Cell: a=12.473(3) b=5.5140(11) c=14.195(3)
 alpha=90 beta=101.88(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	955.4(4)	955.4(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C18 H20 N6 Ni O2 S2	C18 H20 N6 Ni O2 S2
Sum formula	C18 H20 N6 Ni O2 S2	C18 H20 N6 Ni O2 S2
Mr	475.21	475.23
Dx, g cm ⁻³	1.652	1.652
Z	2	2
Mu (mm ⁻¹)	1.206	1.264
F000	492.0	492.0
F000'	493.28	
h, k, lmax	17, 7, 20	17, 7, 20
Nref	2914	2907
Tmin, Tmax	0.675, 0.702	
Tmin'	0.612	

Correction method= Not given

Data completeness= 0.998 Theta(max)= 29.967

R(reflections)= 0.0272(2819)

wR2(reflections)=
0.0692(2907)

S = 1.104

Npar= 134

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

PLAT051_ALERT_1_C	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	4.62 %
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3 Report



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.70000 Ang.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ni --S1 .	6.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ni --N1 .	6.0 s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni (II) .	2.26 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	4 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3 Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	7 Info
PLAT984_ALERT_1_G	The Ni-f'= 0.3393 Deviates from the B&C-Value	0.3420 Check
PLAT984_ALERT_1_G	The S-f'= 0.1246 Deviates from the B&C-Value	0.1218 Check
PLAT985_ALERT_1_G	The Ni-f''= 1.1124 Deviates from the B&C-Value	1.0875 Check
PLAT985_ALERT_1_G	The S-f''= 0.1234 Deviates from the B&C-Value	0.1207 Check

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
16 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT051_shelx
;
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      4.62 %
RESPONSE: ...
;
_vrf_PLAT911_shelx
;
```

PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
RESPONSE: ...
;
end Validation Reply Form

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 28/11/2022; check.def file version of 28/11/2022

