

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 070119_nisech3fe_star_o2_portion2_test

Bond precision: C-C = 0.0063 A Wavelength=1.54184

Cell: a=10.9842 (6) b=11.3750 (3) c=11.6936 (6)
 alpha=74.651 (3) beta=63.420 (5) gamma=87.908 (3)
Temperature: 110 K

| | Calculated | Reported |
|------------------------|-----------------------------------|-----------------------------------|
| Volume | 1254.34 (12) | 1254.34 (11) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C20 H35 Fe N2 Ni O2 S Se, B F4 | C20 H35 Fe N2 Ni O2 S Se, B F4 |
| Sum formula | C20 H35 B F4 Fe N2 Ni O2 S Se | C20 H35 B F4 Fe N2 Ni O2 S Se |
| Mr | 647.87 | 647.89 |
| Dx, g cm ⁻³ | 1.715 | 1.715 |
| Z | 2 | 2 |
| Mu (mm ⁻¹) | 8.457 | 8.457 |
| F000 | 660.0 | 660.0 |
| F000' | 652.42 | |
| h, k, lmax | 13, 14, 14 | 13, 14, 14 |
| Nref | 5396 | 5246 |
| Tmin, Tmax | 0.919, 0.919 | 0.332, 1.000 |
| Tmin' | 0.919 | |

Correction method= # Reported T Limits: Tmin=0.332 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.972

Theta (max)= 78.335

R(reflections)= 0.0580 (5068)

wR2(reflections)=
0.1681 (5246)

S = 1.044

Npar= 305

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

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.07 Report
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00629 Ang.



Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Se1 --Ni1 . 6.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 --O2 . 5.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 --N2 . 5.6 s.u.
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C17 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 8 Note
-8 3 5, -1 3 5, -7 3 1, 8 2 0, -4 2 4, -4 6 7,
-8 2 4, -8 4 6,

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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_PLAT094_070119_nisech3fe_star_o2_portion2_test
;
PROBLEM: Ratio of Maximum / Minimum Residual Density .... 2.07 Report
RESPONSE: ...
;
_vrf_PLAT341_070119_nisech3fe_star_o2_portion2_test
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00629 Ang.
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.

