

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Feqsal_Nimnt_100K

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: Feqsal_Nimnt_100K

Bond precision: C-C = 0.0044 A Wavelength=0.71070

Cell: a=11.5777(7) b=13.6154(4) c=13.9687(11)
 alpha=66.134(8) beta=84.758(12) gamma=65.272(9)
Temperature: 100 K

	Calculated	Reported
Volume	1821.0(3)	1821.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H22 Fe N4 O2, C8 N4 Ni S4	C32 H22 Fe N4 O2, C8 N4 Ni S4
Sum formula	C40 H22 Fe N8 Ni O2 S4	C40 H22 Fe N8 Ni O2 S4
Mr	889.44	889.45
Dx, g cm-3	1.622	1.622
Z	2	2
Mu (mm-1)	1.195	1.195
F000	904.0	904.0
F000'	906.59	
h, k, lmax	15, 17, 18	15, 17, 18
Nref	8364	7972
Tmin, Tmax	0.787, 0.942	0.740, 0.942
Tmin'	0.787	

Correction method= # Reported T Limits: Tmin=0.740 Tmax=0.942
AbsCorr = MULTI-SCAN

Data completeness= 0.953 Theta(max)= 27.497

R(reflections)= 0.0481(6636) wR2(reflections)= 0.1309(7972)

S = 1.115 Npar= 505

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min)

27 Note

Author Response: The reflections below theta(min) were omitted due to the shadow of a direct beam stopper.

Alert level C

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.976 Note

PLAT230_ALERT_2_C Hirshfeld Test Diff for N3 -- C23 .. 6.0 s.u.

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 130 Report

PLAT973_ALERT_2_C Check Calcd Positive Residual Density on Nil 1.14 eA-3

Alert level G

PLAT882_ALERT_1_G Missing datum for _diffn_reflns_av_unetI/netI . Please Check

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 237 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

