checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Feqsal_Nimnt_293K

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_293K

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Bond precision:    C-C = 0.0053 A              Wavelength=0.71070

Cell:          a=11.7638(6)         b=13.5893(5)        c=14.100(1)
               alpha=65.962(11)   beta=85.184(14)   gamma=65.815(9)
Temperature:   293 K

                   Calculated                 Reported
Volume             1868.6(3)                  1868.5(3)
Space group        P -1                       P -1
Hall group         -P 1                       -P 1
Moiety formula     C32 H22 Fe N4 O2, C8 N4 Ni C32 H22 Fe N4 O2, C8 N4 Ni
                   S4                         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          1.581                      1.581
Z                  2                          2
Mu (mm-1)          1.165                      1.165
F000               904.0                      904.0
F000'              906.59
h,k,lmax           15,17,18                   15,17,18
Nref               8648                       8382
Tmin,Tmax          0.792,0.943                0.819,0.943
Tmin'              0.792

Correction method= # Reported T Limits: Tmin=0.819 Tmax=0.943
AbsCorr = MULTI-SCAN

Data completeness= 0.969          Theta(max)= 27.567

R(reflections)= 0.0468( 6421)     wR2(reflections)= 0.1427( 8382)

S = 1.062                    Npar= 505
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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)   11 Note

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

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....   2 Check

        Author Response: The two outliner reflections existed near theta(max) and weak. Therefore, these outliners are considered to give little influence on this crystal structural analysis.

🟡 **Alert level C**
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C20 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600   42 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....   4 Note

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⚪ **Alert level G**
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)   293 Check
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI .   Please Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   213 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
   2 **ALERT level B** = A potentially serious problem, consider carefully
   3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   5 **ALERT level G** = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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

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 27/03/2017; check.def file version of 24/03/2017