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

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Bond precision:   C-C = 0.0055 A             Wavelength=0.71073

Cell:           a=8.7014(8)         b=9.9706(9)        c=11.1502(10)
                alpha=65.851(8)   beta=81.231(8)   gamma=68.810(9)
Temperature:    150 K

                   Calculated                 Reported
Volume          823.02(15)                 823.02(15)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
                C20 H32 N20 Ni2 O2 S2,
Moiety formula                             ?
                2(H2 O)
Sum formula     C20 H36 N20 Ni2 O4 S2      C20 H36 N20 Ni2 O4 S2
Mr              802.19                     802.23
Dx,g cm-3       1.618                      1.619
Z               1                          1
Mu (mm-1)       1.334                      1.334
F000            416.0                      416.0
F000'           417.01
h,k,lmax        12,14,15                   11,13,15
Nref            4955                       4267
Tmin,Tmax       0.875,0.935                0.897,1.000
Tmin'           0.875


Correction method= # Reported T Limits: Tmin=0.897 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.861          Theta(max)= 30.334

R(reflections)= 0.0582( 3433)     wR2(reflections)= 0.1577( 4267)

S = 1.066                    Npar= 230
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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
PLAT420_ALERT_2_B D-H Without Acceptor   O1W   --H1W   .   Please Check

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🟡 Alert level C
PLAT230_ALERT_2_C Hirshfeld Test Diff for   N5   --N6   .   6.2 s.u.
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on   Ni1   1.35 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.72A   From O1W   0.65 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.75A   From N10   0.45 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.83A   From O1W   -0.60 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.43A   From O1W   -0.50 eA-3

⚪ Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   4 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H1W'   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1W   Constrained at   0.5 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X   H1W'   ..H9B   .   1.87 Ang.
                                2-x,1-y,-z =   2_765 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   1 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1   (II)   .   2.07 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   3 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   634 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   1.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   1 Info

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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
   6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  13 **ALERT level G** = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 16/07/2020; check.def file version of 12/07/2020