checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB2

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: MAB2

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Bond precision:    O- B = 0.0056 A            Wavelength=0.68890

Cell:          a=8.5763(5)        b=9.2902(6)        c=9.3493(6)
               alpha=78.098(5)    beta=89.108(5)     gamma=89.110(5)
Temperature:   100 K

                  Calculated                    Reported
Volume            728.75(8)                     728.75(8)
Space group       P -1                          P -1
Hall group        -P 1                          -P 1
Moiety formula    C8 H26 N6 Ni, 2(B5 H4 O10)    C8 H26 N6 Ni, 2(B5 H4 O10)
Sum formula       C8 H34 B10 N6 Ni O20          C8 H34 B10 N6 Ni O20
Mr                701.20                        701.22
Dx,g cm-3         1.598                         1.598
Z                 1                             1
Mu (mm-1)         0.693                         0.699
F000              362.0                         362.0
F000'             362.54
h,k,lmax          11,12,12                      11,12,12
Nref              3340                          3152
Tmin,Tmax                                       0.275,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=0.275 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.944           Theta(max)= 26.572

R(reflections)= 0.0767( 2526)       wR2(reflections)= 0.2109( 3152)

S = 1.077                   Npar= 273
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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

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PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor ....        5.1 Note
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Alert level C

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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.961 Why?
PLAT213_ALERT_2_C Atom O2              has ADP max/min Ratio .....          3.6 prolat
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H12      ..O5      .         2.63 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......       2.770 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         100 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          5 Note
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.96A    From O9            0.41 eA-3
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Alert level G

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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 ..............         14 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.12 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka   0.68890 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.005 Degree
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        93% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         85 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.0 Low
PLAT984_ALERT_1_G The  B-f'=    0.0004 Deviates from the B&C-Value   0.0014 Check
PLAT984_ALERT_1_G The  N-f'=    0.0037 Deviates from the B&C-Value   0.0056 Check
PLAT984_ALERT_1_G The Ni-f'=    0.2866 Deviates from the B&C-Value   0.3428 Check
PLAT984_ALERT_1_G The  O-f'=    0.0071 Deviates from the B&C-Value   0.0101 Check
PLAT985_ALERT_1_G The Ni-f"=    1.0558 Deviates from the B&C-Value   1.0569 Check
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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
   8 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
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   2 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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021