checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB4

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: MAB4

Bond precision: N- C = 0.0045 A Wavelength=0.71075

Cell: a=8.3891(2) b=11.6666(3) c=14.3092(4)
alpha=90 beta=90.035(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1400.47(6)	1400.47(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C8 H24 N4 Ni O2, 2(B5 H4 O10)	2(B5 H4 O10), C8 H24 N4 Ni O2
Sum formula	C8 H32 B10 N4 Ni O22	C8 H32 B10 N4 Ni O22
Mr	703.17	703.18
Dx,g cm-3	1.668	1.668
Z	2	2
Mu (mm-1)	0.791	0.791
F000	724.0	724.0
F000’	725.14	
h,k,lmax	10,15,18	10,15,18
Nref	3224	6239
Tmin,Tmax	0.954,0.969	0.799,1.000
Tmin’	0.764	

Correction method= # Reported T Limits: Tmin=0.799 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.935 Theta(max)= 27.496

R(reflections)= 0.0499(5795) wR2(reflections)= 0.1124(6239)

S = 1.126 Npar= 223

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

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CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           Lilac
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.06 Report
PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem         A         84 %Fit
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.5 Note
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N11      --H11C     .     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.518 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      10.85 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         13 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          9 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         3 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ni1      --O11      .       6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ni1      --N11      .       5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ni1      --N12      .       5.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ni1      --O11B     .       8.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ni1      --N11B     .       8.5 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       53% Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        13 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        10 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1 0-2)         Est.d BASF      0.69 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       1.9 Low
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   3 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
   5 ALERT type 3 Indicator that the structure quality may be low
   7 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

Datablock MAB4 - ellipsoid plot