checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB7

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: MAB7

Bond precision: O- B = 0.0065 A   Wavelength=0.71075

Cell: a=8.5116(7)   b=9.7946(5)   c=9.8073(8)
               alpha=89.873(5)   beta=82.901(7)   gamma=74.372(6)
Temperature: 100 K

	Calculated	Reported
Volume	780.94(10)	780.94(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C2 H18 B6 N2 Ni O15, H2 O	C2 H18 B6 N2 Ni O15, H2 O
Sum formula	C2 H20 B6 N2 Ni O16	C2 H20 B6 N2 Ni O16
Mr	451.75	451.77
Dx,g cm-3	1.921	1.921
Z	2	2
Mu (mm-1)	1.333	1.333
F000	464.0	464.0
F000'	464.99	
h,k,lmax	11,12,12	11,12,12
Nref	3606	5883
Tmin,Tmax	0.953,0.980	0.886,1.000
Tmin'	0.841	

Correction method= # Reported T Limits: Tmin=0.886 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.631   Theta(max)= 27.573

R(reflections)= 0.0682(5320)   wR2(reflections)= 0.1902(5883)

S = 1.022   Npar= 291

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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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.15 Report
PLAT213_ALERT_2_C Atom O13              has ADP max/min Ratio .....       3.7 prolat
PLAT213_ALERT_2_C Atom B2               has ADP max/min Ratio .....       3.5 oblate
PLAT213_ALERT_2_C Atom B4               has ADP max/min Ratio .....       3.9 oblate
PLAT213_ALERT_2_C Atom C1               has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom C2               has ADP max/min Ratio .....       3.6 oblate
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.6 Note
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ........        O1 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H21B     ..O5         .    2.65 Ang.
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .        27 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .     25.84 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         7 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        21 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.13 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
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H13         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A        Constrained at      0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )         8% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2 )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3 )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2 )       1.59 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3 )       1.41 Check
PLAT417_ALERT_2_G Short Inter D-H..H-D       H13A     ..H22B     .      2.13 Ang.
                                    1-x,1-y,1-z  =     2_666 Check
PLAT417_ALERT_2_G Short Inter D-H..H-D       H21A     ..H31D     .      2.10 Ang.
                                    x,y,z  =          1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       12 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      277 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        44 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law        [ 0 1 0] Est.d BASF      0.42 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       1.7 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
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  24 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  14 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