checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_niso_pl

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: mo_niso_pl

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Bond precision:   C-C = 0.0054 A          Wavelength=0.71073

Cell:             a=11.9437(19)     b=6.7402(14)     c=10.6610(18)
                  alpha=90          beta=90          gamma=90
Temperature:      100 K

                 Calculated                  Reported
Volume           858.2(3)                    858.2(3)
Space group      P n n 2                     P n n 2
Hall group       P 2 -2n                     P 2 -2n
Moiety formula   C12 H10 N4 Ni O4, C3 H7 N O C12 H10 N4 Ni O4, C3 H7 N O
Sum formula      C15 H17 N5 Ni O5            C15 H17 N5 Ni O5
Mr               406.03                      406.04
Dx,g cm-3        1.571                       1.571
Z                2                           2
Mu (mm-1)        1.168                       1.168
F000             420.0                       420.0
F000'            420.84
h,k,lmax         19,10,17                    17,10,15
Nref             3663[ 1911]                 2814
Tmin,Tmax        0.845,0.890                 0.811,1.000
Tmin'            0.810

Correction method= # Reported T Limits: Tmin=0.811 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.47/0.77        Theta(max)= 34.537

R(reflections)= 0.0410( 2570)                wR2(reflections)=
                                             0.0941( 2814)
S = 1.075                Npar= 136
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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 C

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PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4 Note
PLAT712_ALERT_1_C ANGLE   Unknown or Inconsistent Label .........      C51B Check
                  C51B        C5B         H52B
PLAT712_ALERT_1_C ANGLE   Unknown or Inconsistent Label .........      C51B Check
                  C51B        C5B         H53B
PLAT712_ALERT_1_C ANGLE   Unknown or Inconsistent Label .........      C52B Check
                  C52B        C5B         H53B
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       14 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....        8 Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..        1 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        5 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        2 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......    Please Check
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records        1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records        1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0200 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53B       Constrained at       0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        12 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .      2.02 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters        3 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers        1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       52 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).        1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      219 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage       67 %
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ        2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.       2 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ        2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.       2 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       2 Info
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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
  7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 37 ALERT level G = General information/check it is not something unexpected

  7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  4 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
 21 ALERT type 4 Improvement, methodology, query or suggestion
  5 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 06/07/2023; check.def file version of 30/06/2023

Datablock mo_niso_pl - ellipsoid plot