checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_4067_auto

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: exp_4067_auto**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0164 A</th>
<th>Wavelength=0.71073</th>
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<td>Cell:</td>
<td>a=29.0676(9)</td>
<td>b=10.4430(3)</td>
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<td>beta=90</td>
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<td>Temperature:</td>
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<tr>
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<td>-P 2n 2ab</td>
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<td>C46 H44 N36 Ni3 O2 W2</td>
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<td>Tmin’</td>
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</table>

Correction method= # Reported T Limits: Tmin=0.586 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.904 Theta(max)= 28.722

R(reflections)= 0.0496( 6309) wR2(reflections)= 0.1114( 7376)
S = 1.209 Npar= 458
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 A**
PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.91Ang From C3 4.79 eA-3

Author Response: We tried to solve this PROBLEM by repeating the single-crystal XRD measurement with better crystal quality; however, even in the best single crystal structure data, this problem still exists. We think that this problem of residual electron density is due to the disorder of the coordination framework related to the C3-N3 bridging cyanide ligand. Such framework disorder can be additionally supported by the evident disorder of the pyrazole ligand.

**Alert level B**
PLAT213_ALERT_2_B Atom C9 has ADP max/min Ratio ..... 4.3 prolat
PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 8.8 Ratio
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.82Ang From C15A 3.11 eA-3

Author Response: We tried to solve this PROBLEM by repeating the single-crystal XRD measurement with better crystal quality; however, even in the best single crystal structure data, this problem still exists. We think that this problem of residual electron density is due to the disorder of the coordination framework related to the C3-N3 bridging cyanide ligand. Such framework disorder can be additionally supported by the evident disorder of the pyrazole ligand.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 2.73Ang From C23 2.96 eA-3

Author Response: We tried to solve this PROBLEM by repeating the single-crystal XRD measurement with better crystal quality; however, even in the best single crystal structure data, this problem still exists. We think that this problem of residual electron density is due to the disorder of the coordination framework related to the C3-N3 bridging cyanide ligand. Such framework disorder can be additionally supported by the evident disorder of the pyrazole ligand.

PLAT975_ALERT_2_B Check Calcd Resid. Dens. 1.03Ang From N3 1.54 eA-3

**Alert level C**
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.40 Report
PLAT213_ALERT_2_C Atom N10 has ADP max/min Ratio ..... 3.8 prolat
Author Response: We tried to solve this PROBLEM by repeating the single-crystal XRD measurement with better crystal quality; however, even in the best single crystal structure data, this problem still exists. We think that this problem of residual electron density is due to the disorder of the coordination framework related to the C3-N3 bridging cyanide ligand. Such framework disorder can be additionally supported by the evident disorder of the pyrazole ligand.

PLAT977_ALERT_2_C Check Negative Difference Density on H11 . -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H18 . -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H19 . -0.33 eA-3
Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite.............. 11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrainted non-H Atoms ............. 9 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension ......... 2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .......................... 6 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large .... 101.50 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records ....... 3 Report
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 ....... 13 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records ....... 5 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used ........ 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used ........ 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used ........ 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used ........ 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used ........ 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used ........ 0.0400 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) ........... 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) ............... 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N13 Constrained at ................. 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N14 Constrained at ................. 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15 Constrained at ................. 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16 Constrained at ................. 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17 Constrained at ................. 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N13A Constrained at .............. 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N14A Constrained at ............... 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15A Constrained at ............... 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16A Constrained at ............... 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17A Constrained at ............... 0.4 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H16A Constrained at ............... 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17 Constrained at ................. 0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A Constrained at ............... 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A Constrained at ............... 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B Constrained at ............... 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A Constrained at ............... 0.4 Check
PLAT301_ALERT_3_G Main Residue Disorder .........................(Resd 1 ) .... 11% Note
PLAT411_ALERT_2_G Short Inter H...H Contact H16A ..H22 . 2.07 Ang. x,-y,-1/2+z = 7_555 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Nil (II) ......................... 2.11 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters ......... 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .......................... 72 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600 .... 764 Note
PLAT933_ALERT_2_G Number of HKL-Omit Records in Embedded .res File ........ 4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ............... 4.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. ........ 0 Info

1 ALERT level A = Most likely a serious problem - resolve or explain
5 ALERT level B = A potentially serious problem, consider carefully
22 ALERT level C = Check. Ensure it is not caused by an omission or oversight
45 ALERT level G = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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.

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**PLATON version of 10/05/2023; check.def file version of 10/05/2023**