checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MADXT5

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: MADXT5

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Bond precision:  C-C = 0.0099 A          Wavelength=0.71073

Cell:            a=13.588(3)     b=19.062(4)         c=16.764(3)
                 alpha=90        beta=100.11(3)      gamma=90
Temperature:     170 K
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	Calculated	Reported
Volume	4274.7(16)	4274.8(15)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C72 H74 K2 N2 Ni4 O14 S12	C72 H74 K2 N2 Ni4 O14 S12
Sum formula	C72 H74 K2 N2 Ni4 O14 S12	C72 H74 K2 N2 Ni4 O14 S12
Mr	1889.01	1889.09
Dx,g cm-3	1.468	1.468
Z	2	2
Mu (mm-1)	1.316	1.316
F000	1948.0	1948.0
F000’	1955.08	
h,k,lmax	16,23,20	16,23,20
Nref	8131	8052
Tmin,Tmax	0.814,0.908	0.826,0.979
Tmin’	0.814	

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Correction method= # Reported T Limits: Tmin=0.826 Tmax=0.979
AbsCorr = NUMERICAL

Data completeness= 0.990          Theta(max)= 25.684

R(reflections)= 0.0568( 4887)     wR2(reflections)= 0.1668( 8052)

S = 0.921                 Npar= 538
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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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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.34 Report
PLAT220_ALERT_2_C NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range        4.7 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1  O   Ueq(max) / Ueq(min) Range        3.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.1 Ratio
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of         N1 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of         K1 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00986 Ang.
PLAT977_ALERT_2_C Check Negative Difference Density on H36E            -0.40 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         18 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.11 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          5 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          4 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        11% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         3 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #       162 Check
              O5   -C22  -K1      1.555   1.555   1.555             38.80 Deg.
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (III)     .       2.94 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni2       (III)     .       2.72 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       245 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        80 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         3 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
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   0 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
   4 ALERT type 3 Indicator that the structure quality may be low
   6 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 22/12/2019; check.def file version of 13/12/2019

Datablock MADXT5 - ellipsoid plot