checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: d505

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Bond precision:   C-C = 0.0085 A            Wavelength=0.71073

Cell:          a=11.1760(11)     b=11.952(1)          c=12.0854(14)
               alpha=68.606(9)   beta=66.295(10)   gamma=77.351(8)
Temperature:   294 K

                 Calculated                Reported
Volume           1371.3(3)                 1371.3(3)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
                 C42 H48 N4 Ni3 O16, 2(H2  C42 H48 N4 Ni3 O16, 2(H2
Moiety formula   O) [+ solvent]            O)
                 C42 H52 N4 Ni3 O18 [+
Sum formula      solvent]                  C40 H46 N4 Ni3 O20
Mr               1076.95                   1078.94
Dx,g cm-3        1.304                     1.307
Z                1                         0
Mu (mm-1)        1.086                     1.089
F000             560.0                     558.0
F000'            561.28
h,k,lmax         13,14,14                  15,15,16
Nref             5399                      5386
Tmin,Tmax        0.710,0.762               0.747,1.000
Tmin'            0.691

Correction method= # Reported T Limits: Tmin=0.747 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.020

R(reflections)= 0.0618( 3799)     wR2(reflections)= 0.1934( 5386)

S = 1.104                    Npar= 313
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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 B
PLAT420_ALERT_2_B D-H Without Acceptor   O9   --H9A   Please Check

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🟡 Alert level C
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.40 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C   Ueq(max)/Ueq(min) Range   3.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   O2   --N1   .   6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for   O3   --C9   .   5.4 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C20   --C21   0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C20 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   O6 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.00853 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C20   - C21   .   1.42 Ang.
PLAT362_ALERT_2_C Short C(sp3)-C(sp2) Bond C8   - C9   .   1.41 Ang.

⚪ Alert level G
FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
          _chemical_formula_sum and _chemical_formula_moiety. This is
          usually due to the moiety formula being in the wrong format.
          Atom count from _chemical_formula_sum: C40 H46 N4 Ni3 O20
          Atom count from _chemical_formula_moiety:C42 H52 N4 Ni3 O18
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
          _chemical_formula_sum and the formula from the _atom_site* data.
          Atom count from _chemical_formula_sum:C40 H46 N4 Ni3 O20
          Atom count from the _atom_site data: C42 H52 N4 Ni3 O18
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
          symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z   1
          From the CIF: _chemical_formula_sum C40 H46 N4 Ni3 O20
          TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	40.00	42.00	-2.00
H	46.00	52.00	-6.00
N	4.00	4.00	0.00
Ni	3.00	3.00	0.00
O	20.00	18.00	2.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   2 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.10 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   2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records   1 Report
PLAT395_ALERT_2_G Deviating X-O-Y   Angle From 120 for O2   110.3 Degree
PLAT395_ALERT_2_G Deviating X-O-Y   Angle From 120 for O3   110.4 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure   261 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   5 Note
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

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 0 ALERT level A = Most likely a serious problem - resolve or explain
 1 ALERT level B = A potentially serious problem, consider carefully
11 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

 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 5 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

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