checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

```
Bond precision:   C-C = 0.0043 A           Wavelength=1.54178

Cell:           a=8.9375(7)        b=12.8596(10)     c=21.1687(17)
                alpha=85.416(3)    beta=82.686(2)    gamma=89.928(3)
Temperature:    100 K

                Calculated                  Reported
Volume          2405.4(3)                   2405.4(3)
Space group     P -1                        P -1
Hall group      -P 1                        -P 1
                2(C14 H6 N2 Ni O8), C4 H20
Moiety formula  N4 Ni O2, C2 H16 N2 Ni O4,  ?
                4(H2 O)
Sum formula     C34 H56 N10 Ni4 O26         C34 H56 N10 Ni4 O26
Mr              1255.65                     1255.72
Dx,g cm-3       1.734                       1.734
Z               2                           2
Mu (mm-1)       2.641                       2.641
F000            1300.0                      1300.0
F000'           1280.11
h,k,lmax        10,15,25                    10,15,25
Nref            8844                        8519
Tmin,Tmax       0.463,0.673                 0.263,0.753
Tmin'           0.420

Correction method= # Reported T Limits: Tmin=0.263 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.963           Theta(max)= 68.364
```

R(reflections)= 0.0559(8443) wR2(reflections)= 0.1577(8519)

S = 1.085 Npar= 692

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 Bond Without Acceptor O3 --H3A . Please Check

Author Response: Due to disordered solvent molecules.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.966 Why?
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.3 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.6 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 3) 2.4 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 4) 2.8 Note
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C12 - C13 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C19 - C20 . 1.53 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor N2 --H2BB . Please Check

Author Response: Due to disordered solvent molecules.

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C14 H6 N2 Ni O8
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.884 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 299 Report

0	2	0,	1	2	0,	1	3	0,	0	4	0,
1	4	0,	2	4	0,	1	5	0,	1	6	0,
1	7	0,	-2	15	0,	0	-15	1,	1	-15	1,
2	-15	1,	-1	-9	1,	-1	-8	1,	-2	-7	1,
-1	-7	1,	1	-7	1,	-2	-6	1,	-1	-6	1,
0	-6	1,	-2	-5	1,	-1	-5	1,	0	-5	1,
1	-5	1,	-2	-4	1,	-1	-4	1,	0	-4	1,
-1	-3	1,	0	-3	1,	1	-3	1,	0	-3	1,
1	-2	1,	2	-2	1,	0	-2	1,	-1	-1	1,
0	-1	1,	1	-1	1,	2	-1	1,	-1	1	1,
0	1	1,	1	1	1,	-1	3	1,	0	3	1,
1	3	1,	2	3	1,	-1	7	1,	1	7	1,
-1	15	1,	0	-15	2,	1	-15	2,	2	-15	2,
-2	-11	2,	-1	-11	2,	-2	-9	2,	-2	-8	2,
-1	-8	2,	0	-8	2,	1	-8	2,	-2	-7	2,
-1	-7	2,	0	-7	2,	1	-7	2,	-2	-6	2,
-1	-6	2,	0	-6	2,	1	-6	2,	-2	-5	2,
-1	-5	2,	0	-5	2,	1	-5	2,	-2	-4	2,
-1	-4	2,	0	-4	2,	1	-4	2,	-2	-3	2,
-1	-3	2,	0	-3	2,	1	-3	2,	-2	-2	2,
-1	-2	2,	0	-2	2,	1	-2	2,	2	-2	2,
0	-1	2,	0	0	2,	0	1	2,	-5	2	2,
1	5	2,	-1	-15	3,	0	-15	3,	1	-15	3,
-2	-14	3,	-2	-13	3,	-1	-13	3,	-2	-12	3,
-1	-12	3,	-2	-11	3,	-1	-11	3,	-2	-10	3,
-3	-9	3,	-2	-9	3,	-2	-8	3,	-1	-8	3,
0	-8	3,	-3	-7	3,	-2	-7	3,	-1	-7	3,
0	-7	3,									

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 5 Note

0	-2	2,	2	-2	2,	-2	-3	3,	-4	-4	4,
2	-2	4,									

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............         32 Report
              H00I  H00J  H4BB  H4AA  H3BB  H3AA  H00K  H00L  H9A   H9B   H10A
              H10B  H1A   H1B   H2A   H2B   H3A   H3B   H4A   H4B   H2AA  H2BB
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         12 Note
              H00I    H00J    H00K    H00L    H4BB    H4AA    H3BB    H3AA
              H2AA    H2BB    H1BB    H1AA
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C14 H6 N2 Ni O8
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
              C4 H20 N4 Ni O2
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
              H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
              H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
              H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          9 Note
              H2 O
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .       2.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni2       (II)      .       1.91 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni3       (II)      .       2.08 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni4       (II)      .       2.08 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni5       (II)      .       1.93 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                0  1  0,   0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         26 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
                1 -4 10,   3 -1  5,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.0 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.478 Note
              Predicted wR2: Based on SigI**2  2.88 or SHELX Weight 14.53
```

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

   1 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
   6 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   7 ALERT type 5 Informative message, check
```

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 15/07/2024; check.def file version of 15/07/2024

Datablock shelx - ellipsoid plot