checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C16H18N3SNiCN4x2H2O

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: C16H18N3SNiCN4x2H2O

```
Bond precision:     C-C = 0.0321 A              Wavelength=0.71073

Cell:               a=16.58(3)       b=16.19(3)           c=13.68(2)
                    alpha=90         beta=96.94(3)        gamma=90
Temperature:        298 K

                    Calculated              Reported
Volume              3645(11)                3646(11)
Space group         C c                     C 1 c 1
Hall group          C -2yc                  C -2yc
Moiety formula      2(C16 H18 N3 S), C4 N4 Ni,  C4 N4 Ni, 2(C16 H18 N3 S),
                    2(H2 O)                 2(H2 O)
Sum formula         C36 H40 N10 Ni O2 S2     C36 H40 N10 Ni O2 S2
Mr                  767.59                  767.61
Dx,g cm-3           1.399                   1.398
Z                   4                       4
Mu (mm-1)           0.695                   0.695
F000                1608.0                  1608.0
F000'               1610.77
h,k,lmax            16,16,13                16,16,13
Nref                3828[ 1918]             3766
Tmin,Tmax           0.959,0.966             0.505,0.745
Tmin'               0.812

Correction method= # Reported T Limits: Tmin=0.505 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.96/0.98        Theta(max)= 20.813

R(reflections)= 0.0740( 1880)       wR2(reflections)= 0.1661( 3766)

S = 0.960                    Npar= 476
```

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**

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
          Calculated sin(theta_max)/wavelength =   0.4999

> **Author Response: The small size and weak diffractive power of the crystal resulted in the low sine(theta_max)/wavelength value.**

🟠 **Alert level B**

PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) ....   4.03 Note

> **Author Response: The small size and weak diffractive power of the crystal resulted in the low amount of parameters.**

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.03208 Ang.

> **Author Response: The small size and weak diffractive power of the crystal resulted in the low resolution.**

🟡 **Alert level C**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
          Rint given   0.164

> **Author Response: Due to the limited resolution, the decision of using as much reflections as possible was made, thus integrating more noise and resulting in a worse Rint.**

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ....   0.164 Report

> **Author Response: Due to the limited resolution, the decision of using as much reflections as possible was made, thus integrating more noise and resulting in a worse Rint.**

PLAT148_ALERT_3_C s.u. on the   a   - Axis is (Too) Large ....   0.030 Ang.

> **Author Response: Due to the limited resolution, the decision of using as much reflections as possible was made, thus integrating more noise and resulting in a worse s.u.**

PLAT148_ALERT_3_C s.u. on the   b   - Axis is (Too) Large ....   0.0300 Ang.

Author Response: Due to the limited resolution, the decision of using as much reflections as possible was made, thus integrating more noise and resulting in a worse s.u.

```
PLAT148_ALERT_3_C s.u. on the     c    - Axis is (Too) Large ....     0.020 Ang.
```

Author Response: Due to the limited resolution, the decision of using as much reflections as possible was made, thus integrating more noise and resulting in a worse s.u.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N6 Check
```

Author Response: Due to the limited resolution of the data, thermal parameters may show poor quality.

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PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C4 Check
```

Author Response: Due to the limited resolution of the data, thermal parameters may show poor quality.

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O2      0.185 Check
```

Author Response: Due to the limited resolution of the data, thermal parameters may show poor quality.

```
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.764 Check
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Author Response: Due to the limited resolution of the data, the value of K results higher than usually advised.

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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.500          2 Report
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Author Response: The small size and weak diffractive power of the crystal resulted in the low amount of reflections that were collected.

⬤ Alert level G

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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 ...        28 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         4 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         2 Report
PLAT721_ALERT_1_G Bond    Calc    0.97000, Rep    0.96000 Dev...      0.01 Ang.
                  C35     -H35B          1.555   1.555 ........    #  70 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       239 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
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 1 ALERT level A = Most likely a serious problem - resolve or explain
 2 ALERT level B = A potentially serious problem, consider carefully
10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
11 ALERT level G = General information/check it is not something unexpected

 2 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
11 ALERT type 3 Indicator that the structure quality may be low
 6 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check
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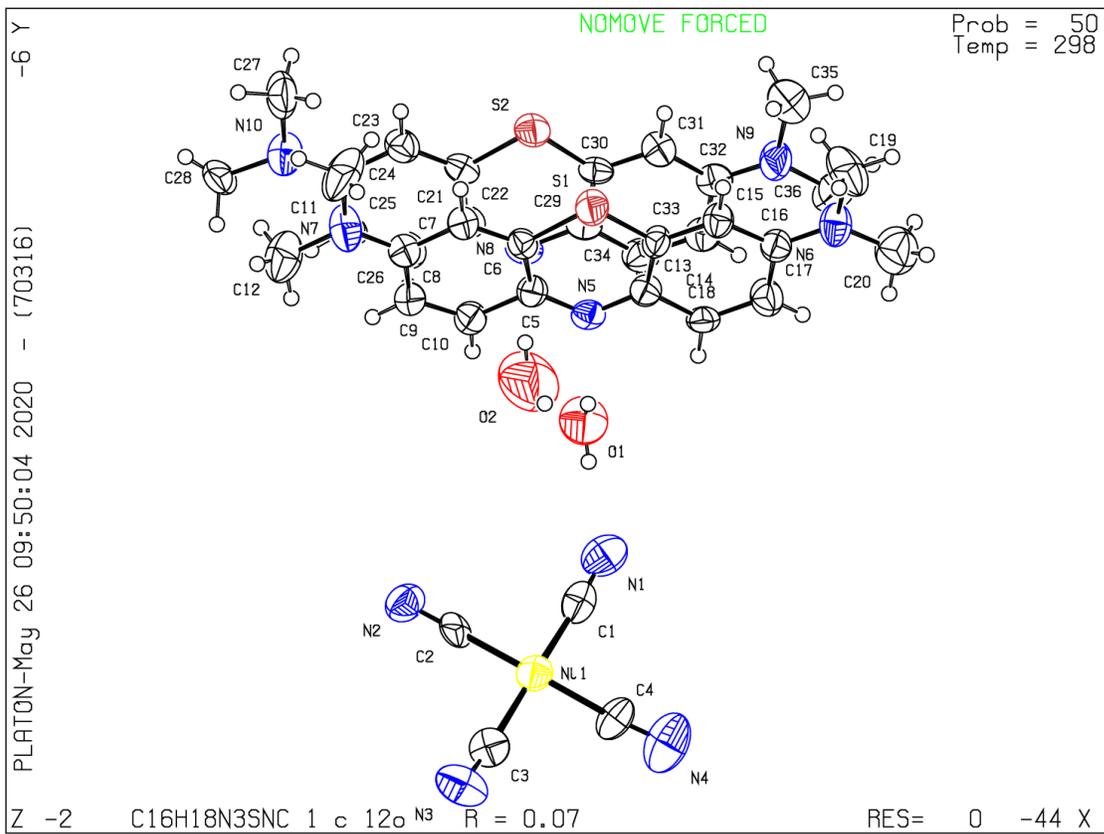
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 22/04/2020; check.def file version of 09/03/2020

NOMOVE FORCED

Prob = 50
Temp = 298

-6 Y

PLATON-May 26 09:50:04 2020 — (70316)

Z -2   C16H18N3SNC 1 c 12o N3   R = 0.07   RES=   O   -44 X