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: ad18

```
Bond precision:   C-C = 0.0039 A             Wavelength=0.71073

Cell:          a=10.6904(15)    b=13.0941(13)      c=10.0521(13)
               alpha=94.104(9)  beta=101.815(11)  gamma=93.942(10)
Temperature:   293 K

                 Calculated                 Reported
Volume           1368.7(3)                  1368.7(3)
Space group      P -1                       P -1
Hall group       -P 1                       ?
Moiety formula   C13 H18 N4 Ni O            ?
Sum formula      C13 H18 N4 Ni O            C13 H18 N4 Ni O
Mr               305.00                     305.02
Dx,g cm-3        1.480                      1.480
Z                4                          4
Mu (mm-1)        1.415                      1.415
F000             640.0                      640.0
F000'            641.50
h,k,lmax         13,16,12                   13,16,12
Nref             5956                       5957
Tmin,Tmax        0.557,0.868                0.814,1.000
Tmin'            0.488

Correction method= # Reported T Limits: Tmin=0.814 Tmax=1.000
AbsCorr = PSI-SCANS

Data completeness= 1.000          Theta(max)= 26.970

R(reflections)= 0.0316( 4690)      wR2(reflections)= 0.0933( 5957)

S = 1.095                  Npar= 343
```

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

```
WEIGH01_ALERT_1_C  Extra text has been found in the
            _refine_ls_weighting_scheme field. This should be in the
            _refine_ls_weighting_details field.
            Weighting scheme given as calc w=1/[\s^2^(Fo^2^)+(0.0394P)^2^+0.7765
            Weighting scheme identified as calc
PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced .........    Please Do !
```

Alert level G

```
ABSTY01_ALERT_1_G  Extra text has been found in the _exptl_absorpt_correction_type
            field, which should be only a single keyword. A literature
            citation should be included in the _exptl_absorpt_process_details
            field.
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni2     --N1B      .        5.2 s.u.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C3A Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C4A Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C3B Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C4B Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      28 Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found    Please Check
PLAT881_ALERT_1_G No Datum for _diffrn_reflns_av_R_equivalents ...    Please Do !
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2016 Note
```

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

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_WEIGH01_ad18
;
PROBLEM: Extra text has been found in the
RESPONSE: ...
;
_vrf_PLAT155_ad18
;
PROBLEM: The Triclinic Unitcell is NOT Reduced ..........    Please Do !
RESPONSE: ...
;
# end Validation Reply Form
```

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 13/08/2017; check.def file version of 12/12/2017