checkCIF/PLATON report

Structure factors have been supplied for datablock(s) IP190LT

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: IP190LT

```
Bond precision:  C-C = 0.0061 A          Wavelength=1.54178

Cell:            a=7.9443(5)     b=10.9970(7)     c=19.0243(13)
                 alpha=90        beta=90          gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	1662.03(19)	1662.03(19)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C16 H16 Br2 N2 Ni	?
Sum formula	C16 H16 Br2 N2 Ni	C16 H16 Br2 N2 Ni
Mr	454.80	454.84
Dx,g cm-3	1.818	1.818
Z	4	4
Mu (mm-1)	7.257	7.257
F000	896.0	896.0
F000’	879.88	
h,k,lmax	9,13,22	9,13,22
Nref	3024[1754]	2982
Tmin,Tmax	0.741,0.748	0.634,0.753
Tmin’	0.533	

```
Correction method= # Reported T Limits: Tmin=0.634 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.99      Theta(max)= 67.841

R(reflections)= 0.0239( 2836)     wR2(reflections)= 0.0616( 2982)

S = 1.057                 Npar= 192
```

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

```
PLAT927_ALERT_1_B Reported and Calculated  wR2 Differ by .........     0.0081 Check
PLAT987_ALERT_1_B The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as Multi-scan
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.576
          From the CIF: _refine_ls_abs_structure_Flack_su    0.016
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00607 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H1     ..  H7      ..       2.12 Ang.
PLAT907_ALERT_2_C Flack x > 0.5, Structure needs to be Inverted? .       0.58 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          7 Report
PLAT926_ALERT_1_C Reported and Calculated   R1 Differ by .........     0.0028 Check
PLAT928_ALERT_1_C Reported and Calculated    S value   Differ by .      0.138
```

Alert level G

```
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.576 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still          90 % Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          6 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Note
```

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 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 27/03/2017; check.def file version of 24/03/2017

Datablock IP190LT - ellipsoid plot