checkCIF/PLATON report

Structure factors have been supplied for datablock(s) NiAs4H10O16

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: NiAs4H10O16

```
Bond precision:  As- O = 0.0030 A        Wavelength=0.71073

Cell:          a=5.4297(7)        b=7.3308(9)      c=8.2795(10)
               alpha=100.356(5)   beta=98.088(5)   gamma=92.982(5)
Temperature:   100 K
```

	Calculated	Reported
Volume	319.95(7)	319.95(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	As4 H10 Ni O16	As4 H10 Ni O16
Sum formula	As4 H10 Ni O16	As4 H10 Ni O16
Mr	624.45	624.47
Dx,g cm-3	3.241	3.241
Z	1	1
Mu (mm-1)	11.869	11.869
F000	298.0	298.0
F000’	298.76	
h,k,lmax	9,12,13	9,12,13
Nref	3190	3000
Tmin,Tmax	0.430,0.622	0.257,0.439
Tmin’	0.340	

```
Correction method= # Reported T Limits: Tmin=0.257 Tmax=0.439
AbsCorr = MULTI-SCAN

Data completeness= 0.940          Theta(max)= 36.705

R(reflections)= 0.0387( 2566)     wR2(reflections)= 0.0880( 3000)

S = 1.082                 Npar= 114
```

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

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O3       ..O7       .       2.88 Ang.
                                          1-x,1-y,2-z  =      2_667 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         10 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.005 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          5 Report
PLAT432_ALERT_2_G Short Inter X...Y Contact  As2      ..O5             3.15 Ang.
                                          1-x,2-y,2-z  =      2_677 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .       1.88 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          5 Note
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 !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        191 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)         Est.d BASF       0.34 Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 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 07/08/2019; check.def file version of 30/07/2019

Datablock NiAs4H10O16 - ellipsoid plot