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:  As- O = 0.0040 A        Wavelength=0.71073

Cell:             a=9.173(3)     b=6.2025(12)        c=7.562(3)
                  alpha=90       beta=114.41(2)      gamma=90
Temperature:      298 K
```

	Calculated	Reported
Volume	391.8(2)	391.8(2)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	As2 H4 Ni2 O10, Sr	?
Sum formula	As2 H4 Ni2 O10 Sr	As2 H4 Ni2 O10 Sr
Mr	518.87	518.91
Dx,g cm-3	4.398	4.399
Z	2	2
Mu (mm-1)	19.963	19.965
F000	488.0	488.0
F000’	486.92	
h,k,lmax	12,8,10	12,8,10
Nref	607	606
Tmin,Tmax	0.625,0.819	0.623,0.815
Tmin’	0.544	

```
Correction method= # Reported T Limits: Tmin=0.623 Tmax=0.815
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 29.540

R(reflections)= 0.0284( 536)      wR2(reflections)= 0.0611( 606)

S = 1.201                 Npar= 48
```

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

PLAT417_ALERT_2_B Short Inter D-H..H-D H1 ..H1 . 2.01 Ang.
1-x,y,1-z = 2_656 Check
PLAT417_ALERT_2_B Short Inter D-H..H-D H1 ..H1 . 2.01 Ang.
1-x,2-y,1-z = 5_676 Check

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.294 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.71A From O1 1.03 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.46A From O2 0.53 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.62A From O4 0.47 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.09A From O3 0.43 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.76A From O1 -0.84 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.86A From O4 -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2 -0.77 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/m I2/m Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1 (II) . 1.99 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 3 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.8 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

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
12 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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 22/03/2021; check.def file version of 19/03/2021

Datablock shelx - ellipsoid plot