checkCIF/PLATON report

Structure factors have been supplied for datablock(s) NiS4

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: NiS4

```
Bond precision:   C-C = 0.0020 A           Wavelength=0.71073

Cell:              a=9.5425(4)      b=26.947(1)      c=27.7314(11)
                   alpha=90         beta=90          gamma=90
Temperature:       150 K
```

	Calculated	Reported
Volume	7130.9(5)	7130.9(5)
Space group	F d d d	F d d d
Hall group	-F 2uv 2vw	-F 2uv 2vw
Moiety formula	C16 H4 Ni O8 S4, 4(C2 H7 N) [+ solvent]	C16 H4 Ni O8 S4, 4(C2 H7 N)
Sum formula	C24 H32 N4 Ni O8 S4 [+ solvent]	C24 H32 N4 Ni O8 S4
Mr	691.47	691.48
Dx,g cm-3	1.288	1.288
Z	8	8
Mu (mm-1)	0.823	0.823
F000	2880.0	2880.0
F000'	2887.76	
h,k,lmax	13,38,39	13,33,34
Nref	2799	2241
Tmin,Tmax		0.631,1.000
Tmin'		

```
Correction method= # Reported T Limits: Tmin=0.631 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.801           Theta(max)= 30.793
```

R(reflections)= 0.0322(2011) wR2(reflections)= 0.1010(2241)

S = 1.087 Npar= 97

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

PLAT430_ALERT_2_A Short Inter D...A Contact O003 ..O003 . 2.46 Ang.
3/4-x,3/4-y,z = 2_555 Check

Author Response: The two O003 on benzenedicarboxyl moiety are twisted to each other that O003 and O003(3/4-x, 3/4-y,z) on adjacent molecule come closer and the distance between these two O003 was shortened to 2.46 angstrom to trigger this alert.

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
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N007 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.1 Note
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.88Ang From N007 . 0.60 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From N007 . 0.57 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From N007 . -0.62 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H007 . -0.62 eA-3

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
H007
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 18.97 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni01 --S1 . 6.7 s.u.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 143 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 18 Note
Ni01 O003 O004 C005 C006 N007 H007 C008
C009 H009 C00A H00A H00B H00C C00B H00D
H00E H00F
PLAT794_ALERT_5_G Tentative Bond Valency for Ni01 (III) . 2.82 Info
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 409 Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 5 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 5 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 5 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 5 Units

```
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       4.90 Note
              Predicted wR2: Based on SigI**2  2.06 or SHELX Weight  9.50
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
```

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

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   5 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 06/01/2024; check.def file version of 05/01/2024

Datablock NiS4 - ellipsoid plot