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: tennantite-Ni

Bond precision: = 0.0000 A Wavelength=1.54184

Cell: a=10.2957(9) b=10.2957(9) c=10.2957(9)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1091.4(3)	1091.4(3)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	As5.88 Cu21.12 Fe0.96 Ni1.92 S26 Sb2.12	As2.94 Cu10.56 Fe0.48 Ni0.96 S13 Sb1.06
Sum formula	As5.88 Cu21.12 Fe0.96 Ni1.92 S26 Sb2.12	As2.94 Cu10.56 Fe0.48 Ni0.96 S13 Sb1.06
Mr	3040.70	1520.25
Dx,g cm-3	4.626	4.626
Z	1	2
Mu (mm-1)	40.928	40.930
F000	1409.4	1409.0
F000'	1364.54	
h,k,lmax	12,12,12	8,12,10
Nref	202[119]	184
Tmin,Tmax	0.745,0.849	0.421,1.000
Tmin'	0.721	

Correction method= # Reported T Limits: Tmin=0.421 Tmax=1.000
AbsCorr = ?

Data completeness= 1.55/0.91 Theta(max)= 64.790

R(reflections)= 0.0423(163)

wR2(reflections)= 0.1158(184)

S = 1.161 Npar= 21

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

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PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) ........       5.67 Note
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Alert level C

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STRVA01_ALERT_4_C           Flack parameter is too small
           From the CIF: _refine_ls_abs_structure_Flack   -0.320
           From the CIF: _refine_ls_abs_structure_Flack_su    0.180
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
            Calculated sin(theta_max)/wavelength =    0.5868
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full           ! Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...       1.14 Do !
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.30 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          3 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Sb         Constrained at      0.265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As         Constrained at      0.735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cu1        Constrained at       0.76 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ni1        Constrained at       0.16 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1        Constrained at       0.08 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        79% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           4 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.          2 Units
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  1 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
  9 ALERT type 4 Improvement, methodology, query or suggestion
  4 ALERT type 5 Informative message, check
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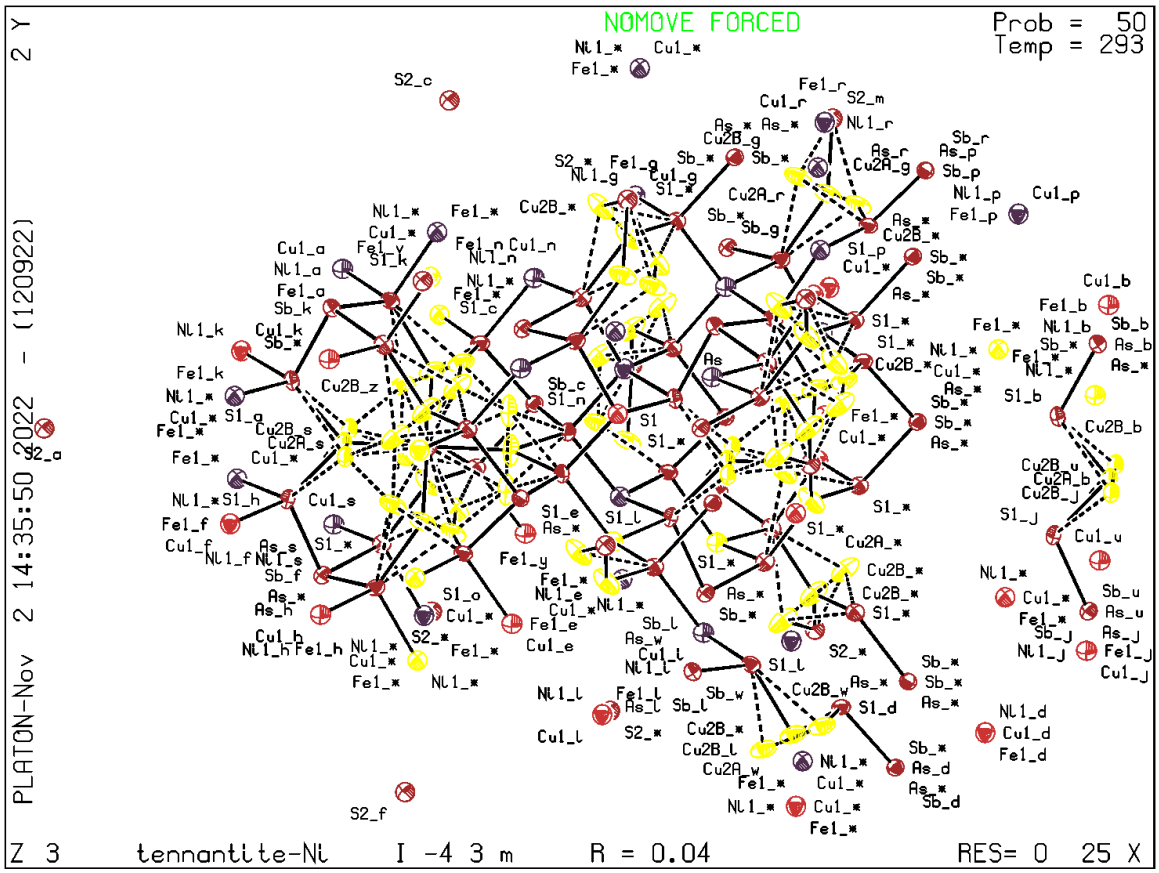
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 12/09/2022; check.def file version of 09/08/2022

Datablock tennantite-Ni - ellipsoid plot