checkCIF/PLATON report

Structure factors have been supplied for datablock(s) wort_empa

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: wort_empa

Bond precision: Te- O = 0.0267 A Wavelength=0.71073

Cell: a=9.2215(13) b=9.2215(13) c=7.5150(15)
alpha=90 beta=90 gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	553.43(19)	553.43(19)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	Fe0.26 Ni3.74 O18 Te6, 0.156(Ni4), 0.02(Mn4), 0.075(Mg4), 12(O0	Fe0.26 Ni3.74 O18 Te6, Mg1.15 Mn0.08 Ni0.75 O6
Sum formula	Fe0.26 Mg1.15 Mn0.08 Ni4.51 O24 Te6	Fe0.13 Mg0.57 Mn0.04 Ni2.26 O12 Te3
Mr	1461.28	730.80
Dx,g cm-3	4.385	4.385
Z	1	2
Mu (mm-1)	11.873	11.877
F000	652.9	653.0
F000'	651.76	
h,k,lmax	11,11,9	7,7,5
Nref	361	100
Tmin,Tmax	0.495,0.552	0.239,0.423
Tmin'	0.167	

Correction method= # Reported T Limits: Tmin=0.239 Tmax=0.423
AbsCorr = ?

Data completeness= 0.277 Theta(max)= 25.242

R(reflections)= 0.0544(94)

wR2(reflections)= 0.1393(100)

S = 1.168 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 A

PLAT088_ALERT_3_A Poor Data / Parameter Ratio ..... 4.76 Note

Author Response: Crystal structure has been checked and average structrure is crystal-c

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Alert level B

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree
O1 O2
PLAT920_ALERT_1_B Theta(Max) in CIF and FCF Differ by ..... 9.49 Degree

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Alert level C

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) ... 1.11 Do !
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.28 Report
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.33Ang From Ow 1.88 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.99Ang From O1 . -0.54 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From O1 . -0.54 eA-3

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: Fe0.13 Mg0.57 Mn.04 Ni2.26 O1
Atom count from _chemical_formula_moiety:Fe0.26 Mg1.15 Mn.08 Ni4.49 O2
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
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 45.45 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 3 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Ni1 Constrained at 0.935 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1 Constrained at 0.065 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ni3 Constrained at 0.1559 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mn3 Constrained at 0.0196 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of Mg3        Constrained at     0.0745 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ow         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ni2        Constrained at     0.0756 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mg2        Constrained at     0.4244 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        29% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        Ow Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         1 Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
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 !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        86% Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ          4 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ          4 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.         4 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.         4 Units
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
36 **ALERT level G** = General information/check it is not something unexpected

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
21 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 10/05/2023; check.def file version of 10/05/2023

Datablock wort_empa - ellipsoid plot