# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) wort_nosubs

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_nosubs

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Bond precision:   Ni- O = 0.0300 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
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| | 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 | Ni2 O9 Te3, 0.108(Ni4), 2.94(O), 0.604(Mg) | Ni2 O9 Te3, 0.108(Ni4), 2.94(O), 0.604(Mg) |
| Sum formula | Mg0.60 Ni2.43 O11.94 Te3 | Fe0 Mg0.60 Mn0 Ni2.43 O11.97 Te3 |
| Mr | 731.31 | 731.76 |
| Dx,g cm-3 | 4.389 | 4.391 |
| Z | 2 | 2 |
| Mu (mm-1) | 11.957 | 11.957 |
| F000 | 653.8 | 654.0 |
| F000' | 652.65 | |
| h,k,lmax | 11,11,9 | 7,7,5 |
| Nref | 361 | 100 |
| Tmin,Tmax | 0.493,0.550 | 0.239,0.423 |
| Tmin' | 0.165 | |

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

Data completeness= 0.277            Theta(max)= 25.242
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R(reflections)= 0.0548( 94)

wR2(reflections)= 0.1382( 100)

S = 1.164 Npar= 22

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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.

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**Alert level A**

PLAT088_ALERT_3_A Poor Data / Parameter Ratio ..... 4.55 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**

PLAT041_ALERT_1_C Calc. and Reported SumFormula 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) ... 1.12 Do !
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.26 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 1 Check
M2
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.29Ang From Ow 1.88 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.94Ang From O1 . -0.55 eA-3

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**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: Mg0.6 Ni2.43 O11.97 Te3
Atom count from _chemical_formula_moiety:Mg0.604 Ni2.432 O11.94 Te3
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:Mg0.6 Ni2.43 O11.97 Te3
Atom count from the _atom_site data: Mg0.6038 Ni2.433 O11.94 Te3
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum Fe0 Mg0.60 Mn0 Ni2.43 O11.97 Te3
TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|---|---|---|---|
| Fe | 2.00 | 0.00 | 2.00 |
| Mg | 1.20 | 1.21 | -0.01 |
| Mn | 2.00 | 0.00 | 2.00 |
| Ni | 4.86 | 4.87 | -0.01 |
| O | 23.94 | 23.88 | 0.06 |
| Te | 6.00 | 6.00 | 0.00 |

| | | | |
|---|---|---|---|
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 3 | Report |
| PLAT004_ALERT_5_G | Polymeric Structure Found with Maximum Dimension | 3 | Info |
| PLAT017_ALERT_1_G | Check Scattering Type Consistency of M2 as | MG | |
| PLAT017_ALERT_1_G | Check Scattering Type Consistency of M3 as | NI | |
| PLAT068_ALERT_1_G | Reported F000 Differs from Calcd (or Missing)... | Please | Check |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large | 50.47 | Why ? |
| PLAT300_ALERT_4_G | Atom Site Occupancy of M3 Constrained at | 0.2165 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of M2 Constrained at | 0.6038 | Check |
| 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 |
| PLAT311_ALERT_2_G | Isolated Disordered Oxygen Atom (No H's ?) ..... | Ow | Check |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels ..... | 3 | Note |
| PLAT802_ALERT_4_G | CIF Input Record(s) with more than 80 Characters | 1 | 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
27 **ALERT level G** = General information/check it is not something unexpected

13 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
10 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.

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**PLATON version of 10/05/2023; check.def file version of 10/05/2023**

**Datablock wort_nosubs** - ellipsoid plot