# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

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Bond precision: = 0.0000 A Wavelength=0.71073

Cell: a=10.3734(8) b=10.3734(8) c=20.6910(12)
alpha=90 beta=90 gamma=120
Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1928.2(3) | 1928.2(2) |
| Space group | R -3 | R -3 |
| Hall group | -R 3 | -R 3 |
| Moiety formula | Mg6.90 O114 Ti49.23 Zr4.77, 2.631(Sr) | ? |
| Sum formula | Mg6.90 O114 Sr2.63 Ti49.23 Zr4.77 | Sr Zr Ti18 Mg2 O38 |
| Mr | 5014.08 | 1751.50 |
| Dx,g cm-3 | 4.318 | 4.525 |
| Z | 1 | 3 |
| Mu (mm-1) | 7.412 | 8.387 |
| F000 | 2368.7 | 2369.0 |
| F000' | 2365.44 | |
| h,k,lmax | 13,13,26 | 13,13,26 |
| Nref | 1000 | 1001 |
| Tmin,Tmax | 0.747,0.778 | 0.619,1.000 |
| Tmin' | 0.428 | |

Correction method= # Reported T Limits: Tmin=0.619 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.001 Theta(max)= 27.550

R(reflections)= 0.0285( 781)

wR2(reflections)= 0.0612( 1001)

S = 1.340 Npar= 116

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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**

PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 11.62 %

**Author Response: In order to estimate mean atomic numbers of mixed sites, the scattering factors of dominant cations were used together with refinement of occupancies, which led to the discrepancy between reported (ideal) and refined formulas.**

PLAT075_ALERT_1_A Occupancy 1.150 Greater Than 1.0 for ..... T

**Author Response: In order to estimate mean atomic number of mixed T site, the scattering factor of Mg (as dominant cation) was used together with occupancy refinement. Since other cations of this mixed site have higher Z, the effective occupancy becomes > 1.**

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**Alert level B**

ABSMU01_ALERT_1_B The ratio of given/expected absorption coefficient lies outside the range 0.95 <> 1.05
Calculated value of mu = 7.891
Value of mu given = 8.387

**Author Response: In order to estimate mean atomic numbers of mixed sites, the scattering factors of dominant cations were used together with refinement of occupancies, which led to the discrepancy between reported (ideal) and refined formulas.**

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 240.42 Check

**Author Response: In order to estimate mean atomic numbers of mixed sites, the scattering factors of dominant cations were used together with refinement of occupancies, which led to the discrepancy between reported (ideal) and refined formulas.**

## Alert level C

```
CHEMW01_ALERT_1_C  The ratio of given/expected molecular weight as calculated
            from the _chemical_formula_sum lies outside
            the range 0.99 <> 1.01
            Calculated formula weight =  1697.6272
            Formula weight given      =  1751.5000
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
PLAT088_ALERT_3_C Poor Data / Parameter Ratio .....................      8.63 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.29 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     4.242 Check
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## Alert level G

```
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:Mg2 O38 Sr1 Ti18 Zr1
            Atom count from the _atom_site data:  Mg2.3 O38 Sr0.877 Ti16.41 Zr1.59
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    3
           From the CIF: _chemical_formula_sum  Sr Zr Ti18 Mg2 O38
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           Sr         3.00      2.63    0.37
           Zr         3.00      4.77   -1.77
           Ti        54.00     49.23    4.77
           Mg         6.00      6.90   -0.90
           O        114.00    114.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT017_ALERT_1_G Check Scattering Type Consistency of A        as         SR
PLAT017_ALERT_1_G Check Scattering Type Consistency of B        as         ZR
PLAT017_ALERT_1_G Check Scattering Type Consistency of C1       as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of C2       as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of C3       as         TI
PLAT017_ALERT_1_G Check Scattering Type Consistency of T        as         MG
PLAT017_ALERT_1_G Check Scattering Type Consistency of X1       as         ZR
PLAT017_ALERT_1_G Check Scattering Type Consistency of X2       as         ZR
PLAT017_ALERT_1_G Check Scattering Type Consistency of X3       as         ZR
PLAT017_ALERT_1_G Check Scattering Type Consistency of X4       as         ZR
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     0.333 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        32% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        10 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 !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         2 Check
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  2 ALERT level A = Most likely a serious problem - resolve or explain
  2 ALERT level B = A potentially serious problem, consider carefully
  6 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

 23 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  2 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
  3 ALERT type 4 Improvement, methodology, query or suggestion
  5 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 I** - ellipsoid plot