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: zilbermintsite

Bond precision: Si- O = 0.0116 A   Wavelength=0.71073

Cell: a=8.9605(5)   b=5.7295(2)   c=25.1033(13)
               alpha=90   beta=116.616(7)   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1152.21(12)	1152.21(12)
Space group	P 21/m	P 21/m
Hall group	-P 2yb	-P 2yb
Moiety formula	Al5.90 Ce10.09 Fe3.08 Mg0.72 Mn0.30 O62 Si14, 1.91(Ca)	?
Sum formula	Al5.90 Ca1.91 Ce10.09 Fe3.08 Mg0.72 Mn0.30 O62 Si14	Al2.95 Ca0.96 Ce5.05 Fe1.54 Mg0.36 Mn0.15 O31 Si7
Mr	3240.69	1620.40
Dx,g cm-3	4.670	4.671
Z	1	2
Mu (mm-1)	11.624	11.625
F000	1488.3	1488.0
F000'	1489.59	
h,k,lmax	11,7,33	11,7,33
Nref	3023	2857
Tmin,Tmax	0.175,0.621	0.312,0.763
Tmin'	0.144	

Correction method= # Reported T Limits: Tmin=0.312 Tmax=0.763
AbsCorr = GAUSSIAN

Data completeness= 0.945   Theta(max)= 27.870

R(reflections)= 0.0757(2677)

wR2(reflections)=
0.1994(2857)

S = 1.262   Npar= 274

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 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 gaussian
DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
           _refine_diff_density_min given =   -5.479
           Test value =   -4.350
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density   5.59 eA-3
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density   -5.48 eA-3
PLAT213_ALERT_2_C Atom Si2   has ADP max/min Ratio .....   3.2 prolat
PLAT213_ALERT_2_C Atom O18   has ADP max/min Ratio .....   4.0 oblate
PLAT213_ALERT_2_C Atom O21   has ADP max/min Ratio .....   3.1 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1 O   Ueq(max)/Ueq(min) Range   6.0 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   A5CE Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O21 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Si2 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Si5 Check
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ....   O4 Check
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ....   O17 Check

⚪ Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   2 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   21.25 Why ?
PLAT158_ALERT_4_G The Input Unitcell is NOT Standard/Reduced .....   Please Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records   5 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   5 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   2 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 M1FE   Constrained at   0.57 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M3FE   Constrained at   0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M3MN   Constrained at   0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M1AL   Constrained at   0.17 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M1MG   Constrained at   0.26 Check
PLAT300_ALERT_4_G Atom Site Occupancy of M3MG   Constrained at   0.1 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of O23          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O24          Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd   1)           17% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd   2)          100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         17 Note
                 A1CE    A1CA    A2CE    A3CE    A4CE    A5CE    A6CE    M1AL
                 M1FE    M1MG    M2FE    M2AL    M3MG    M3FE    M3MN    M4FE
                 M4AL
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         12 Note
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
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        3 Note
                 0  1 17,   4  2 14,   2  0 14,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged   Please Check
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
 18 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

  8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 ALERT type 2 Indicator that the structure model may be wrong or deficient
  2 ALERT type 3 Indicator that the structure quality may be low
 16 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 06/01/2024; check.def file version of 05/01/2024

Datablock zilbermintsite - ellipsoid plot