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

Bond precision: = 0.0000 A Wavelength=0.03350

Cell: a=10.2(2) b=10.2(2) c=14.9(3)
alpha=90 beta=90 gamma=120
Temperature: 293 K

	Calculated	Reported
Volume	1343(60)	1340(50)
Space group	P 6/m c c	P 6/m c c
Hall group	-P 6 2c	-P 6;-2c
Moiety formula	Al14.40 O64 Si17.60, 0.52(Sr), 4.5(Ca), 1.159(K)	?
Sum formula	Al14.40 Ca4.50 K1.16 O64 Si17.60 Sr0.52	Al7.2 Ca2.25 K0.58 O32 Si8.8 Sr0.26
Mr	2178.12	1089.00
Dx,g cm-3	2.690	2.694
Z	1	2
Mu (mm-1)	0.000	0.000
F000	0.0	1077.0
F000'	1077.19	
h,k,lmax		12,12,18
Nref		5728
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= Theta(max)= 1.210

R(reflections)= 0.1432(3052) wR2(reflections)= wR= 0.1572(5728)

S = 2.540 Npar= 113

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

ATOM007_ALERT_1_A _atom_site_aniso_label is missing
Unique label identifying the atom site.

Author Response: All atoms were refined with one isotropic displacement parameter.

PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value .... Please Do !

Author Response: Cell parameters were determined by the software PETS. No output information for this parameter was given.

PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ..... Please Do !

Author Response: Cell parameters were determined by the software PETS. No output information for this parameter was given.

PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ..... Please Do !

Author Response: Cell parameters were determined by the software PETS. No output information for this parameter was given.

PLAT881_ALERT_1_A No Datum for _diffrn_reflns_av_R_equivalents ... Please Do !

Author Response: Data were refined dynamically considering separetely each electron diffraction pattern.

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 2.540
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
PLAT082_ALERT_2_C High R1 Value ..... 0.14 Report
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P 6;-2 c
PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large .... 0.200 Ang.
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large .... 0.300 Ang.
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 2 Check
Ca1 K1
PLAT799_ALERT_4_C Numeric Label on Displacement Par. Record ..... ? Check

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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         10 Units
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 Si1        Constrained at       0.55 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Si2        Constrained at     0.5499 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al1        Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al2        Constrained at       0.45 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca1        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of K1         Constrained at     0.5796 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        40% 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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )       0.01 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )       0.19 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )       0.05 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Si1      ..Si1             3.02 Ang.
                                                 y,-x+y,z  =      5_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Si1      ..Si1             3.02 Ang.
                                                 x-y,x,z  =       6_555 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
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 !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold  of        3.0 Sig(I)
PLAT970_ALERT_5_G Refinement Requires Electron Scattering Factors.     Please Check
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   5 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  28 ALERT level G = General information/check it is not something unexpected

  13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
  16 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 13/07/2021; check.def file version of 13/07/2021

Datablock I - ellipsoid plot