

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	Si- O = 0.0020 A	Wavelength=0.71073	
Cell:	a=14.5596 (4)	b=5.2213 (1)	c=19.8270 (4)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1507.25 (6)	1507.25 (6)	
Space group	P c c a	P c c a	
Hall group	-P 2a 2ac	-P 2a 2ac	
	Ce3.94 Fe3.32 O68 Si24		
Moiety formula	Zn0.68, 2.708 (Ba),	?	
	1.292 (Sr), 3.888 (Na),		
	Ba2.71 Ce3.94 Fe3.32		
Sum formula	Na12.31 O68 Si24 Sr1.29	Ba0.50 Ce Fe0.50 Na3 O17	
	Zn0.68	Si6 Sr0.50 Zn0.50	
Mr	3312.83	822.72	
Dx, g cm-3	3.650	3.626	
Z	1	4	
Mu (mm-1)	7.538	7.951	
F000	1551.6	1544.0	
F000'	1552.16		
h, k, lmax	21, 7, 29	20, 7, 28	
Nref	2508	2362	
Tmin, Tmax	0.795, 0.902	0.750, 0.953	
Tmin'	0.626		

Correction method= # Reported T Limits: Tmin=0.750 Tmax=0.953
AbsCorr = GAUSSIAN

Data completeness= 0.942 Theta(max) = 31.455

R(reflections)= 0.0246 (1902) wR2(reflections)= 0.0665 (2362)

S = 1.072 Npar= 140

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

PLAT075_ALERT_1_A Occupancy 1.053 Greater Than 1.0 for NA2

Alert level B

PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 5.20 %

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 21.95 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.666 Check
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Ce1 1.12 eA-3

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:Ba0.5 Ce1 Fe0.5 Na3 O17 Si6 Sr0.
Atom count from the _atom_site data: Ba0.677 Ce0.986 Fe0.83 Na3.078 O
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 4
From the CIF: _chemical_formula_sum Ba0.50 Ce Fe0.50 Na3 O17 Si6 Sr0.5
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Ba	2.00	2.71	-0.71
Ce	4.00	3.94	0.06
Fe	2.00	3.32	-1.32
Na	12.00	12.31	-0.31
O	68.00	68.00	0.00
Si	24.00	24.00	0.00
Sr	2.00	1.29	0.71
Zn	2.00	0.68	1.32

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffraction_ambient_temperature (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 14% 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
PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O1 132.1 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O3 125.3 Degree
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 141 Note

1 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

11 **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
2 **ALERT type 3** Indicator that the structure quality may be low
7 **ALERT type 4** Improvement, methodology, query or suggestion
1 **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 05/12/2020; check.def file version of 05/12/2020

