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: 2

Bond precision: O- C = 0.0170 A Wavelength=0.71073

Cell: a=10.075(3) b=10.075(3) c=12.639(5)
alpha=90 beta=90 gamma=120
Temperature: 293 K

	Calculated	Reported
Volume	1111.1(9)	1111.2(7)
Space group	P 63 m c	P63mc
Hall group	P 6c -2c	P 6c -2c
Moiety formula	C3 O9, 4(C O3), C O3, Rb, 5(Ca), 5(Na)	?
Sum formula	C8 Ca5 Na5 O24 Rb	C8 Ca5 Na5 O24 Rb
Mr	880.90	880.90
Dx,g cm-3	2.633	2.633
Z	2	2
Mu (mm-1)	3.600	3.600
F000	864.0	864.0
F000’	865.20	
h,k,lmax	13,13,16	13,13,16
Nref	991[519]	982
Tmin,Tmax	0.806,0.835	0.911,1.000
Tmin’	0.698	

Correction method= # Reported T Limits: Tmin=0.911 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.89/0.99 Theta(max)= 27.460

R(reflections)= 0.0450(967) wR2(reflections)= 0.1129(982)

S = 1.240 Npar= 88

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 B

PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) ..... 5.90 Note
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT732_ALERT_1_B Angle Calc 60.09(13), Rep 60.08(3) ..... 4.33 s.u.-R
O2 -C2 -CA1 1.555 1.555 1.555 .... # 358 Check

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 Multi-scan
PLAT036_ALERT_1_C No s.u. Given for Flack Parameter ..... Please Do !
PLAT220_ALERT_2_C Non-Solvent Resd 2 O Ueq(max)/Ueq(min) Range 4.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3 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:C8 Ca5 Na5 O24 Rb1
Atom count from the _atom_site data: C8 Ca4.99 Na5.01 O24.01 Rb1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C8 Ca5 Na5 O24 Rb
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	16.00	16.00	0.00
Ca	10.00	9.98	0.02
Na	10.00	10.02	-0.02
O	48.00	48.02	-0.02
Rb	2.00	2.00	0.00

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 1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 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 >O7 is Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Ca2 is Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Na2 is Constrained at 0.6667 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 10 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 13 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
16 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
  4 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 11/08/2016; check.def file version of 04/08/2016

Datablock 2 - ellipsoid plot