

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lgjc040_0ma_a

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: lgjc040_0ma_a

Bond precision: Si- O = 0.0007 A Wavelength=0.71073

Cell: a=16.1805 (3) b=5.5466 (1) c=10.0276 (2)
 alpha=90 beta=90 gamma=90

Temperature: 294 K

	Calculated	Reported
Volume	899.95 (3)	899.94 (3)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	Al6 H2 O26 Si6, 4 (Ca)	?
Sum formula	Al6 Ca4 H2 O26 Si6	Al3 H Ca2 O13 Si3
Mr	908.76	454.37
Dx, g cm ⁻³	3.354	3.354
Z	2	4
Mu (mm ⁻¹)	2.054	2.042
F000	904.0	985.0
F000'	907.99	
h, k, lmax	26, 8, 16	26, 8, 16
Nref	2144	2142
Tmin, Tmax	0.745, 0.903	0.679, 0.747
Tmin'	0.736	

Correction method= # Reported T Limits: Tmin=0.679 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta (max)= 35.013

R(reflections)= 0.0124 (2049)

wR2(reflections)=
0.0321 (2142)

S = 1.130


Npar= 125

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**

PLAT927_ALERT_1_B Reported and Calculated wR2 Differ by -0.0113 Check
PLAT928_ALERT_1_B Reported and Calculated S value Differ by . -0.398 Check

 **Alert level C**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by -0.0022 Check

 **Alert level G**

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
PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O9 . 173.6 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Al3 (III) . 2.57 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al12 (III) . 2.94 Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT982_ALERT_1_G The O-f'= 0.0080 Deviates from IT-value = 0.0106 Check

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

- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
3 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 28/11/2022; check.def file version of 28/11/2022

