checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 18360_calcinaxite_auto2

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: 18360_calcinaxite_auto2

Bond precision: Si- O = 0.0032 A   Wavelength=0.71073

Cell: a=7.0155(4)   b=8.0721(4)   c=10.0275(4)
                alpha=104.420(4)   beta=99.764(4)   gamma=115.126(5)
Temperature: 293 K

	Calculated	Reported
Volume	472.74(5)	472.74(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	O10 Si4, Ca, K, Na	Ca K Na O10 Si4
Sum formula	Ca K Na O10 Si4	Ca K Na O10 Si4
Mr	374.53	374.53
Dx,g cm-3	2.631	2.631
Z	2	2
Mu (mm-1)	1.701	1.701
F000	372.0	372.0
F000'	373.75	
h,k,lmax	9,11,13	9,10,13
Nref	2587	2078
Tmin,Tmax	0.815,0.918	0.966,1.000
Tmin'	0.815	

Correction method= # Reported T Limits: Tmin=0.966 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.803   Theta(max)= 29.308

R(reflections)= 0.0353(1896)   wR2(reflections)= 0.0852(2078)

S = 1.115   Npar= 154

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

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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.967 Why?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ    Please Check
             Calc: O10 Si4, Ca, K, Na
             Rep.: Ca K Na O10 Si4
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      O7 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     Si3 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.648 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600       56 Report
              -7  1  0,  -7  2  0,   6 -1  1,   7 -1  1,   7  0  1,  -8  2  1,
              -7  2  1,   6 -1  2,   7 -1  2,   6  0  2,   5 -5  3,   6 -1  3,
               6  0  3,   6 -7  4,   6 -6  4,   5 -5  4,   6 -1  4,   6 -7  5,
               5 -6  5,   4 -5  5,   5 -5  5,   6 -7  6,   5 -6  6,   4 -5  6,
               5 -7  7,   4 -6  7,   5 -6  7,   3 -5  7,   4 -5  7,   2 -4  7,
               3 -4  7,   4 -7  8,   4 -6  8,   3 -5  8,   3 -6  9,   4 -6  9,
               2 -5  9,   3 -5  9,   2 -6 10,   3 -6 10,  -1 -5 10,   1 -5 10,
               2 -5 10,  -2 -4 10,  -1 -4 10,  -4 -3 10,  -3 -3 10,  -2 -5 11,
              -1 -5 11,   0 -5 11,   1 -5 11,  -3 -4 11,  -2 -4 11,  -1 -4 11,
               0 -4 11,  -3 -3 11,
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From O5       .      -0.48 eA-3
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension      3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF    Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)     293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)     293 Check
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O1       .   137.4 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O4       .   140.0 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O8       .   134.0 Degree
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
              0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600     443 Note
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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
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
   1 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.

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