checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kokch_sc_test1

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: kokch_sc_test1

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Bond precision:  = 0.0000 A              Wavelength=0.28970

Cell:            a=10.5757(3)     b=10.5757(3)     c=15.6404(6)
                 alpha=90         beta=90          gamma=120
Temperature:     293 K

                Calculated                Reported
Volume          1514.94(12)               1514.94(10)
Space group     P 6/m c c                 P 6/m c c
Hall group      -P 6 2c                   -P 6 2c
Moiety formula  Al8 O64 Si24, 8(K)        ?
Sum formula     Al8 K8 O64 Si24           Al K O8 Si3
Mr              2226.80                   278.35
Dx,g cm-3       2.441                     2.441
Z               1                         8
Mu (mm-1)       0.128                     0.110
F000            1104.0                    1104.0
F000'           1104.29
h,k,lmax        18,18,27                  16,17,26
Nref            1558                      1455
Tmin,Tmax       0.996,0.998               0.916,1.000
Tmin'           0.996

Correction method= # Reported T Limits: Tmin=0.916 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.934          Theta(max)= 15.000

R(reflections)= 0.0683( 648)      wR2(reflections)= 0.2635( 1455)

S = 1.135                 Npar= 44
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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

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group P6/mmm Check

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -1.795
Test value = -1.425
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.26	Report
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density	-1.79	eA-3
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	O1	Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.2	Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	114.477	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	12.450	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	3.967	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.503	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	30	Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF	14	Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.27A From Si1	-1.86	eA-3
PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on K1	-1.45	eA-3
PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on K2	-1.43	eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.86A From O1'	-0.50	eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...	0.13	Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.12	Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.28970	Ang.
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ...	?	Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem c/2	100	%Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem C	100	%Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem a/2	100	%Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem b/2	100	%Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem I	100	%Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem B	100	%Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem A	100	%Fit
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...	2	Units
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 _diffrn_ambient_temperature ..... (K)	293	Check
PLAT300_ALERT_4_G Atom Site Occupancy of Si1 Constrained at	0.75	Check
PLAT300_ALERT_4_G Atom Site Occupancy of Si2 Constrained at	0.75	Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al1 Constrained at	0.25	Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al2 Constrained at	0.25	Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1)	40%	Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 2	0.08	Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 3	0.25	Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell .	56.67%	Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	68	Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units
PLAT984_ALERT_1_G The Al-f'= 0.0184 Deviates from the B&C-Value	0.0048	Check
PLAT984_ALERT_1_G The K-f'= 0.0671 Deviates from the B&C-Value	0.0346	Check
PLAT984_ALERT_1_G The O-f'= 0.0031 Deviates from the B&C-Value	-0.0010	Check
PLAT984_ALERT_1_G The Si-f'= 0.0239 Deviates from the B&C-Value	0.0082	Check

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

 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
  9 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 07/08/2019; check.def file version of 30/07/2019

Datablock kokch_sc_test1 - ellipsoid plot