checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kap1150b

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: kap1150b

Bond precision: O- B = 0.0040 A Wavelength=0.71073

Cell:	a=15.5471(19)	b=14.3403(17)	c=11.7315(15)
	alpha=90	beta=90	gamma=90
Temperature:	301 K		

	Calculated	Reported
Volume	2615.5(6)	2615.5(6)
Space group	C m c a	C m c a
Hall group	-C 2bc 2	-C 2bc 2
Moiety formula	B4 O56 Si16 U4, 7.104(K), 4.896(Na)	B K1.78 Na1.22 O14 Si4 U
Sum formula	B4 K7.10 Na4.90 O56 Si16 U4	B K1.78 Na1.22 O14 Si4 U
Mr	2731.13	682.77
Dx,g cm-3	3.468	3.468
Z	2	8
Mu (mm-1)	13.461	13.460
F000	2497.7	2498.0
F000’	2428.24	
h,k,lmax	25,23,18	25,23,18
Nref	2969	2963
Tmin,Tmax	0.622,0.764	0.114,0.164
Tmin’	0.578	

Correction method= # Reported T Limits: Tmin=0.114 Tmax=0.164
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 35.003

R(reflections)= 0.0356(2822) wR2(reflections)= 0.0686(2963)

S = 1.251 Npar= 120

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.34A From O1 4.17 eA-3

Author Response: This peak is an artefact from a unknown crystal defect. It is also located 1.82 A from the uranium atom. The second-highest residual density peak is 2.25 eA-3, located trans to the 4.17 eA-3 peak across the U atom. These two peaks may represent oxygen atoms of uranyl group from a disordered domain in the crystal. These residual peaks appeared in refinements from multiple crystals despite extensive crystal screening. Because of their relatively small magnitudes in a uranium structure, they do not alter the good precision of the refinement from the dominant average domain.

Alert level C

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 ..... 7.995 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.059 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.36A From O2 2.45 eA-3

Author Response: This peak is an artefact from a unknown crystal defect. It is also located 1.82 A from the uranium atom. The second-highest residual density peak is 2.25 eA-3, located trans to the 4.17 eA-3 peak across the U atom. These two peaks may represent oxygen atoms of uranyl group from a disordered domain in the crystal. These residual peaks appeared in refinements from multiple crystals despite extensive crystal screening. Because of their relatively small magnitudes in a uranium structure, they do not alter the good precision of the refinement from the dominant average domain.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.70A From O5 -2.07 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.40A From K2 -1.88 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.44A From K1C -1.53 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.67A From O2 0.74 eA-3

Alert level G

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 8
From the CIF: _chemical_formula_sum B K1.78 Na1.22 O14 Si4 U
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
B	8.00	8.00	0.00
K	14.24	14.21	0.03
Na	9.76	9.79	-0.03
O	112.00	112.00	0.00
Si	32.00	32.00	0.00

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           U          8.00      8.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         2 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.25 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      41.16 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O7             133.5 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si   Angle From 150 for O4             124.6 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si   Angle From 150 for O5             137.2 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for U1        (VI)      .       5.93 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          7 Note
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1 **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
20 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 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
9 ALERT type 4 Improvement, methodology, query or suggestion
2 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 10/08/2020; check.def file version of 06/08/2020

Datablock kap1150b - ellipsoid plot