checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound_2_uco3_10

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: Compound_2_uco3_10

```
Bond precision:  O- N = 0.0200 A         Wavelength=0.71073

Cell:            a=7.8596(2)    b=15.8675(3)       c=10.6823(2)
                 alpha=90       beta=90.141(2)     gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1332.21(5)	1332.21(5)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	Cl3 N O5 U, N O3, 3(K)	0.5(Cl3 N O5 U), Cl1.5 K0.5 N0.5 O2.5 U0.5, 2.5(K), N O3
Sum formula	Cl3 K3 N2 O8 U	Cl3 K3 N2 O8 U
Mr	617.70	617.70
Dx,g cm-3	3.080	3.080
Z	4	4
Mu (mm-1)	13.747	13.747
F000	1112.0	1112.0
F000’	1078.57	
h,k,lmax	13,26,17	13,26,17
Nref	13026[6697]	11537
Tmin,Tmax	0.064,0.167	0.637,1.000
Tmin’	0.030	

```
Correction method= # Reported T Limits: Tmin=0.637 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.89      Theta(max)= 36.420

R(reflections)= 0.0254( 8552)     wR2(reflections)= 0.0501( 11537)

S = 1.019                 Npar= 356
```

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

PLAT111_ALERT_2_B ADDSYM Detects New (Pseudo) Centre of Symmetry . 100 %Fit

Author Response: There are more than 350 reflections with >3sig(I), which should be absent in P21/n space group.

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem n 100 %Fit

Author Response: There are more than 350 reflections with >3sig(I), which should be absent in P21/n space group.

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group P21/n Check

Author Response: There are more than 350 reflections with >3sig(I), which should be absent in P21/n space group.

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.488
From the CIF: _refine_ls_abs_structure_Flack_su 0.015
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of U1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of U2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N4 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
Cl3 N O5 U
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report

---

Alert level G

PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.488 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 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 O11A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O11B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O12A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O12B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O13A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O13B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O14A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O14B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O15A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O15B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O16A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O16B Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 75% Note

```
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )        75% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  O15A     ..N3              2.61 Ang.
                                                    x,y,z  =      1_555 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             Cl3 N O5 U
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             K
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
             K
PLAT794_ALERT_5_G Tentative Bond Valency for U1        (VI)      .       5.81 Info
PLAT794_ALERT_5_G Tentative Bond Valency for U2        (VI)      .       5.93 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        392 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.6 Low
```

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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
  23 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 18/09/2020; check.def file version of 20/08/2020

Datablock Compound_2_uco3_10 - ellipsoid plot