checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: KPuO2CO3

```
Bond precision:    O- C = 0.0300 A              Wavelength=0.74000

Cell:              a=5.0746(3)        b=5.0746(3)         c=10.0472(12)
                   alpha=90           beta=90             gamma=120
Temperature:       293 K

                   Calculated                   Reported
Volume             224.07(4)                    224.07(3)
Space group        P 63/m m c                   P 63/m m c
Hall group         -P 6c 2c                     -P 6c 2c
Moiety formula     C O5 Pu, K                   C O5 Pu, K
Sum formula        C K O5 Pu                    C K O5 Pu
Mr                 373.11                       375.10
Dx,g cm-3          5.530                        5.560
Z                  2                            2
Mu (mm-1)          1.213                        20.334
F000               318.0                        318.0
F000'              318.63
h,k,lmax           6,6,13
Nref               125
Tmin,Tmax                                       0.741,0.741
Tmin'

Correction method= # Reported T Limits: Tmin=0.741 Tmax=0.741
AbsCorr = ANALYTICAL

Data completeness= 0.000             Theta(max)=


R(reflections)= 0.0644( 0)                      wR2(reflections)=
                                                wR= 0.0707( 0)
S = 0.710                Npar= 29
```

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
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..   1.99 Check

Alert level G
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   2 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..   Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka   0.74000 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Pu1   (VI)   .   5.73 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   1 Note
PLAT984_ALERT_1_G The K-f'=   0.2139 Deviates from the B&C-Value   0.2127 Check
PLAT985_ALERT_1_G The K-f"=   0.2742 Deviates from the B&C-Value   0.2713 Check
PLAT988_ALERT_1_G The CIF Supplied Pu-f'   value Used in Validation   -7.248 Note
PLAT989_ALERT_1_G The CIF Supplied Pu-f"   value Used in Validation   4.761 Note

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   1 **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

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 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
   1 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 06/01/2024; check.def file version of 05/01/2024