checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

```
Bond precision:   Ag-Ag = 0.0020 A          Wavelength=0.71073

Cell:               a=4.6654(18)       b=16.142(6)       c=18.874(7)
                    alpha=90           beta=90           gamma=90
Temperature:        293 K

                  Calculated                    Reported
Volume            1421.4(9)                     1421.4(9)
Space group       C m c m                       C m c m
Hall group        -C 2c 2                       -C 2c 2
Moiety formula    Ag6 Ce4 Te10, 2(Rb)           ?
Sum formula       Ag6 Ce4 Rb2 Te10              Ag3 Ce2 Rb Te5
Mr                2654.64                       1327.32
Dx,g cm-3         6.203                         6.203
Z                 2                             4
Mu (mm-1)         23.746                        23.746
F000              2216.0                        2216.0
F000'             2190.05
h,k,lmax          6,21,25                       6,21,25
Nref              1075                          1072
Tmin,Tmax         0.116,0.093                   0.407,0.746
Tmin'             0.074

Correction method= # Reported T Limits: Tmin=0.407 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997            Theta(max)= 28.822

R(reflections)= 0.0386( 845)                  wR2(reflections)=
                                              0.0832( 1072)
S = 0.995                  Npar= 37
```

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

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.98Ang From Ce1 2.07 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From Te3 1.89 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.20Ang From Te4 1.72 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.85Ang From Ce1 1.68 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From Te2 1.68 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.08Ang From Te4 1.61 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From Te4 1.58 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.20Ang From Te3 1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.15Ang From Ce1 -1.81 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.65Ang From Ag6 -1.76 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 2.49Ang From Rb7 -1.73 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.68Ang From Ce1 -1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 2.15Ang From Ag6 -1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.65Ang From Ce1 -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.59Ang From Te4 -1.54 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.39Ang From Te2 -1.54 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.81Ang From Te2 -1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.69Ang From Rb7 -1.51 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 1.183 Note
Predicted wR2: Based on SigI**2 7.03 or SHELX Weight 8.36

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
18 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 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 13/05/2024; check.def file version of 04/05/2024

Datablock shelx - ellipsoid plot

