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

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Bond precision:   Pd-Pd = 0.0010 A         Wavelength=0.71073

Cell:              a=7.7198(2)      b=7.7198(2)      c=43.1237(11)
                   alpha=90         beta=90          gamma=120
Temperature:       293 K

                 Calculated                  Reported
Volume           2225.66(13)                 2225.66(13)
Space group      R -3 c                      R -3 c :H
Hall group       -R 3 2"c                    -R 3 2"c
Moiety formula   As2.78 Bi18.73 Pd96 Te14.50 ?
Sum formula      As2.78 Bi18.73 Pd96 Te14.50 As0.23 Bi1.56 Pd8 Te1.21
Mr               16185.58                    1348.80
Dx,g cm-3        12.076                      12.076
Z                1                           12
Mu (mm-1)        61.347                      61.347
F000             6815.7                      6815.7
F000'            6642.18
h,k,lmax         11,11,63                    11,11,63
Nref             851                         841
Tmin,Tmax        0.239,0.375                 0.502,0.628
Tmin'            0.221

Correction method= # Reported T Limits: Tmin=0.502 Tmax=0.628
AbsCorr = MULTI-SCAN

Data completeness= 0.988           Theta(max)= 31.739

R(reflections)= 0.0267( 761)                    wR2(reflections)=
                                                0.0594( 841)
S = 1.135                 Npar= 39
```

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.85Ang From M1BI 3.24 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.87Ang From Bi1 2.68 eA-3

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 ..... 2.122 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From Pd4 2.41 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From M1BI 2.23 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From Pd1 1.75 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.86Ang From Pd4 1.73 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From Pd3 1.63 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.74Ang From Te3 1.60 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.76Ang From Pd2 1.58 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.083 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 72.53 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 3 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 52% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 2 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! 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 11 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 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
5 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 28/11/2022; check.def file version of 28/11/2022

Datablock shelx - ellipsoid plot