checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Se3.73Te0.27W2

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: Se3.73Te0.27W2

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Bond precision:   = 0.0000 A              Wavelength=1.54184

Cell:               a=3.3074(5)      b=3.3074(5)      c=13.180(2)
                    alpha=90         beta=90          gamma=120
Temperature:        298 K

                 Calculated                Reported
Volume           124.86(4)                 124.86(5)
Space group      P 63/m m c                P 63/m m c
Hall group       -P 6c 2c                  -P 6c 2c
Moiety formula   Se3.73 Te0.27 W2          Se3.73 Te0.27 W2
Sum formula      Se3.73 Te0.27 W2          Se3.73 Te0.27 W2
Mr               696.85                    696.85
Dx,g cm-3        9.268                     9.268
Z                1                         1
Mu (mm-1)        125.904                   125.910
F000             288.9                     289.0
F000'            275.37
h,k,lmax         4,4,16                    4,4,16
Nref             72                        72
Tmin,Tmax        0.006,0.284               0.343,1.000
Tmin'            0.000

Correction method= # Reported T Limits: Tmin=0.343 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 76.035

R(reflections)= 0.0363( 71)                wR2(reflections)=
                                           0.0981( 72)
S = 1.263                Npar= 6
```

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. 2.02Ang From Te1 2.72 eA-3

Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.39Ang From Te1 -3.23 eA-3

Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

Alert level C

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

Author Response: The synthesis produced substitutional disorder in the Se atoms with Te

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.180 Check

Author Response: This is a frequent problem for integration of low-intensity reflections in high-background images. It does not have a significant efect on the refinement results.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From Te1 2.25 eA-3

Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.91Ang From W1 1.99 eA-3

Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.80Ang From W1 1.66 eA-3

Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.90Ang From Te1 1.53 eA-3

Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.74Ang From W1 -2.48 eA-3

Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.69Ang From Te1           -1.88 eA-3
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Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.18Ang From Te1           -1.78 eA-3
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Author Response: The crystal measured is very tiny. Considering that the compound crystallizes in layers, this measured crystal was a tiny layer smaller than 0.1 mm. Despite that the unit cell was calculated using up to 85 % of the reflections, unaccounted for twinning is not discarted. We tried to consider twins in our refinement but the best results are reported in this cif file. The wrong assigning of atoms is not possible because other techniques confirmed the composition.

Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
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          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Te1        Constrained at     0.0685 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Se1        Constrained at     0.9315 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        85% Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
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   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
   9 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
```

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  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
  6 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 18/05/2022; check.def file version of 17/05/2022

Datablock Se3.73Te0.27W2 - ellipsoid plot