checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Se3.96Te0.04W2

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: Se3.96Te0.04W2

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Bond precision:   = 0.0000 A                Wavelength=1.54184

Cell:               a=3.2857(5)      b=3.2857(5)      c=12.9773(15)
                    alpha=90         beta=90          gamma=120
Temperature:        298 K

                  Calculated                  Reported
Volume            121.33(4)                   121.33(4)
Space group       P 63/m m c                  P 63/m m c
Hall group        -P 6c 2c                    -P 6c 2c
Moiety formula    Se3.96 Te0.04 W2            Se3.96 Te0.04 W2
Sum formula       Se3.96 Te0.04 W2            Se3.96 Te0.04 W2
Mr                685.47                      685.47
Dx,g cm-3         9.381                       9.420
Z                 1                           1
Mu (mm-1)         120.696                     121.003
F000              284.7                       284.7
F000'             270.95
h,k,lmax          4,4,16                      4,4,16
Nref              69                          69
Tmin,Tmax         0.008,0.298                 0.038,1.000
Tmin'             0.000

Correction method= # Reported T Limits: Tmin=0.038 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000            Theta(max)= 75.918

R(reflections)= 0.0320( 65)                    wR2(reflections)=
                                               0.0808( 69)
S = 1.161                  Npar= 6
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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

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.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.50Ang From W1 1.94 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 90 % 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. 1.91Ang From Te1 -1.87 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 90 % 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. 1.63Ang From Te1 -1.61 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 90 % 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.

PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on W1 -1.03 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 90 % 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       0.01 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Se1        Constrained at       0.99 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        85% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
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
   0 ALERT level B = A potentially serious problem, consider carefully
   5 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
   5 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
   5 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 19/02/2022; check.def file version of 19/02/2022

Datablock Se3.96Te0.04W2 - ellipsoid plot