Checkcif Report

Datablock: FFSM21B_K1

```
Bond precision:       = 0.0000 A                  Wavelength=0.29460
Cell:        a=8.9166(3)    b=8.9166(3)   c=8.9166(3)
             alpha=90       beta=90       gamma=90
Temperature: 293 K
                   Calculated                        Reported
Volume             708.92(7)                         708.93(6)
Space group        I m -3                            I m -3
Hall group         -I 2 2 3                          -I 2 2 3
Moiety formula     Co8 Ge5.93 Sb12.24 Te5.93         ?
Sum formula        Co8 Ge5.93 Sb12.24 Te5.93         Co Ge0.74 Sb1.53 Te0.74
Mr                 3148.63                           393.6
Dx,g cm-3          7.375                             7.375
Z                  1                                 8
Mu (mm-1)          10.267                            10.267
F000               1338.2                            1338.2
F000'              1335.90
h,k,lmax           17,17,17                          17,17,17
Nref               567                               562
Tmin,Tmax          0.998,0.999                       0.491,1.000
Tmin'              0.997
Correction method= # Reported T Limits: Tmin=0.491
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.991        Theta(max)= 17.133
R(reflections)= 0.0353( 470)       wR2(reflections)= 0.0827( 562)
S = 1.202             Npar= 10
```

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's comment: This is a consequence of mixed atom sites in a disordered compound, and in addition minor rounding artifacts.

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.
Author's comment: synchrotron radiation, μ calculated with NIST database.

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
Author's comment: correct.

PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.13 Ratio
Author's comment: Z was chosen so that the nominal composition of this solid.state compound corresponds to one formula unit.

PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag Ka .. 0.2946 Ang.
Author's comment: correct, synchrotron radiation.

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
Author's comment: mixed cation site.

PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
Author's comment: correct, measurement at room temperature.
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2 is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Te2 is Constrained at 0.247 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Ge2 is Constrained at 0.247 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_a is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_b is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_c is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_d is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_i is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_j is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_l is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_m is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_n is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_o is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_p is Constrained at 0.510 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Sb2_q is Constrained at 0.510 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 44 Note
Author's comment: all these alerts are due to the mixed cation site 24g.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
Author's comment: ADDSYM was done separately without assuming shared positions, no higher symmetry was found.
PLAT984_ALERT_1_G The Co-f'= 0.191 Deviates from the B&C-Value 0.120 Check
PLAT984_ALERT_1_G The Ge-f'= 0.287 Deviates from the B&C-Value 0.182 Check
PLAT984_ALERT_1_G The Sb-f'= 0.054 Deviates from the B&C-Value -0.222 Check
PLAT984_ALERT_1_G The Te-f'= -0.051 Deviates from the B&C-Value -0.345 Check
PLAT985_ALERT_1_G The Ge-f''= 0.361 Deviates from the B&C-Value 0.364 Check
PLAT985_ALERT_1_G The Sb-f''= 2.071 Deviates from the B&C-Value 2.087 Check
PLAT985_ALERT_1_G The Te-f''= 2.218 Deviates from the B&C-Value 2.233 Check
Author's comment: The dispersion correction terms were taken from the NIST database, the deviations from checkcif's values are very small.

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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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
31 **ALERT level G** = General information/check it is not something unexpected

Checkcif Report

Datablock: FFSM21B_matrix

```
Bond precision:      = 0.0000 A                    Wavelength=0.29460
Cell:         a=4.2348(11)   b=4.2348(11)   c=10.373(3)
              alpha=90       beta=90        gamma=120
Temperature: 293 K
                    Calculated                        Reported
Volume              161.10(11)                        161.10(11)
Space group         R 3 m                             R 3 m :h
Hall group          R 3 -2"                           R 3 -2"
Moiety formula      Ge2.31 Sb0.46 Te3                 ?
Sum formula         Ge2.31 Sb0.46 Te3                 Ge0.77 Sb0.15 Te
Mr                  606.56                            202.19
Dx,g cm-3           6.252                             6.252
Z                   1                                 3
Mu (mm-1)           9.051                             9.051
F000                253.4                             253.4
F000'               252.76
h,k,lmax            7,7,18                            7,7,18
Nref                283[ 143]                         871
Tmin,Tmax           0.997,0.999                       0.450,1.000
Tmin'               0.995
Correction method= # Reported T Limits: Tmin=0.450
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 6.09/3.08    Theta(max)= 15.361
R(reflections)= 0.0314( 871)       wR2(reflections)= 0.0885( 138)
S = 1.055             Npar= 9
```

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.320
From the CIF: _refine_ls_abs_structure_Flack_su 0.040

Author's comment: As the refinement already takes into accound a 4-component twin, additional inversion twinning renders the refinement unstable. Also, the calculation of the Flack parameter is not reliable in multi-component twins. It is clear that inversion twinning is present, because twinning occurs are a consequence of a phase transition upon cooling a Fm-3m high-temperature phase.

PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms … Please Check

Author's comment: This is a consequence of mixed atom sites in a disordered compound.

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

Author's comment: synchrotron radiation, μ calculated with NIST database.

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info

Author's comment: correct.

PLAT021_ALERT_4_G Ratio Unique / Expected Reflections too High ... 6.091
Author's comment: This is due to a SHELX HKLF5 refinement.
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.33 Ratio
Author's comment: Z = 3 was chosen as it is a rhombohedral structure (hexagonal setting) with 3 layers per unit cell. This standard is nit detected by checkcif due to the cation disorder.
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag Ka .. 0.2946 Ang.
Author's comment: correct, synchrotron radiation.
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
Author's comment: mixed cation site.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
Author's comment: correct, measurement at room temperature.
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1 is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >Ge1 is Constrained at 0.769 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_a is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_b is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_c is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_d is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_e is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_f is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_* is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_* is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_* is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_* is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_* is Constrained at 0.154 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Sb1_* is Constrained at 0.154 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 18 Note
Author's comment: all these alerts are due to the mixed cation site.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
Author's comment: ADDSYM was done separately without assuming shared positions, no higher symmetry was found. The space group choice is confirmed by the cations' z parameter which significantly deviates from 0.
PLAT984_ALERT_1_G The Ge-f'= 0.287 Deviates from the B&C-Value 0.182 Check
PLAT984_ALERT_1_G The Sb-f'= 0.054 Deviates from the B&C-Value -0.222 Check
PLAT984_ALERT_1_G The Te-f'= -0.051 Deviates from the B&C-Value -0.345 Check
PLAT985_ALERT_1_G The Ge-f''= 0.361 Deviates from the B&C-Value 0.364 Check
PLAT985_ALERT_1_G The Sb-f''= 2.071 Deviates from the B&C-Value 2.087 Check
PLAT985_ALERT_1_G The Te-f''= 2.218 Deviates from the B&C-Value 2.233 Check
Author's comment: The dispersion correction terms were taken from the NIST database, the deviations from checkcif's values are very small.

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