checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 250422a_2m_a

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: 250422a_2m_a

Bond precision: C-C = 0.0088 A Wavelength=0.71073

Cell: a=10.8448(6) b=11.3293(6) c=13.4356(8)
alpha=105.810(2) beta=105.661(2) gamma=100.719(2)
Temperature: 173 K

	Calculated	Reported
Volume	1468.10(15)	1468.10(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H96 Ge2 K2 O2 Si8	?
Sum formula	C40 H96 Ge2 K2 O2 Si8	C6.67 H16 Ge0.33 K0.33 O0.33 Si1.33
Mr	1057.31	176.21
Dx,g cm-3	1.196	1.196
Z	1	6
Mu (mm-1)	1.357	1.357
F000	566.0	566.0
F000'	567.43	
h,k,lmax	12,13,15	12,13,15
Nref	5193	5185
Tmin,Tmax	0.850,0.873	0.533,0.679
Tmin'	0.762	

Correction method= # Reported T Limits: Tmin=0.533 Tmax=0.679
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.050

R(reflections)= 0.0624(4913) wR2(reflections)= 0.1666(5185)

S = 1.248 Npar= 256

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

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.133
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C40 H96 Ge2 K2 O2 Si8
             Rep.: C6.67 H16 Ge0.33 K0.33 O0.33 Si1.33
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.0 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         K1 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00883 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.377 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.596          8 Report
              -1  1  0,   0  1  0,  -1  0  1,   1  0  1,   2  8  7,   4  2 11,
              -1  6 11, -10 -2 13,
PLAT977_ALERT_2_C Check Negative Difference Density on H8C       .      -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H12A      .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15A      .      -0.32 eA-3
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Alert level G

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CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z    6
          From the CIF: _chemical_formula_sum  C6.67 H16 Ge0.33 K0.33 O0.33 Si1.3
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         40.02     40.00    0.02
          H         96.00     96.00    0.00
          Ge         1.98      2.00   -0.02
          K          1.98      2.00   -0.02
          O          1.98      2.00   -0.02
          Si         7.98      8.00   -0.02
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.133 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.167 Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.002 Degree
PLAT303_ALERT_2_G Full Occupancy Atom H10B      with # Connections       2.00 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.10 Ratio
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: K1       --K1        ..       4.50 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      41.00 Deg.
             K1   -C10  -H10B    2_667   1_555   1_555 ......     #  111 Check
PLAT793_ALERT_4_G Model has Chirality at C1          (Centro SpGr)          R Verify
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        92% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
              -1  0  1,   1  0  1,   0  1  0,  -1  1  0,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.095 Note
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             Predicted wR2: Based on SigI**2  5.38 or SHELX Weight 13.35
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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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
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 02/02/2025; check.def file version of 02/02/2025

Datablock 250422a_2m_a - ellipsoid plot