checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 250807_byx_0806_bn

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: 250807_byx_0806_bn

```
Bond precision:   Si- C = 0.0034 A         Wavelength=1.34139

Cell:             a=16.7818(12)     b=6.9005(5)         c=21.8834(14)
                  alpha=90          beta=108.776(2)     gamma=90
Temperature:      170 K

                  Calculated                  Reported
Volume            2399.3(3)                   2399.3(3)
Space group       P 21/c                      P 1 21/c 1
Hall group        -P 2ybc                     -P 2ybc
Moiety formula    C16 H42 Ge Si4              C16 H42 Ge Si4
Sum formula       C16 H42 Ge Si4              C16 H42 Ge Si4
Mr                419.47                      419.44
Dx,g cm-3         1.161                       1.161
Z                 4                           4
Mu (mm-1)         2.364                       2.425
F000              904.0                       904.0
F000'             902.09
h,k,lmax          21,8,28                     21,8,28
Nref              5528                        5466
Tmin,Tmax         0.865,0.886                 0.569,0.752
Tmin'             0.483

Correction method= # Reported T Limits: Tmin=0.569 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.989            Theta(max)= 60.856

                                                    wR2(reflections)=
R(reflections)= 0.0501( 4361)                       0.1327( 5466)
S = 1.128                  Npar= 264
```

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

```
PLAT051_ALERT_1_C Mu(calc) and Mu(cif) Ratio Differs from 1.0 by .       2.52 %
PLAT213_ALERT_2_C Atom C4A            has ADP max/min Ratio .....        3.5 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       4.1 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Si04 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  Ge1      --H1A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  Ge1      --H1B      .     Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         8 Report
              -3  1  3,   2  0  4,  -6  2  8,   8  0  8, -19  2 13, -19  1 14,
              -7  5 20,  -6  0 26,
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        11 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records         1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for SecondPar    0.0200 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0100 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)       24% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H1B      ..H10C     .      2.06 Ang.
                                                     x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H7A      ..H2D      .      2.07 Ang.
                                                     x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H15C     ..H2C      .      2.10 Ang.
                                                     x,y,z  =     1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        8 Note
              Si03    Si04    Si05    Si06    H2AA    H2AB    H3AA    H3AB
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       26 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        54 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        1 Note
               -3  1  3,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     2.228 Note
              Predicted wR2: Based on SigI**2  5.96 or SHELX Weight 11.77
PLAT984_ALERT_1_G The  C-f'=    0.0148 Deviates from the B&C-Value    0.0137 Check
```

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

   3 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
  7 ALERT type 3 Indicator that the structure quality may be low
  6 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 04/06/2025; check.def file version of 30/05/2025

Datablock 250807_byx_0806_bn - ellipsoid plot