checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 250925a_0m_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: 250925a_0m_a

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Bond precision:   C-C = 0.0037 A          Wavelength=0.71073

Cell:           a=12.0180(3)       b=14.4718(4)       c=16.6526(4)
                alpha=113.767(1)   beta=104.872(1)    gamma=90.080(1)
Temperature:    173 K

                 Calculated                 Reported
Volume           2543.78(12)                2543.78(11)
Space group      P -1                       P -1
Hall group       -P 1                       -P 1
Moiety formula   C32 H82 Ge2 K2 Si8         C32 H82 Ge2 K2 Si8
Sum formula      C32 H82 Ge2 K2 Si8         C32 H82 Ge2 K2 Si8
Mr               915.12                     915.07
Dx,g cm-3        1.195                      1.195
Z                2                          2
Mu (mm-1)        1.554                      1.554
F000             976.0                      976.0
F000'            978.79
h,k,lmax         15,18,21                   15,18,21
Nref             10803                      10789
Tmin,Tmax        0.830,0.856                0.644,0.747
Tmin'            0.733

Correction method= # Reported T Limits: Tmin=0.644 Tmax=0.747
AbsCorr = MULTI-SCAN
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Data completeness= 0.999 Theta(max)= 26.732

R(reflections)= 0.0391(8733) wR2(reflections)= 0.1005(10789)

S = 1.121 Npar= 429

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

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si7 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  Ge1      --H1       .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  Ge2      --H2       .     Please Check
PLAT601_ALERT_2_C Unit-Cell Contains Solvent Accessible VOIDS .LE.         35 Ang**3
PLAT910_ALERT_3_C Missing FCF Reflection(s) Below Theta(Min)[Deg]=       2.21 Note
                1  0  0,   0  1  0,   0 -1  1,  -1  0  1,   0  0  1,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          9 Report
                0  2  0,   1 -2  1,  -4  0  1,  -3  0  1,  -2  0  1,   1  0  1,
                3  0  1,   0 -2  2,   0  0  2,
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Alert level G

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PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT303_ALERT_2_G Full Occupancy Atom H1        with # Connections       2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H2        with # Connections       2.00 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: K1       --K1        ..       4.18 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: K2       --K2        ..       4.16 Ang.
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                0  2  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          7 Note
               -1  0  1,   1  0  1,   0  0  2,   0  2  0,   1 -2  1,   3  0  1,
                0 -2  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.785 Note
             Predicted wR2: Based on SigI**2  5.63 or SHELX Weight  8.97
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
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   1 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

Datablock 250925a_0m_a - ellipsoid plot