checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: compound3

```
Bond precision:    C-C = 0.0086 A              Wavelength=0.71075

Cell:           a=12.6367(7)          b=16.9170(6)      c=20.4887(10)
                alpha=91.3815(14)  beta=105.252(2)  gamma=109.642(3)
Temperature:  103 K

                   Calculated                    Reported
Volume             3949.2(3)                     3949.2(3)
Space group        P -1                          P -1
Hall group         -P 1                          -P 1
                   C62 H108 Cl4 Ge2 Si9, C4   C62 H108 Cl4 Ge2 Si9, C4
Moiety formula     H8 O                          H8 O
Sum formula        C66 H116 Cl4 Ge2 O Si9     C66 H116 Cl4 Ge2 O Si9
Mr                 1465.42                       1465.37
Dx,g cm-3          1.232                         1.232
Z                  2                             2
Mu (mm-1)          1.070                         1.070
F000               1556.0                        1556.0
F000'              1559.52
h,k,lmax           15,20,24                      15,20,24
Nref               14713                         14641
Tmin,Tmax          0.938,0.958                   0.939,0.958
Tmin'              0.938

Correction method= # Reported T Limits: Tmin=0.939 Tmax=0.958
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 25.500

R(reflections)= 0.0683( 10301)     wR2(reflections)= 0.1359( 14641)

S = 1.117                   Npar= 767
```

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

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.84 Report
PLAT213_ALERT_2_C Atom C68          has ADP max/min Ratio .....          3.4 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range       3.7 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range       4.3 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C28 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C64 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00864 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        35 Ang3
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Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     15.58 Why ?
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..        4% Note
PLAT398_ALERT_2_G Deviating  C-O-C  Angle from 120 Deg for O1          106.9 Degree
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
          C4 H8 O
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         5 Note
```

```
   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
   6 ALERT level G = General information/check it is not something unexpected

   1 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
   3 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: compound5

```
Bond precision:   C-C = 0.0085 A          Wavelength=0.71075

Cell:          a=11.6792(2)      b=15.7581(3)      c=24.7906(5)
               alpha=76.264(1)   beta=88.080(1)   gamma=70.251(1)
Temperature:   103 K
```

	Calculated	Reported
Volume	4165.89(14)	4165.89(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H108 Cl2 Ge2 Si8, 2(C6 H6)	C62 H108 Cl2 Ge2 Si8, 2 (C6 H6)
Sum formula	C74 H120 Cl2 Ge2 Si8	C74 H120 Cl2 Ge2 Si8
Mr	1450.55	1450.49
Dx,g cm-3	1.156	1.156
Z	2	2
Mu (mm-1)	0.937	0.937
F000	1548.0	1548.0
F000'	1550.78	
h,k,lmax	13,18,29	13,18,29
Nref	14665	14555
Tmin,Tmax	0.914,0.972	0.914,0.972
Tmin'	0.911	

Correction method= # Reported T Limits: Tmin=0.914 Tmax=0.972
AbsCorr = MULTI-SCAN

Data completeness= 0.992   Theta(max)= 25.000

R(reflections)= 0.0637(13024)   wR2(reflections)= 0.1311(14555)

S = 1.289   Npar= 805

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
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of   C67 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C68 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   3.0 Note
PLAT331_ALERT_2_C Small Average Phenyl   C-C Dist. C69   -C71_a   1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00849 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .   32 Ang3

⚪ Alert level G
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical   ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   10.84 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.001 Degree
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...   3 Note

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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
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   6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   4 **ALERT level G** = General information/check it is not something unexpected

```
2 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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 13/08/2017; check.def file version of 27/07/2017

NOMOVE FORCED

Prob = 50
Temp = 103

-36 Y

PLATON-Oct 22 15:12:59 2017 - (70316)

Z -93   compound3 P -1   R = 0.07   RES=   0   -9 X

NOMOVE FORCED

Prob = 50
Temp = 103

71 Y

PLATON-Oct 22 15:13:04 2017 - (70316)

Z 123   compound5 P -1   R = 0.06   RES=   0   -23 X