checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 30r5-006

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: 30r5-006

```
Bond precision:   Ga-Cl = 0.0041 A          Wavelength=0.71073

Cell:             a=12.3962(8)      b=7.1340(5)          c=42.127(3)
                  alpha=90          beta=93.799(2)       gamma=90
Temperature:      298 K
```

	Calculated	Reported
Volume	3717.3(4)	3717.3(4)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	Hg18 Se8, 8(Cl4 Ga)	Hg9 Se4, 4(Cl4 Ga)
Sum formula	Cl32 Ga8 Hg18 Se8	Cl16 Ga4 Hg9 Se4
Mr	5934.46	2967.23
Dx,g cm-3	5.302	5.302
Z	2	4
Mu (mm-1)	44.924	44.923
F000	5008.0	5008.0
F000'	4948.09	
h,k,lmax	16,9,54	16,9,54
Nref	4269	4250
Tmin,Tmax	0.475,0.638	0.015,0.047
Tmin'	0.441	

```
Correction method= # Reported T Limits: Tmin=0.015 Tmax=0.047
AbsCorr = MULTI-SCAN

Data completeness= 0.996            Theta(max)= 27.464

R(reflections)= 0.0463( 3692)                    wR2(reflections)=
                                                 0.1213( 4250)
S = 1.137                  Npar= 150
```

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

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: Cl32 Ga8 Hg18 Se8
             Rep.: Cl16 Ga4 Hg9 Se4
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: Hg18 Se8, 8(Cl4 Ga)
             Rep.: Hg9 Se4, 4(Cl4 Ga)
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Ga1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Ga2 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.859 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          8 Report
               1  1  1,  -2  0  2,  -4  0  4,  -4  0  6,   6  0 30,   3  1 31,
              -2  2 34,   0  0 36,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.72Ang From Se2              1.69 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.80Ang From Hg4              1.51 eA-3
PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on       Hg5      -1.28 eA-3
```

Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     151.49 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Hg5       (II)      .       1.66 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ga1       (III)     .       3.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ga2       (III)     .       3.06 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
               0  0  2,   0  0  4,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          9 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          5 Note
              -2  2 34,   0  0  4,   0  0 36,   3  1 31,   6  0 30,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.856 Note
             Predicted wR2: Based on SigI**2  4.25 or SHELX Weight 10.67
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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
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

3 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
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
5 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 02/02/2025; check.def file version of 02/02/2025

Datablock 30r5-006 - ellipsoid plot