checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3_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: 3_a

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Bond precision:   S-Mg = 0.0130 A          Wavelength=0.71073

Cell:              a=16.7154(5)      b=16.7154(5)      c=7.4147(3)
                   alpha=90          beta=90           gamma=120
Temperature:       297 K
```

	Calculated	Reported
Volume	1794.15(13)	1794.15(13)
Space group	P -6	P -6
Hall group	P -6	P -6
Moiety formula	2(Ga6 La Mg3 S15), Ga6 La Mg6 S18, 6(Mg)	?
Sum formula	Ga18 La3 Mg18 S48	Ga18 La3 Mg18 S48
Mr	3648.15	3648.16
Dx,g cm-3	3.376	3.376
Z	1	1
Mu (mm-1)	9.949	9.949
F000	1713.0	1713.0
F000'	1722.95	
h,k,lmax	20,20,8	20,20,8
Nref	2360[1184]	2340
Tmin,Tmax	0.368,0.503	0.001,0.092
Tmin'	0.316	

```
Correction method= # Reported T Limits: Tmin=0.001 Tmax=0.092
AbsCorr = 'N

Data completeness= 1.98/0.99        Theta(max)= 25.342

R(reflections)= 0.0423( 1921)                    wR2(reflections)=
                                                 0.1283( 2340)
S = 1.184                  Npar= 152
```

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

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 Numerical Mu From Formula
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.78 Note

Alert level G

ABSTY01_ALERT_1_G Extra text has been found in the _exptl_absorpt_correction_type field, which should be only a single keyword. A literature citation should be included in the _exptl_absorpt_process_details field.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.53 Why ?
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem 20 86 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group P-6m2 Check
Check Model Parameter Symmmetry for Reflection Data Support
PLAT794_ALERT_5_G Tentative Bond Valency for La1 (III) . 2.53 Info
PLAT794_ALERT_5_G Tentative Bond Valency for La2 (III) . 2.32 Info
PLAT794_ALERT_5_G Tentative Bond Valency for La3 (III) . 2.49 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ga1 (III) . 2.95 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ga2 (III) . 2.91 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ga3 (III) . 2.92 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.13 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (1 0 0) Est.d BASF 0.57 Check

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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
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
1 ALERT type 4 Improvement, methodology, query or suggestion
8 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 06/07/2023; check.def file version of 30/06/2023

Datablock 3_a - ellipsoid plot