

Structure factors have been supplied for datablock(s) mjr\_ra\_412\_300k

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	Si- O = 0.0010 Å	Wavelength=0.68890	
Cell:	a=8.2725(1) alpha=90	b=8.2725(1) beta=90	c=8.2725(1) gamma=90
Temperature:	300 K		
	Calculated	Reported	
Volume	566.12(2)	566.12(2)	
Space group	P 21 3	P 21 3	
Hall group	P 2ac 2ab 3	P 2ac 2ab 3	
Moiety formula	O4 Si, Cl, O, 7(Li)	Cl1 Li7 O5 Si1	
Sum formula	Cl Li7 O5 Si	Cl Li7 O5 Si	
Mr	192.12	192.12	
Dx, g cm-3	2.254	2.254	
Z	4	4	
Mu (mm-1)	0.744	0.760	
F000	368.0	368.0	
F000'	369.06		
h,k,lmax	12,12,12	12,12,12	
Nref	710[ 415]	726	
Tmin,Tmax	0.977,0.985	0.574,1.000	
Tmin'	0.977		

Data completeness= 1.75/1.02                      Theta(max)= 31.892

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R(reflections)= 0.0229( 718)      wR2(reflections)=
S = 1.136                        0.0605( 726)
Npar= 48
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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.

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#### **Alert level B**

PLAT306\_ALERT\_2\_B Isolated Oxygen Atom (H-atoms Missing ?) ..... 03 Check

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#### **Alert level C**

STRVA01\_ALERT\_4\_C                      Flack parameter is too small  
                    From the CIF: \_refine\_ls\_abs\_structure\_Flack    -0.250  
                    From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su    0.050  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 2.25 Report

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#### **Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
                    not performed for this radiation type.  
PLAT042\_ALERT\_1\_G Calc. and Reported Moiety Formula Strings Differ            Please Check  
PLAT092\_ALERT\_4\_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka            0.68890 Ang.  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 6 )            100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 7 )            100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 2 )            0.33 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 3 )            0.33 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 6 )            0.28 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 7 )            0.05 Check  
PLAT870\_ALERT\_4\_G ALERTS Related to Twinning Effects Suppressed ..            ! Info  
PLAT916\_ALERT\_2\_G Hooft y and Flack x Parameter Values Differ by .            0.33 Check  
PLAT931\_ALERT\_5\_G CIFcalcFCF Twin Law ( 0 1-1)            Est.d BASF            0.34 Check  
PLAT961\_ALERT\_5\_G Dataset Contains no Negative Intensities .....            Please Check

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
13 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
9 ALERT type 4 Improvement, methodology, query or suggestion  
2 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. 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.

