checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2LiCl

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: 2LiCl

```
Bond precision:  C-C = 0.0079 A          Wavelength=0.71073

Cell:           a=27.6951(9)    b=9.7813(3)         c=14.2023(5)
                alpha=90        beta=103.951(3)     gamma=90
Temperature:    103 K
```

	Calculated	Reported
Volume	3733.8(2)	3733.8(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C30 H22 Al Cl F10 Li P), 4(C3.50 H4)	2(C30 H22 Al Cl F10 Li P), 4(C3.50 H4)
Sum formula	C81 H68 Al2 Cl2 F20 Li2 P2	C40.50 H34 Al Cl F10 Li P
Mr	1622.03	811.01
Dx,g cm-3	1.443	1.443
Z	2	4
Mu (mm-1)	0.249	0.249
F000	1660.0	1660.0
F000’	1662.29	
h,k,lmax	33,11,17	33,11,16
Nref	6758	6745
Tmin,Tmax	0.985,0.993	0.677,1.000
Tmin’	0.983	

```
Correction method= # Reported T Limits: Tmin=0.677 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 25.250

R(reflections)= 0.0841( 5830)     wR2(reflections)= 0.2188( 6745)

S = 1.155                 Npar= 531
```

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 .... 2.58 Report
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.7 Note
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C18 -C23 1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C24 -C29 1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00792 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 9.541 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.405 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 11 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

---

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C40.5 H34 Al1 Cl1 F10 Li1 P1
Atom count from _chemical_formula_moiety:C74 H60 Al2 Cl2 F20 Li2 P2
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 16.39 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of C37 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C38 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C39 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C40 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C43 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H38 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H39 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H40 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43B Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 15 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT898_ALERT_4_G Second Reported H-M Symbol in CIF Ignored ..... ! Check
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 70% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

---

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
25 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
18 ALERT type 4 Improvement, methodology, query or suggestion
1 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 07/08/2019; check.def file version of 30/07/2019

Datablock 2LiCl - ellipsoid plot