checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0083_0m

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: mo_b0083_0m

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=12.2143(5) b=12.0951(6) c=14.2648(7)
alpha=90 beta=113.848(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1927.46(16)	1927.46(16)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C36 H58 Fe2 Li2 N2 O Si2	0.5(C36 H58 Fe2 Li2 N2 O Si2)
Sum formula	C36 H58 Fe2 Li2 N2 O Si2	C18 H29 Fe Li N O0.50 Si
Mr	716.60	358.30
Dx,g cm-3	1.235	1.235
Z	2	4
Mu (mm-1)	0.843	0.843
F000	764.0	764.0
F000’	765.87	
h,k,lmax	16,15,18	16,15,18
Nref	9300[4869]	9291
Tmin,Tmax	0.788,0.862	0.267,0.320
Tmin’	0.627	

Correction method= # Reported T Limits: Tmin=0.267 Tmax=0.320
AbsCorr = MULTI-SCAN

Data completeness= 1.91/1.00 Theta(max)= 27.999

R(reflections)= 0.0180(9109) wR2(reflections)= 0.0527(9291)

S = 1.129 Npar= 438

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 B

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check

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Alert level C

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ... 4.8 Ratio
PLAT313_ALERT_2_C Oxygen with three covalent bonds (rare) ..... O1 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 81.60

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.50 Ratio
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 2 Report
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 4 Note
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C3 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C19 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 3 Report

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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
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **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
9 ALERT type 3 Indicator that the structure quality may be low
1 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*, 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 21/06/2015; check.def file version of 21/06/2015

Datablock mo_b0083_0m - ellipsoid plot

