

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: cu_b0089_0m

Bond precision:	C-C = 0.0050 A	Wavelength=1.54178	
Cell:	a=10.8656(4)	b=10.9386(5)	c=19.3571(8)
	alpha=90	beta=102.672(2)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2244.64(16)	2244.64(16)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C32 H78 Li8 N6 O6	C16 H39 Li4 N3 O3	
Sum formula	C32 H78 Li8 N6 O6	C16 H39 Li4 N3 O3	
Mr	698.52	349.26	
Dx,g cm-3	1.033	1.034	
Z	2	4	
Mu (mm-1)	0.520	0.520	
F000	768.0	768.0	
F000'	770.00		
h,k,lmax	13,13,23	13,13,23	
Nref	4179	4026	
Tmin,Tmax	0.872,0.892	0.650,0.754	
Tmin'	0.834		

Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.963 Theta(max)= 68.998

R(reflections)= 0.1116(3592) wR2(reflections)= 0.4055(4026)

S = 1.995 Npar= 280

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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.41 Report
PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.23 eA-3

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.965 Why?
PLAT082_ALERT_2_C High R1 Value 0.11 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.54 Report
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.005 Ang.
PLAT350_ALERT_3_C Short C-H (X0.96,N1.08A) C1 - H1B 0.81 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C1 - H1A .. 1.15 Ang.

Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 12% Note
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C1 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 4 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.26 Ratio

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

