

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sv0468

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: sv0468

Bond precision: C-C = 0.0031 A Wavelength=1.54186

Cell: a=10.2172(3) b=17.3386(6) c=34.6955(9)
 alpha=90 beta=90.735(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	6145.9(3)	6145.9(3)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C24 H42 Fe Li N2 P3, 0.5(C6 H14)	C24 H42 Fe Li N2 P3, 0.5(C6 H14)
Sum formula	C27 H49 Fe Li N2 P3	C27 H49 Fe Li N2 P3
Mr	557.38	557.38
Dx, g cm-3	1.205	1.205
Z	8	8
Mu (mm-1)	5.526	5.526
F000	2392.0	2392.0
F000'	2394.37	
h,k,lmax	12,20,42	12,20,41
Nref	5717	5340
Tmin,Tmax	0.428,0.833	0.539,0.834
Tmin'	0.323	

Correction method= # Reported T Limits: Tmin=0.539 Tmax=0.834
AbsCorr = INTEGRATION

Data completeness= 0.934 Theta(max)= 68.990

R(reflections)= 0.0309(4654) wR2(reflections)= 0.0733(5340)

S = 1.021 Npar= 318

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

PLAT029_ALERT_3_B	_diffrn_measured_fraction_theta_full value Low .	0.942	Note
PLAT911_ALERT_3_B	Missing # FCF Refl Between THmin & STh/L= 0.600	322	Report

Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	8.50	Why ?
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
PLAT793_ALERT_4_G	The Model has Chirality at P1 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at P3 (Centro SPGR)	S	Verify
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	52	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	5	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
0 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
4 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* 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 13/08/2017; check.def file version of 27/07/2017

