

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) c2c

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: c2c

Bond precision: C-C = 0.0039 Å Wavelength=0.71073

Cell: a=23.29(2) b=13.532(9) c=21.12(3)
 alpha=90 beta=121.01(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	5705(10)	5705(10)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C40 H96 K4 Li4 N4 O10	C20 H48 K2 Li2 N2 O5
Sum formula	C40 H96 K4 Li4 N4 O10	C20 H48 K2 Li2 N2 O5
Mr	977.37	488.68
Dx,g cm-3	1.138	1.138
Z	4	8
Mu (mm-1)	0.360	0.360
F000	2128.0	2128.0
F000'	2131.98	
h,k,lmax	29,17,26	0,0,0
Nref	6229	6223
Tmin,Tmax	0.914,0.927	0.595,0.647
Tmin'	0.914	

Correction method= # Reported T Limits: Tmin=0.595 Tmax=0.647
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.999

R(reflections)= 0.0428(5033) wR2(reflections)= 0.0907(6223)

S = 1.070 Npar= 377

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 A

PLAT881_ALERT_1_A No Datum for _diffrn_reflns_av_R_equivalents ... Please Do !

Alert level C

PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large 0.030 Ang.
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.8 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 8.964 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note

Alert level G

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
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 10.39 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 14 Note
PLAT300_ALERT_4_G Atom Site Occupancy of O3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9AA Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9AB Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9BC Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9BD Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12E Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12F Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 10% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 4 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.60 Ratio
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: K2 --K2 .. 4.99 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 209 Check
C11B -O3B -C11 1.555 1.555 1.555 27.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 275 Check
O4 -C13 -LI2 1.555 1.555 2.656 40.45 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 319 Check
H9AA -C9 -H9BC 1.555 1.555 1.555 17.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 322 Check
H9AB -C9 -H9BD 1.555 1.555 1.555 18.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 324 Check
O3 -C9 -O3B 1.555 1.555 1.555 18.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 392 Check
O3B -C11B -O3 1.555 1.555 1.555 18.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 397 Check
C12B -C11B -C12 1.555 1.555 1.555 39.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 405 Check
C11 -C11B -C12B 1.555 1.555 1.555 28.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 423 Check
C11 -C12B -C11B 1.555 1.555 1.555 24.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 441 Check

C12B -C12 -C11	1.555	1.555	1.555	39.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				445 Check
C11 -C12 -C11B	1.555	1.555	1.555	30.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				467 Check
O3 -C11 -O3B	1.555	1.555	1.555	14.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				474 Check
C11B -O3 -C11	1.555	1.555	1.555	30.80 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #				10 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...				2 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities				Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.				5 Info

1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
46 **ALERT level G** = General information/check it is not something unexpected

4 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
4 **ALERT type 2** Indicator that the structure model may be wrong or deficient
5 **ALERT type 3** Indicator that the structure quality may be low
38 **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 23/04/2018; check.def file version of 23/04/2018

