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: Jiang20220201

Bond precision: C-C = 0.0030 A Wavelength=1.54187

Cell: a=10.5397(3) b=12.5200(3) c=20.9594(5)
alpha=78.167(6) beta=81.725(6) gamma=65.527(5)
Temperature: 123 K

	Calculated	Reported
Volume	2458.36(15)	2458.36(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C48 H64 B2 Li2 O8 [+ solvent]	C48 H64 B2 Li2 O8,0.5(C6 H14)
Sum formula	C48 H64 B2 Li2 O8 [+ solvent]	C51 H71 B2 Li2 O8
Mr	804.49	847.57
Dx,g cm-3	1.087	1.145
Z	2	2
Mu (mm-1)	0.560	0.582
F000	864.0	914.0
F000'	866.46	
h,k,lmax	12,15,25	12,15,25
Nref	9009	8833
Tmin,Tmax	0.875,0.943	0.734,1.000
Tmin'	0.875	

Correction method= # Reported T Limits: Tmin=0.734 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.980 Theta(max)= 68.253

R(reflections)= 0.0631(7647) wR2(reflections)= 0.1749(8833)

S = 1.065 Npar= 553

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 G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C51 H71 B2 Li2 O8
           Atom count from the _atom_site data:  C48 H64 B2 Li2 O8
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C51 H71 B2 Li2 O8
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        102.00     96.00    6.00
           H        142.00    128.00   14.00
           B          4.00      4.00    0.00
           Li         4.00      4.00    0.00
           O         16.00     16.00    0.00
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT014_ALERT_1_G No       _shelx_fab_checksum Found in CIF ......     Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.10 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        245 A**3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      41.54 Deg.
             O3   -B2   -LI1     1_555   1_555   1_555 ......     #   14 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      41.40 Deg.
             O4   -B2   -LI2     1_555   1_555   1_555 ......     #   20 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      41.37 Deg.
             O8   -C47  -LI2     1_555   1_555   1_555 ......     #  285 Check
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   5 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
   0 ALERT type 3 Indicator that the structure quality may be low
   5 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 28/11/2022; check.def file version of 28/11/2022

Datablock Jiang20220201 - ellipsoid plot