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: mo_b0517_0m

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Bond precision:    C-C = 0.0017 A            Wavelength=0.71073

Cell:              a=15.696(3)      b=9.3886(17)        c=19.721(4)
                   alpha=90         beta=92.353(7)      gamma=90
Temperature:       100 K

                   Calculated                 Reported
Volume             2903.7(10)                 2903.8(10)
Space group        P 21/c                     P 1 21/c 1
Hall group         -P 2ybc                    -P 2ybc
Moiety formula     C22 H50 Li4 N2 O6          C22 H50 Li4 N2 O6
Sum formula        C22 H50 Li4 N2 O6          C22 H50 Li4 N2 O6
Mr                 466.40                     466.40
Dx,g cm-3          1.067                      1.067
Z                  4                          4
Mu (mm-1)          0.073                      0.073
F000               1024.0                     1024.0
F000'              1024.44
h,k,lmax           19,11,24                   19,11,24
Nref               5714                       5705
Tmin,Tmax          0.980,0.990                0.619,0.647
Tmin'              0.975

Correction method= # Reported T Limits: Tmin=0.619 Tmax=0.647
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.000

R(reflections)= 0.0358( 4797)     wR2(reflections)= 0.0915( 5705)

S = 1.058                    Npar= 340
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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 C
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             dull

Alert level G
PLAT343_ALERT_2_G Unusual sp?   Angle Range in Main Residue for   C21   Check
PLAT343_ALERT_2_G Unusual sp?   Angle Range in Main Residue for   C22   Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .   1.19 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #   46 Check
             O6   -C18 -LI4   1.555   1.555   1.555   42.48 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #   126 Check
             O3   -C8   -LI1   1.555   1.555   1.555   42.67 Deg.
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES ....   7 Note

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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
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   6 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 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
   3 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 11/08/2016; check.def file version of 04/08/2016