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_b0133_0m

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Bond precision:  C-Li = 0.0098 A         Wavelength=1.54178

Cell:            a=12.1310(3)    b=15.2270(4)       c=16.3851(4)
                 alpha=90        beta=92.206(2)     gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           3024.39(13)               3024.39(13)
Space group      P 21/n                    P 1 21/n 1
Hall group       -P 2yn                    -P 2yn
Moiety formula   C40 H104 Li16 N8 O11      C40 H104 Li16 N8 O11
Sum formula      C40 H104 Li16 N8 O11      C40 H104 Li16 N8 O11
Mr               984.35                    984.35
Dx,g cm-3        1.081                     1.081
Z                2                         2
Mu (mm-1)        0.561                     0.561
F000             1072.0                    1072.0
F000'            1074.87
h,k,lmax         14,18,19                  14,18,19
Nref             5731                      5646
Tmin,Tmax        0.898,0.928
Tmin'            0.839

Correction method= Not given

Data completeness= 0.985          Theta(max)= 69.986

R(reflections)= 0.0962( 4257)     wR2(reflections)= 0.3136( 5646)

S = 1.319                 Npar= 494
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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 A

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SHFSU01_ALERT_2_A  The absolute value of parameter shift to su ratio > 0.20
           Absolute value of the parameter shift to su ratio given   5.947
           Additional refinement cycles may be required.
PLAT080_ALERT_2_A Maximum Shift/Error ..........................       5.95 Why ?
PLAT241_ALERT_2_A High   'MainMol' Ueq as Compared to Neighbors of       C17A Check
PLAT351_ALERT_3_A Long   C-H (X0.96,N1.08A)  C18      - H18A     ..       1.33 Ang.
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H17A     ..H17D             1.14 Ang.
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H17A     ..H17E             1.01 Ang.
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H17B     ..H17E             1.17 Ang.
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H17B     ..H17F             1.25 Ang.
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H17C     ..H17D             1.43 Ang.
PLAT412_ALERT_2_A Short Intra XH3 .. XHn     H17C     ..H17F             0.79 Ang.
PLAT770_ALERT_2_A Suspect C-H Bond in CIF:  C18      --H18A      .       1.34 Ang.
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Alert level B

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DIFMN02_ALERT_2_B  The minimum difference density is < -0.1*ZMAX*1.00
           _refine_diff_density_min given =     -0.845
           Test value =     -0.800
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       0.97 eA-3
PLAT098_ALERT_2_B Large Reported Min.  (Negative) Residual Density      -0.85 eA-3
PLAT220_ALERT_2_B Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        7.0 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for   C17A     --C17B      .       10.5 s.u.
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        Li7 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        Li8 Check
PLAT412_ALERT_2_B Short Intra XH3 .. XHn     H17A     ..H17F             1.75 Ang.
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Alert level C

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DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT074_ALERT_1_C Occupancy Parameter = 0.0 for .................       CNT1 Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.31 Report
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .       CNT1 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .       CNT1 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       CNT1 Check
PLAT220_ALERT_2_C Non-Solvent  Resd 1  O   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        8.7 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N3       --C10A             0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3       --C11A             0.25 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O6B Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N3 Check
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C19      - H19B     ..       1.12 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C19      - H19C     ..       1.13 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        24 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        12 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for   N2       --C8A       .       5.8 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   N2       --C6        .       7.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   N3       --C10       .       7.0 s.u.
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PLAT230_ALERT_2_G Hirshfeld Test Diff for   N3       --C11       .        5.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of CnT1       Constrained at        0.0 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        32% Note
PLAT343_ALERT_2_G Unusual       sp?Angle Range in Main Residue for       C17A Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for        C18 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C19 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         29 Note
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.98010 Dev...       0.01 Ang.
              C12A     -H12D            1.555   1.555 ........     #  191 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      110.20 Dev...       1.20 Degree
              O6B     -C17B    -H17B       1.555  1.555  1.555     #  784 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      110.30 Dev...       1.30 Degree
              CNT1    -C17A    -H17D       1.555  1.555  1.555     #  789 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.35 Ratio
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        73 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        28 Note
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  11 ALERT level A = Most likely a serious problem - resolve or explain
   8 ALERT level B = A potentially serious problem, consider carefully
  16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  24 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  32 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
  11 ALERT type 4 Improvement, methodology, query or suggestion
   1 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

Datablock cu_b0133_0m - ellipsoid plot