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: 3167tri

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Bond precision:  O-Li = 0.0084 A         Wavelength=0.71073

Cell:             a=13.9966(5)     b=22.8582(8)     c=44.793(2)
                  alpha=90         beta=90          gamma=90
Temperature:      173 K

                 Calculated                Reported
Volume           14330.9(10)               14330.9(10)
Space group      P b c a                   P b c a
Hall group       -P 2ac 2ab                -P 2ac 2ab
Moiety formula   C40 H101.52 K4 Li4 O12 Si8 C40 H101.51 K4 Li4 O12 Si8
Sum formula      C40 H101.52 K4 Li4 O12 Si8 C40 H104 K4 Li4 O12 Si8
Mr               1183.62                   1186.11
Dx,g cm-3        1.097                     1.099
Z                8                         8
Mu (mm-1)        0.424                     0.424
F000             5100.2                    5120.0
F000'            5113.34
h,k,lmax         17,28,55                  17,28,55
Nref             14069                     14062
Tmin,Tmax        0.863,0.903               0.929,1.000
Tmin'            0.862

Correction method= # Reported T Limits: Tmin=0.929 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 25.999

R(reflections)= 0.0796( 9588)     wR2(reflections)= 0.1933( 14062)

S = 1.131                 Npar= 821
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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

```
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   2.009
           Additional refinement cycles may be required.
PLAT080_ALERT_2_A Maximum Shift/Error ..........................       2.01 Why ?
PLAT213_ALERT_2_A Atom C27B           has ADP max/min Ratio .....        5.3 prolat
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Alert level B

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PLAT213_ALERT_2_B Atom C29B           has ADP max/min Ratio .....        4.1 prolat
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Alert level C

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..      2.49 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT213_ALERT_2_C Atom C25A           has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C30B           has ADP max/min Ratio .....        4.0 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 1  O   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   Si6      --C16       .        5.4 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Si4      --C11              0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Si6      --C17              0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Si6      --C18              0.18 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         K2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si7 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si8 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H1C      ..H33A             2.05 Ang.
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C40 H104 K4 Li4 O12 Si8
           Atom count from _chemical_formula_moiety:C40 H101.51 K4 Li4 O12 Si8
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:C40 H104 K4 Li4 O12 Si8
           Atom count from the _atom_site data:  C40 H101.5200 K4 Li4 O12 Si8
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    8
          From the CIF: _chemical_formula_sum  C40 H104 K4 Li4 O12 Si8
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        320.00    320.00    0.00
          H        832.00    812.16   19.84
          K         32.00     32.00    0.00
          Li        32.00     32.00    0.00
          O         96.00     96.00    0.00
          Si        64.00     64.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         40 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      36.05 Why ?
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          4 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        29% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  1        169.52 Check
PLAT722_ALERT_1_G Angle   Calc      112.00, Rep      110.60 Dev...       1.40 Degree
             C28B    -C27B    -H27B       1.555  1.555  1.555     #  574 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      110.50 Dev...       1.50 Degree
             C27B    -C28B    -H28A       1.555  1.555  1.555     #  578 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      113.00 Dev...       2.00 Degree
             O10B    -C29B    -H29A       1.555  1.555  1.555     #  581 Check
PLAT722_ALERT_1_G Angle   Calc      113.00, Rep      110.50 Dev...       2.50 Degree
             C30B    -C29B    -H29B       1.555  1.555  1.555     #  586 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      111.60 Dev...       1.60 Degree
             C29B    -C30B    -H30A       1.555  1.555  1.555     #  587 Check
PLAT722_ALERT_1_G Angle   Calc      112.00, Rep      117.00 Dev...       5.00 Degree
             O11B    -C33B    -H33A       1.555  1.555  1.555     #  605 Check
PLAT722_ALERT_1_G Angle   Calc      112.00, Rep      108.00 Dev...       4.00 Degree
             O11B    -C33B    -H33B       1.555  1.555  1.555     #  606 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      108.90 Dev...       1.10 Degree
             H33A    -C33B    -H33B       1.555  1.555  1.555     #  608 Check
PLAT722_ALERT_1_G Angle   Calc      114.00, Rep      109.20 Dev...       4.80 Degree
             C34B    -C35B    -H35A       1.555  1.555  1.555     #  612 Check
PLAT722_ALERT_1_G Angle   Calc      113.00, Rep      122.80 Dev...       9.80 Degree
             C34B    -C35B    -H35B       1.555  1.555  1.555     #  613 Check
PLAT722_ALERT_1_G Angle   Calc      114.00, Rep      108.40 Dev...       5.60 Degree
             C36B    -C35B    -H35A       1.555  1.555  1.555     #  616 Check
PLAT722_ALERT_1_G Angle   Calc      114.00, Rep      115.40 Dev...       1.40 Degree
             C36B    -C35B    -H35B       1.555  1.555  1.555     #  617 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.90 Dev...       1.10 Degree
             C38B    -C39B    -H39A       1.555  1.555  1.555     #  631 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      111.30 Dev...       1.30 Degree
             C38B    -C39B    -H39B       1.555  1.555  1.555     #  632 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.80 Dev...       1.20 Degree
             C40B    -C39B    -H39A       1.555  1.555  1.555     #  635 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      112.20 Dev...       1.20 Degree
             O9A     -C25A    -H2         1.555  1.555  1.555     #  656 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      112.10 Dev...       1.10 Degree
             C26A    -C25A    -H2         1.555  1.555  1.555     #  660 Check
PLAT722_ALERT_1_G Angle   Calc      112.00, Rep      110.90 Dev...       1.10 Degree
             C25A    -C26A    -H3         1.555  1.555  1.555     #  661 Check
PLAT722_ALERT_1_G Angle   Calc      112.00, Rep      110.90 Dev...       1.10 Degree
             C33A    -C34A    -H19        1.555  1.555  1.555     #  709 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      113.20 Dev...       2.20 Degree
             C35A    -C34A    -H19        1.555  1.555  1.555     #  713 Check
PLAT722_ALERT_1_G Angle   Calc      112.00, Rep      110.60 Dev...       1.40 Degree
             C35A    -C34A    -H1D        1.555  1.555  1.555     #  714 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      112.80 Dev...       1.80 Degree
             C34A    -C35A    -H1E        1.555  1.555  1.555     #  715 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.90 Dev...       1.10 Degree
             C34A    -C35A    -H1F        1.555  1.555  1.555     #  716 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      108.80 Dev...       2.20 Degree
             O11A    -C36A    -H1H        1.555  1.555  1.555     #  723 Check
PLAT722_ALERT_1_G Angle   Calc      113.00, Rep      114.30 Dev...       1.30 Degree
             O12A    -C37A    -H37D       1.555  1.555  1.555     #  728 Check
PLAT722_ALERT_1_G Angle   Calc      112.00, Rep      113.20 Dev...       1.20 Degree
             C38A    -C39A    -H39D       1.555  1.555  1.555     #  735 Check
PLAT722_ALERT_1_G Angle   Calc      113.00, Rep      110.50 Dev...       2.50 Degree
             C40A    -C39A    -H39C       1.555  1.555  1.555     #  738 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.17 Ratio
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
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PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 470 Note

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

35 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
21 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
8 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 30/01/2018; check.def file version of 30/01/2018

Datablock 3167tri - ellipsoid plot