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_b1032_0m

```
Bond precision:   C-C = 0.0020 A            Wavelength=0.71073

Cell:             a=9.8606(18)     b=19.160(2)          c=20.638(3)
                  alpha=90         beta=91.536(6)       gamma=90
Temperature:      100 K

                  Calculated                 Reported
Volume            3897.7(10)                 3897.8(10)
Space group       P 21/c                     P 1 21/c 1
Hall group        -P 2ybc                    -P 2ybc
Moiety formula    C28 H68 Li4 O3 Si4         C28 H68 Li4 O3 Si4
Sum formula       C28 H68 Li4 O3 Si4         C28 H68 Li4 O3 Si4
Mr                592.94                     592.94
Dx,g cm-3         1.010                      1.010
Z                 4                          4
Mu (mm-1)         0.176                      0.176
F000              1312.0                     1312.0
F000'             1313.64
h,k,lmax          12,24,26                   12,24,26
Nref              8523                       8504
Tmin,Tmax         0.949,0.974                0.678,0.746
Tmin'             0.942

Correction method= # Reported T Limits: Tmin=0.678 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 27.000

R(reflections)= 0.0315( 7278)     wR2(reflections)= 0.0814( 8504)

S = 1.059                   Npar= 396
```

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

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for  Si3      --C11       ..        5.4 s.u.
```

Alert level G

```
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......    Please Check
PLAT303_ALERT_2_G Full Occupancy Atom H5A      with # Connections       2.00 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for         C5 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .     1.15 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       21 Check
            C5   -SI2  -LI4    1.555   1.555   1.555          44.69 Deg.
```

```
   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
   5 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 09/11/2017; check.def file version of 08/11/2017

NOMOVE FORCED

Prob = 50
Temp = 100

47 Y

PLATON-Nov 27 11:57:36 2017 - (70316)

Z 105   mo_b1032_OP 1 21/c 1   R = 0.03   RES=   0 -111 X