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: I

Bond precision: $S - P = 0.0287 \text{ A}$ Wavelength=$1.54056$

Cell:

\begin{align*}
\text{a} &= 10.51452(6) \\
\text{b} &= 10.51452(6) \\
\text{c} &= 6.59148(8) \\
\text{alpha} &= 90 \\
\text{beta} &= 90 \\
\text{gamma} &= 120
\end{align*}

Temperature: 298 K

Calculated vs. Reported

\begin{align*}
\text{Volume} &: 631.092(12) \quad 631.092(10) \\
\text{Space group} &: P 3 2 1 \quad P 3 2 1 \\
\text{Hall group} &: P 3 2" \quad P 3 2" \\
\text{Moiety formula} &: P2 S6, 4(Li) \quad P2 S6, 4(Li) \\
\text{Sum formula} &: Li4 P2 S6 \quad Li4 P2 S6 \\
\text{Mr} &: 282.06 \quad 282.07 \\
\text{Dx, g cm}^{-3} &: 2.227 \quad 2.230 \\
\text{Z} &: 3 \quad 3 \\
\text{Mu (mm}^{-1}) &: 17.600 \quad 17.929 \\
\text{F000} &: 414.0 \quad 0.0 \\
\text{F000'} &: 421.98 \\
\text{h, k, lmax} &: 13,13,8 \quad 8,8,6 \\
\text{Nref} &: 971[ 565] \quad 220 \\
\text{Tmin, Tmax} & \text{Not given}
\end{align*}

Correction method= Not given

Data completeness= 0.39/0.23 Theta(max) = 89.200

R(reflections) = wR2(reflections) =

\begin{align*}
\text{S} &= \quad \text{Npar}=\quad
\end{align*}

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

_REFI015_ALERT_1_C  _refine_ls_shift/su_max is missing
Maximum shift/s.u. ratio after final refinement cycle.
The following tests will not be performed
SHFSU_01

Alert level G

_PLAT004_ALERT_5_G  Polymeric Structure Found with Maximum Dimension
_PLAT092_ALERT_4_G  Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka
_PLAT112_ALERT_2_G  ADDSYM Detects New (Pseudo) Symm. Elem
_PLAT112_ALERT_2_G  ADDSYM Detects New (Pseudo) Symm. Elem
_PLAT112_ALERT_2_G  ADDSYM Detects New (Pseudo) Symm. Elem
_PLAT113_ALERT_2_G  ADDSYM Suggests Possible Pseudo/New Space Group
_PLAT152_ALERT_1_G  The Supplied and Calc. Volume s.u. Differ by ...
_PLAT802_ALERT_4_G  CIF Input Record(s) with more than 80 Characters
_PLAT981_ALERT_1_G  No non-zero f" Anomalous Scattering Values Found Please Check
_PLAT986_ALERT_1_G  No non-zero f’ Anomalous Scattering Values Found Please Check

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
11 ALERT level G = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level G

_PUBL017_ALERT_1_G  The _publ_section_references section is missing or empty.

0 ALERT level A = Data missing that is essential or data in wrong format
1 ALERT level G = General alerts. Data that may be required is missing
**Publication of your CIF**

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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**PLATON version of 23/04/2018; check.def file version of 23/04/2018**

_Datablock I_ - ellipsoid plot