

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) elbaitw

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: elbaitw

| | | |
|-----------------|---|-------------------------------|
| Bond precision: | O- B = 0.0025 A | Wavelength=0.71073 |
| Cell: | a=15.8117(2) | b=15.8117(2) c=7.0937(1) |
| | alpha=90 | beta=90 gamma=120 |
| Temperature: | 293 K | |
| | Calculated | Reported |
| Volume | 1535.89(4) | 1535.89(4) |
| Space group | R 3 m | R 3 m :H |
| Hall group | R 3 -2" | R 3 -2" |
| | Al23.85 B9.56 H10.50 O93 | |
| Moiety formula | Si17.44, 1.908(Na), 3.15(Li) | ? |
| Sum formula | Al23.85 B9.56 H10.50 Li3.15 H3.50 Al7.95 B3.19 Li1.05 Na1.91 O93 Si17.44 | Na0.64 O30.75 Si5.81 |
| Mr | 2801.05 | 929.74 |
| Dx, g cm-3 | 3.028 | 3.016 |
| Z | 1 | 3 |
| Mu (mm-1) | 0.924 | 0.922 |
| F000 | 1387.0 | 1381.0 |
| F000' | 1390.72 | |
| h, k, lmax | 27, 27, 12 | 24, 26, 12 |
| Nref | 1953[983] | 1783 |
| Tmin, Tmax | 0.895, 0.912 | 0.688, 0.747 |
| Tmin' | 0.895 | |

Correction method= # Reported T Limits: Tmin=0.688 Tmax=0.747
AbsCorr = MULTII-SCAN

Data completeness= 1.81/0.91 Theta(max)= 37.473

R(reflections)= 0.0193(1713)

wR2(reflections)=
0.0414(1783)

S = 1.086

Npar= 95

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

| | | | |
|-------------------|--|----------------|--------------|
| PLAT041_ALERT_1_C | Calc. and Reported SumFormula | Strings Differ | Please Check |
| | Calc: Al7.95 B3.19 H3.50 Li1.05 Na0.64 O31 Si5.81 | | |
| | Rep.: H3.50 Al7.95 B3.19 Li1.05 Na0.64 O30.75 Si5.81 | | |
| PLAT043_ALERT_1_C | Calculated and Reported Mol. Weight Differ by .. | 11.83 | Check |
| PLAT068_ALERT_1_C | Reported F000 Differs from Calcd (or Missing)... | | Please Check |
| PLAT077_ALERT_4_C | Unitcell Contains Non-integer Number of Atoms .. | | Please Check |
| PLAT220_ALERT_2_C | NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range | 3.7 | Ratio |



Alert level G

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:H3.5 Al7.95 B3.19 Li1.05 Na0.64
Atom count from the _atom_site data: H3.5011 Al7.95 B3.186 Li1.05 Na0
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 3
From the CIF: _chemical_formula_sum H3.50 Al7.95 B3.19 Li1.05 Na0.64 O
TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|------|-----------|-----------|-------|
| H | 10.50 | 10.50 | -0.00 |
| Al | 23.85 | 23.85 | -0.00 |
| B | 9.57 | 9.56 | 0.01 |
| Li | 3.15 | 3.15 | 0.00 |
| Na | 1.92 | 1.91 | 0.01 |
| O | 92.25 | 93.00 | -0.75 |
| Si | 17.43 | 17.44 | -0.01 |

| | | | |
|-------------------|--|--------|-------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 4 | Note |
| PLAT004_ALERT_5_G | Polymeric Structure Found with Maximum Dimension | 1 | Info |
| PLAT045_ALERT_1_G | Calculated and Reported Z Differ by a Factor ... | 0.333 | Check |
| PLAT168_ALERT_4_G | The CIF-Embedded .res File Contains EXYZ Records | 2 | Report |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records | 2 | Report |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | 2 | Report |
| PLAT199_ALERT_1_G | Reported _cell_measurement_temperature (K) | 293 | Check |
| PLAT200_ALERT_1_G | Reported _diffrn_ambient_temperature (K) | 293 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H1 Constrained at | 0.5011 | Check |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 1) | 17% | Note |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 2) | 100% | Note |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 3) | 100% | Note |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | 5 | Note |
| | LiY AlY AlZ SiT Bt | | |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 2 | Note |
| PLAT883_ALERT_1_G | No Info/Value for _atom_sites_solution_primary . | | Please Do ! |

| | | |
|---|----------------------|-----------|
| PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= | 0.600 | 29 Note |
| PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ | | 3 Units |
| PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value | | 2.42 Note |
| Predicted wR2: Based on SigI**2 | 1.71 or SHELX Weight | 3.92 |

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

9 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
2 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT041_elbaitw
;
PROBLEM: Calc. and Reported SumFormula      Strings Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT043_elbaitw
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..      11.83 Check
RESPONSE: ...
;
_vrf_PLAT068_elbaitw
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...      Please Check
RESPONSE: ...
;
_vrf_PLAT077_elbaitw
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..      Please Check
RESPONSE: ...
;
_vrf_PLAT220_elbaitw
;
PROBLEM: NonSolvent   Resd 1   0   Ueq(max)/Ueq(min) Range      3.7 Ratio
RESPONSE: ...
;
# end Validation Reply Form
```

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 06/01/2024; check.def file version of 05/01/2024

