checkCIF/PLATON report

Structure factors have been supplied for datablock(s) VESTA_phase_1

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: VESTA_phase_1

```
Bond precision:   = 0.0000 A                Wavelength=0.71073

Cell:             a=4.21998(16)     b=4.21998(16)     c=4.21998(16)
                  alpha=90          beta=90           gamma=90
Temperature:      0 K
```

	Calculated	Reported
Volume	75.150	75
Space group	F m -3 m	F m -3 m
Hall group	-F 4 2 3	?
Moiety formula	0.889(O), 0.523(Nb), 0.811(Li), 0.444(D)	?
Sum formula	D0.44 Li0.81 Nb0.52 O0.89	?
Mr	69.29	0.00
Dx,g cm-3	4.593	0.000
Z	3	0
Mu (mm-1)	5.818	0.000
F000	94.2	0.0
F000'	90.95	
h,k,lmax		
Nref		
Tmin,Tmax		
Tmin'		

```
Correction method= Not given

Data completeness=                Theta(max)=

R(reflections)=                                   wR2(reflections)=
S =                      Npar=
```

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

SYMM001_ALERT_1_A _symmetry_cell_setting is missing
The cell setting should be one of the following
* triclinic
* monoclinic
* orthorhombic
* tetragonal
* rhombohedral
* trigonal
* hexagonal
* cubic
The following tests will not be performed.
SYMMS_01,SYMMS_02

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.

GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.

GEOM002_ALERT_1_A _geom_bond_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM003_ALERT_1_A _geom_bond_distance is missing
Distance between atom sites 1 and 2.

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.000 Why?
PLAT043_ALERT_1_A Calculated and Reported Mol. Weight Differ by .. 69.29 Check
PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value .... Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ..... Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ..... Please Do !
PLAT197_ALERT_1_A Missing _cell_measurement_temperature Datum .... Please Add
PLAT198_ALERT_1_A Missing _diffrn_ambient_temperature Datum .... Please Add
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ..... Please Do !
PLAT880_ALERT_1_A No datum for _diffrn_reflns_number supplied .... Please Do !
PLAT881_ALERT_1_A No Datum for _diffrn_reflns_av_R_equivalents ... Please Do !
PLAT902_ALERT_1_A No (Interpretable) Reflections Found in FCF .... Please Check

Alert level C

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT151_ALERT_1_C No s.u. (esd) Given on Volume ..... Please Do !

Alert level G

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PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          0 Check
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with       Fm-3m Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at     0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Nb1        Constrained at     0.3919 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Li1        Constrained at     0.6081 Check
PLAT300_ALERT_4_G Atom Site Occupancy of D1         Constrained at     0.3333 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        100% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    2)        100% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    3)        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    1)       0.01 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       0.01 Check
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT980_ALERT_1_G No Anomalous Scattering Factors Found in CIF ...     Please Check
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20 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
16 **ALERT level G** = General information/check it is not something unexpected

25 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
2 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 22/08/2024; check.def file version of 21/08/2024

Datablock VESTA_phase_1 - ellipsoid plot