

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nabimusaite

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: nabimusaite

Bond precision:	S- O = 0.0011 A	Wavelength=0.70848
Cell:	a=7.1966(1)	b=7.1966(1) c=41.2146(5)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	
	Calculated	Reported
Volume	1848.57(6)	1848.57(4)
Space group	R -3 m	R -3 m
Hall group	-R 3 2"	?
Moiety formula	12(O4 Si), 2(O12 S3), 3(F O), 3(O), 0.108(Ba), 36(Ca), 2.892(K)	?
Sum formula	Ba0.11 Ca36 F3 K2.89 O78 S6	Ba0.036 Ca12 F1 K0.964 O26 Si12 S2 Si4
Mr	3405.23	1135.00
Dx, g cm-3	3.059	3.059
Z	1	3
Mu (mm-1)	3.178	3.157
F000	1696.0	1696.0
F000'	1707.31	
h, k, lmax	11, 11, 66	11, 9, 65
Nref	1069	1036
Tmin, Tmax	0.492, 0.388	0.877, 1.000
Tmin'	0.369	

Correction method= # Reported T Limits: Tmin=0.877 Tmax=1.000
AbsCorr = MULTII-SCAN

Data completeness= 0.969

Theta(max)= 34.640

R(reflections)= 0.0197(932)

wR2(reflections)=

wR= 0.0279(1036)

S = 1.640

Npar= 57

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

EXPT108_ALERT_1_A The magnitudes of the crystal dimensions do not
match the min, mid and max definitions
GEOM005_ALERT_1_A _geom_angle_atom_site_label_1 is missing
Label identifying the atom site 1.
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.
PLAT902_ALERT_1_A No (Interpretable) Reflections Found in FCF Please Check

Alert level B

CRYSS01_ALERT_1_B The magnitudes of the crystal dimensions do not
match the min, mid and max definitions
SHFSU01_ALERT_2_B The absolute value of parameter shift to su ratio > 0.10
Absolute value of the parameter shift to su ratio given 0.168
Additional refinement cycles may be required.
PLAT080_ALERT_2_B Maximum Shift/Error 0.17 Why ?
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 08 Check

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given Please Do !

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
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
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.70848 Ang.
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
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 F7 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7 Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9) 100% Note

PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	07	Check
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2	Units
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0	Sig(I)
PLAT984_ALERT_1_G	The Ba-f' = -0.2823 Deviates from the B&C-Value	-0.2860	Check
PLAT984_ALERT_1_G	The Ca-f' = 0.2282 Deviates from the B&C-Value	0.2267	Check
PLAT984_ALERT_1_G	The K-f' = 0.2016 Deviates from the B&C-Value	0.2005	Check
PLAT984_ALERT_1_G	The S-f' = 0.1258 Deviates from the B&C-Value	0.1242	Check
PLAT984_ALERT_1_G	The Si-f' = 0.0833 Deviates from the B&C-Value	0.0823	Check
PLAT985_ALERT_1_G	The Ba-f" = 2.2981 Deviates from the B&C-Value	2.2830	Check
PLAT985_ALERT_1_G	The Ca-f" = 0.3092 Deviates from the B&C-Value	0.3059	Check
PLAT985_ALERT_1_G	The K-f" = 0.2519 Deviates from the B&C-Value	0.2493	Check
PLAT985_ALERT_1_G	The S-f" = 0.1248 Deviates from the B&C-Value	0.1237	Check

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

23 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 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
 8 ALERT type 4 Improvement, methodology, query or suggestion
 5 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
 _publ_contact_author_name and _publ_contact_author_address.
 PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.
 PUBL006_ALERT_1_A _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'
 PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
 PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
 PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
 PUBL012_ALERT_1_A _publ_section_abstract is missing.
 Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
 empty.

7 **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 level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
```

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RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_EXPT108_nabimusaite
;
PROBLEM: The magnitudes of the crystal dimensions do not
RESPONSE: ...
;
_vrf_GEOM005_nabimusaite
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_GEOM006_nabimusaite
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_nabimusaite
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_nabimusaite
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT902_nabimusaite
;
PROBLEM: No (Interpretable) Reflections Found in FCF ....      Please Check
RESPONSE: ...
;
# end Validation Reply Form

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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.

