

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zadovite

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: zadovite

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Bond precision:	P- O = 0.0018 A	Wavelength=0.70848
Cell:	a=7.0896(1)	b=7.0896(1)      c=25.4317(5)
	alpha=90	beta=90      gamma=120
Temperature:	293 K	
	Calculated	Reported
Volume	1107.01(4)	1107.00(3)
Space group	R -3 m	R -3 m
Hall group	-R 3 2"	?
Moiety formula	2(O12 Si3), 2(O12 P3), 3(F), 3(Ba), 18(Ca)	?
Sum formula	Ba3 Ca18 F3 O48 P6 Si6	Ba1 Ca6 F1 O16 P2 Si2
Mr	2312.79	770.90
Dx, g cm-3	3.469	3.469
Z	1	3
Mu (mm-1)	5.154	5.160
F000	1113.0	1113.0
F000'	1117.90	
h,k,lmax	11,11,40	11,10,40
Nref	646	618
Tmin,Tmax	0.884,0.950	0.982,1.000
Tmin'	0.857	

Correction method= # Reported T Limits: Tmin=0.982 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.957      Theta(max)= 34.680

R(reflections)= 0.0188( 547)	wR2(reflections)=
S = 1.250	wR= 0.0231( 618)
Npar= 35	

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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.

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### Alert level A

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.

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### Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT125_ALERT_4_C	No '_symmetry_space_group_name_Hall'	Given .....	Please Do !
PLAT431_ALERT_2_C	Short Inter HL..A Contact F1	..02 .	2.88 Ang.
		1-x+y,-x,z =	3_455 Check
PLAT431_ALERT_2_C	Short Inter HL..A Contact F1	..02 .	2.88 Ang.
		1-y,1+x-y,z =	2_665 Check
PLAT431_ALERT_2_C	Short Inter HL..A Contact F1	..02 .	2.88 Ang.
		x,-1+y,z =	1_545 Check

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### 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	1 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.	
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	(K) 293 Check	
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	(K) 293 Check	
PLAT431_ALERT_2_G	Short Inter HL..A Contact F1	..02 .	2.88 Ang.
		-x,-1-x+y,-z =	6_545 Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact F1	..02 .	2.88 Ang.
		-1+y,x,-z =	4_455 Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact F1	..02 .	2.88 Ang.
		1+x-y,1-y,-z =	5_665 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2 Note	
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 !	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	27 Note	
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked	! Info	
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 P-f' = 0.1035 Deviates from the B&C-Value	0.1021 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	

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4 **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  
22 **ALERT level G** = General information/check it is not something unexpected

16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 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  
4 ALERT type 4 Improvement, methodology, query or suggestion  
5 ALERT type 5 Informative message, check

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## checkCIF publication errors

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### **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.

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### **Alert level G**

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or  
empty.

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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

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## 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_GEOM005_zadovite
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_GEOM006_zadovite
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_zadovite
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_zadovite
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
# end Validation Reply Form

```

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.

