

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: stibiotantalite

Bond precision: Sb- O = 0.0063 A Wavelength=0.71073

Cell: a=5.5419(2) b=4.9200(2) c=11.8003(5)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	321.75(2)	321.75(2)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	Nb0.84 O16 Sb4 Ta3.16	Nb0.211 O4 Sb Ta0.789
Sum formula	Nb0.84 O16 Sb4 Ta3.16	Nb0.21 O4 Sb Ta0.79
Mr	1392.53	347.99
Dx, g cm ⁻³	7.187	7.184
Z	1	4
Mu (mm ⁻¹)	35.788	35.742
F000	597.0	597.0
F000'	591.28	
h, k, lmax	7, 6, 16	7, 6, 15
Nref	890 [465]	775
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= 1.67/0.87 Theta(max)= 29.394

R(reflections)= 0.0173(766)

wR2(reflections)=
0.0436(775)

S = 1.158

Npar= 58

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**

STRVA01_ALERT_4_C Flack test results are ambiguous.
 From the CIF: `_refine_ls_abs_structure_Flack` 0.380
 From the CIF: `_refine_ls_abs_structure_Flack_su` 0.030
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

● **Alert level G**

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT012_ALERT_1_G No `_shelx_res_checksum` Found in CIF Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT199_ALERT_1_G Reported `_cell_measurement_temperature` (K) 293 Check
PLAT200_ALERT_1_G Reported `_diffrn_ambient_temperature` (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 17% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Sb (III) . 2.88 Info
PLAT883_ALERT_1_G No Info/Value for `_atom_sites_solution_primary` . Please Do !

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

- 10 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
1 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
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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.

