

# 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: I

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Bond precision:    Y- O = 0.0343 A                      Wavelength=0.82526

Cell:                a=10.42959(5)      b=6.10154(3)            c=24.82182(11)  
                      alpha=90            beta=94.8293(3)        gamma=90

Temperature:        293 K

|                | Calculated         | Reported        |
|----------------|--------------------|-----------------|
| Volume         | 1573.968(13)       | 1573.968(12)    |
| Space group    | P 2/c              | P 1 2/c 1       |
| Hall group     | -P 2yc             | -P 2yc          |
| Moiety formula | O27 Ti4 Y6, 10(Ba) | ?               |
| Sum formula    | Ba10 O27 Ti4 Y6    | Ba10 O27 Ti4 Y6 |
| Mr             | 2530.24            | 2530.30         |
| Dx,g cm-3      | 5.339              | 5.339           |
| Z              | 2                  | 2               |
| Mu (mm-1)      | 22.272             | 22.507          |
| F000           | 2196.0             | 1632.0          |
| F000'          | 2177.19            |                 |
| h,k,lmax       | 24,14,58           |                 |
| Nref           | 21168              |                 |
| Tmin,Tmax      |                    |                 |
| Tmin'          |                    |                 |

Correction method= Not given

Data completeness= 0.000                      Theta(max)=

R(reflections)= 0.0467( 0)                      wR2(reflections)= wR= 0.0630( 0)

S = 10.410                                      Npar= 124

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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**

PLAT699\_ALERT\_1\_A Missing \_exptl\_crystal\_description Value ..... Please Do !

**Author Response: As per the IUCR guidelines, this is not required for powder data**

**Alert level C**

SHFSU01\_ALERT\_2\_C The absolute value of parameter shift to su ratio > 0.05  
 Absolute value of the parameter shift to su ratio given 0.058  
 Additional refinement cycles may be required.

**Author Response: This is the standard convergence criteria for Jana2006**

PLAT080\_ALERT\_2\_C Maximum Shift/Error ..... 0.06 Why ?

**Author Response: Refinement does not fully converge as it's refining a commensurate model against incommensurate data**

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Ti2 Check

**Author Response: This is probably as a result of this refinement being an commensurate approximation of an incommensurate structure**

PLAT799\_ALERT\_4\_C Numeric Label on Displacement Par. Record ..... ? Check

**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   |
| PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka | 0.82526 | Ang.   |
| PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing .....          | 0.00003 | Ang.   |
| PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing .....          | 0.00011 | Ang.   |
| PLAT145_ALERT_4_G s.u. on beta Small or Missing .....              | 0.0003  | Degree |
| PLAT794_ALERT_5_G Tentative Bond Valency for Y1 (III) .            | 3.17    | Info   |
| PLAT794_ALERT_5_G Tentative Bond Valency for Y2 (III) .            | 3.35    | Info   |
| PLAT794_ALERT_5_G Tentative Bond Valency for Y3 (III) .            | 3.24    | Info   |
| PLAT794_ALERT_5_G Tentative Bond Valency for Ti2 (IV) .            | 4.46    | Info   |
| PLAT984_ALERT_1_G The Ba-f' = -0.0916 Deviates from the B&C-Value  | -0.1008 | Check  |
| PLAT984_ALERT_1_G The Y-f' = -1.7511 Deviates from the B&C-Value   | -1.7394 | Check  |
| PLAT985_ALERT_1_G The Ba-f" = 2.9970 Deviates from the B&C-Value   | 2.9766  | Check  |
| PLAT985_ALERT_1_G The Ti-f" = 0.5980 Deviates from the B&C-Value   | 0.5943  | Check  |
| PLAT985_ALERT_1_G The Y-f" = 0.6750 Deviates from the B&C-Value    | 0.6647  | Check  |

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 15 **ALERT level G** = General information/check it is not something unexpected
- 7 **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  
0 ALERT type 3 Indicator that the structure quality may be low  
5 ALERT type 4 Improvement, methodology, query or suggestion  
5 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.

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