**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 1487\_0m\_a

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](http://journals.iucr.org/services/cif/checking/checkcifreport.html)

**Datablock: 1487\_0m\_a**

Bond precision: C-C = 0.0033 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=10.268(3) | b=10.442(5) | c=10.873(3) |
|  | alpha=79.95(2) | beta=66.827(12) | gamma=73.585(16) |
| Temperature: | 293 K |  |  |

Calculated Reported Volume 1025.4(7) 1025.4(6) Space group P -1 P -1

Hall group -P 1 -P 1

Moiety formula 2(C20 H20 P), Cl6 Hf Cl6 Hf, 2(C20 H20 P) Sum formula C40 H40 Cl6 Hf P2 C40 H40 Cl6 Hf P2

Mr 973.85 973.85

Dx,g cm-3 1.577 1.577

Z 1 1

|  |  |  |
| --- | --- | --- |
| Mu (mm-1) | 3.040 | 3.040 |
| F000 | 484.0 | 484.0 |
| F000’ | 484.63 |  |
| h,k,lmax | 17,18,18 | 17,17,18 |
| Nref | 11073 | 11001 |
| Tmin,Tmax | 0.421,0.544 | 0.473,0.581 |
| Tmin’ | 0.410 |  |

Correction method= # Reported T Limits: Tmin=0.473 Tmax=0.581

AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 37.870

R(reflections)= 0.0313( 9243) wR2(reflections)= 0.0601( 11001) S = 1.020 Npar= 224

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 B**

PLAT973\_ALERT\_2\_B Check Calcd Positive Resid. Density on Hf1 1.61 eA-3

**Alert level C**

[ABSTY02\_ALERT\_1\_C](http://journals.iucr.org/services/cif/checking/ABSTY_02.html) An \_exptl\_absorpt\_correction\_type has been given without a literature citation. This should be contained in the

\_exptl\_absorpt\_process\_details field. Absorption correction given as multi-scan

|  |  |  |  |
| --- | --- | --- | --- |
| PLAT244\_ALERT\_4\_C Low | ’Solvent’ Ueq as Compared to Neighbors of | Hf1 | Check |
| PLAT910\_ALERT\_3\_C Missi | ng # of FCF Reflection(s) Below Theta(Min). | 8 | Note |

 **Alert level G**

PLAT012\_ALERT\_1\_G No \_shelx\_res\_checksum Found in CIF ...... Please Check PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check PLAT794\_ALERT\_5\_G Tentative Bond Valency for Hf1 (IV) . 3.34 Info PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 63 Note PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 2 Note PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 10 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

5 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

1 ALERT type 3 Indicator that the structure quality may be low

2 ALERT type 4 Improvement, methodology, query or suggestion

1 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](http://journals.iucr.org/services/cif/checking/checkform.html) 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 17/03/2019; check.def file version of 04/03/2019**

**Datablock 1487\_0m\_a- ellipsoid plot**

>­

(Y)

tD

tD

(Y)

0

r-

NOMOVE FORCED Prob

Temp

50

293

L CL2a

Q\_

CI

I

:z:

0

f-

CI

\_j

o\_

z -140 1487 Om a p -1 R 0.03 RES= 0 171 X