**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 1238\_0ma\_b

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: 1238\_0ma\_b**

Bond precision: C-C = 0.0137 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=29.593(18) | b=9.374(4) | c=23.543(12) |
|  | alpha=90 | beta=130.124(19) | gamma=90 |
| Temperature: | 293 K |  |  |

Calculated Reported Volume 4994(5) 4994(4) Space group C 2 C 1 2 1

Hall group C 2y C 2y

Moiety formula 2(C26 H21 N P), Cl6 Hf 0.5(Cl6 Hf), C26 H21 N P

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sum formula | C52 H42 Cl6 Hf | N2 | P2 | C52 H42 Cl6 Hf N2 P2 |
| Mr | 1148.01 |  |  | 1148.01 |
| Dx,g cm-3 | 1.527 |  |  | 1.527 |
| Z | 4 |  |  | 4 |
| Mu (mm-1) | 2.511 |  |  | 2.511 |
| F000 | 2288.0 |  |  | 4576.0 |
| F000’ | 2290.59 |  |  |  |
| h,k,lmax | 50,15,40 |  |  | 49,15,38 |
| Nref | 25901[ 13559] |  |  | 24247 |
| Tmin,Tmax | 0.208,0.590 |  |  | 0.109,0.419 |
| Tmin’ | 0.126 |  |  |  |

Correction method= # Reported T Limits: Tmin=0.109 Tmax=0.419

AbsCorr = MULTI-SCAN

Data completeness= 1.79/0.94 Theta(max)= 37.280

R(reflections)= 0.0567( 17788) wR2(reflections)= 0.1427( 24247) S = 1.094 Npar= 571

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**



[PLAT029\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT029.html) \_diffrn\_measured\_fraction\_theta\_full value Low . 0.943 Why? [PLAT910\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT910.html) Missing # of FCF Reflection(s) Below Theta(Min). 12 Note [PLAT934\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT934.html) Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 5 Check [PLAT971\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 0.88A From Hf1 3.33 eA-3

[PLAT971\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 0.92A From Hf2 2.53 eA-3

[PLAT972\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 1.87A From Cl1 -3.30 eA-3

[PLAT972\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 1.90A From Cl5 -3.10 eA-3

[PLAT987\_ALERT\_1\_B](http://journals.iucr.org/services/cif/checking/PLAT987.html) The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

**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

[PLAT068\_ALERT\_1\_C](http://journals.iucr.org/services/cif/checking/PLAT068.html) Reported F000 Differs from Calcd (or Missing)... Please Check [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C13 --C14 . 0.20 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C43 --C44 . 0.18 Ang. [PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of C3 Check [PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of C13 Check [PLAT244\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT244.html) Low ’Solvent’ Ueq as Compared to Neighbors of Hf1 Check [PLAT244\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT244.html) Low ’Solvent’ Ueq as Compared to Neighbors of Hf2 Check [PLAT342\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT342.html) Low Bond Precision on C-C Bonds ............... 0.01371 Ang. [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 2.281 Check [PLAT911\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT911.html) Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report [PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 0.36A From Hf1 -1.99 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 0.44A From Cl5 -1.76 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 0.48A From Cl1 -1.64 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 0.56A From Hf2 -1.55 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 0.55A From Hf2 -1.55 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 0.54A From Hf1 -1.52 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 0.58A From Hf1 -1.52 eA-3

[PLAT978\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT978.html) Number C-C Bonds with Positive Residual Density. 0 Info

**Alert level G**



[FORMU01\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/FORMU_01.html) There is a discrepancy between the atom counts in the

\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is usually due to the moiety formula being in the wrong format. Atom count from \_chemical\_formula\_sum: C52 H42 Cl6 Hf1 N2 P2

Atom count from \_chemical\_formula\_moiety:C26 H21 Cl3 Hf0.5 N1 P1

[PLAT012\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT012.html) No \_shelx\_res\_checksum Found in CIF ...... Please Check [PLAT033\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT033.html) Flack x Value Deviates > 3.0 \* sigma from Zero . 0.054 Note [PLAT042\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT042.html) Calc. and Reported MoietyFormula Strings Differ Please Check [PLAT063\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT063.html) Crystal Size Likely too Large for Beam Size .... 0.79 mm [PLAT083\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT083.html) SHELXL Second Parameter in WGHT Unusually Large 13.06 Why ? [PLAT128\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT128.html) Alternate Setting for Input Space Group C2 I2 Note [PLAT199\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT199.html) Reported \_cell\_measurement\_temperature ..... (K) 293 Check [PLAT200\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT200.html) Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check [PLAT233\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT233.html) Hirshfeld (M-X Solvent) Hf2 --Cl7 . 6.3 s.u. [PLAT790\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT790.html) Centre of Gravity not Within Unit Cell: Resd. # 2 Note

C26 H21 N P

[PLAT794\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT794.html) Tentative Bond Valency for Hf1 (IV) . 3.46 Info [PLAT794\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT794.html) Tentative Bond Valency for Hf2 (IV) . 3.40 Info [PLAT912\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT912.html) Missing # of FCF Reflections Above STh/L= 0.600 712 Note [PLAT933\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT933.html) Number of OMIT Records in Embedded .res File ... 1 Note [PLAT952\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT952.html) Calculated (ThMax) and CIF-Reported Lmax Differ 2 Units [PLAT958\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT958.html) Calculated (ThMax) and Actual (FCF) Lmax Differ 2 Units [PLAT992\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT992.html) Repd & Actual \_reflns\_number\_gt Values Differ by 1 Check

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

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

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

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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

16 ALERT type 2 Indicator that the structure model may be wrong or deficient

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

10 ALERT type 4 Improvement, methodology, query or suggestion

4 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.

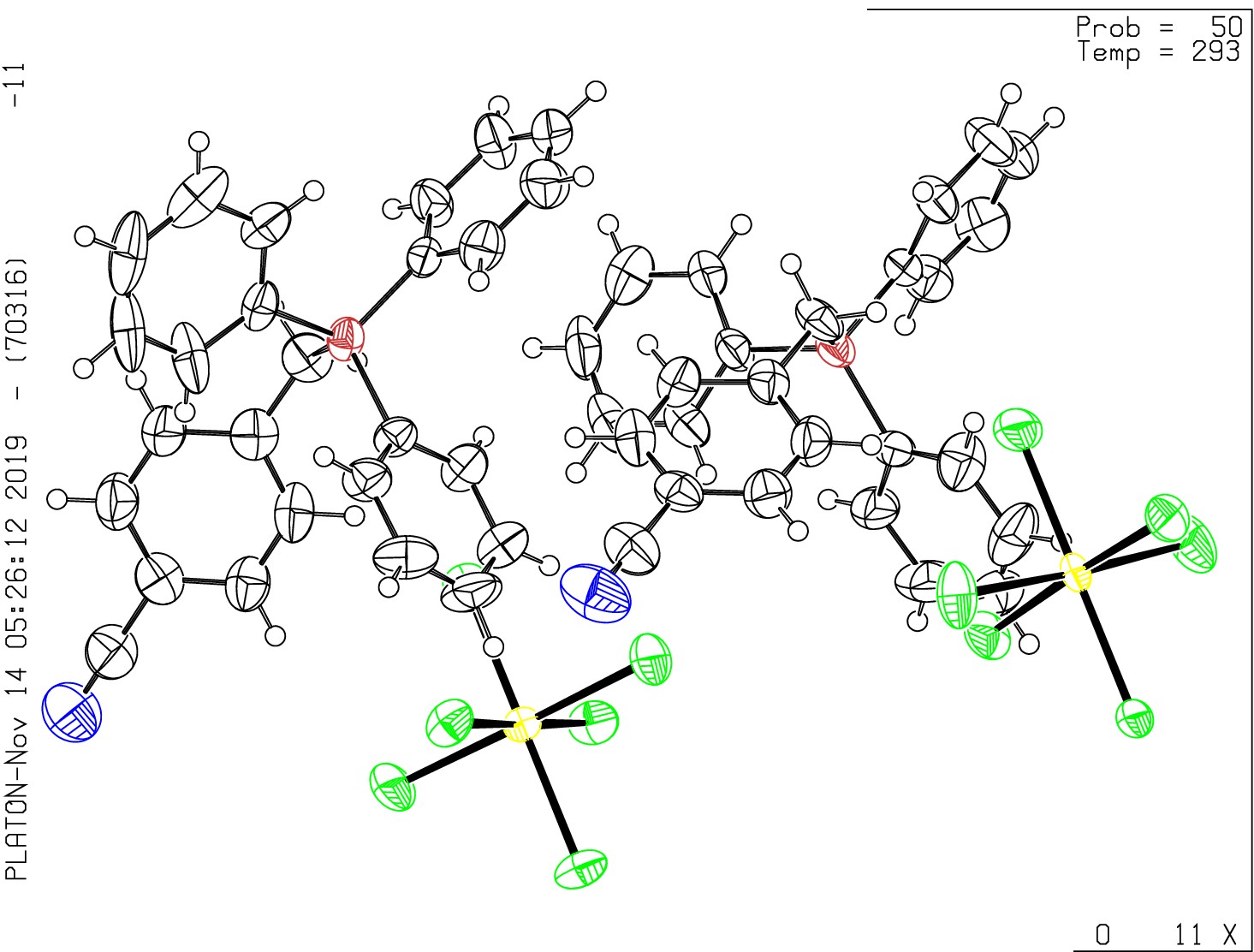
**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to

CIF submission.

**PLATON version of 07/08/2019; check.def file version of 30/07/2019**

**Datablock 1238**-**0ma\_b- ellipsoid plot**



>- NOMOVE FORCED

z -20 1238-0ma\_bC 1 2 1 R = 0.06 RES=