**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 1239\_0ma\_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: 1239\_0ma\_a**

Bond precision: C-C = 0.0175 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=19.876(16) | b=12.878(7) | c=21.395(10) |
|  | alpha=90 | beta=116.73(3) | gamma=90 |
| Temperature: | 293 K |  |  |

|  |  |  |  |
| --- | --- | --- | --- |
|  | Calculated | Reported |  |
| Volume | 4891(5) | 4891(5) |
| Space group | P 21/c | P 1 21/c | 1 |
| Hall group | -P 2ybc | -P 2ybc |  |

Moiety formula 2(C25 H21 F P), Cl6 Hf Cl6 Hf, 2(C25 H21 F P)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Sum formula | C50 H42 Cl6 | F2 | Hf | P2 | C50 H42 Cl6 F2 Hf P2 |
| Mr | 1133.97 |  |  |  | 1133.97 |
| Dx,g cm-3 | 1.540 |  |  |  | 1.540 |
| Z | 4 |  |  |  | 4 |
| Mu (mm-1) | 2.567 |  |  |  | 2.567 |
| F000 | 2256.0 |  |  |  | 2256.0 |
| F000’ | 2258.70 |  |  |  |  |
| h,k,lmax | 29,19,32 |  |  |  | 29,17,27 |
| Nref | 17324 |  |  |  | 13346 |
| Tmin,Tmax | 0.237,0.418 |  |  |  | 0.267,0.476 |
| Tmin’ | 0.159 |  |  |  |  |

Correction method= # Reported T Limits: Tmin=0.267 Tmax=0.476

AbsCorr = MULTI-SCAN

Data completeness= 0.770 Theta(max)= 32.230

R(reflections)= 0.0738( 9744) wR2(reflections)= 0.1869( 13346) S = 1.159 Npar= 550

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 A**

[PLAT029\_ALERT\_3\_A](http://journals.iucr.org/services/cif/checking/PLAT029.html) \_diffrn\_measured\_fraction\_theta\_full value Low . 0.770 Why?

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| [PLAT330\_ALERT\_2\_A](http://journals.iucr.org/services/cif/checking/PLAT330.html) | Large | Aver | Phenyl | C-C | Dist | C61 | -C66 | . | 1.44 | Ang. |
| [PLAT331\_ALERT\_2\_A](http://journals.iucr.org/services/cif/checking/PLAT331.html) | Small | Aver | Phenyl | C-C | Dist | C51 | -C56 | . | 1.34 | Ang. |
|  **Alert level B** |
| [PLAT330\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT330.html) | Large | Aver | Phenyl | C-C | Dist | C21 | -C26 | . | 1.42 | Ang. |
| [PLAT910\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT910.html) Missing # of FCF Reflection(s) Below Theta(Min). 15 Note[PLAT934\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT934.html) Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 7 Check |
| [PLAT971\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT971.html) | Check Calcd Resid. Dens. 2.08A | From | C23 |  | 3.23 | eA-3 |
| [PLAT971\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT971.html) | Check Calcd Resid. Dens. 1.57A | From | Cl1 |  | 2.59 | 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

[PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C34 Check [PLAT244\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT244.html) Low ’Solvent’ Ueq as Compared to Neighbors of Hf1 Check [PLAT330\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT330.html) Large Aver Phenyl C-C Dist C41 -C46 . 1.42 Ang. [PLAT331\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT331.html) Small Aver Phenyl C-C Dist C11 -C16 . 1.36 Ang. [PLAT332\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT332.html) Large Phenyl C-C Range C41 -C46 . 0.16 Ang. [PLAT342\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT342.html) Low Bond Precision on C-C Bonds ............... 0.01748 Ang. [PLAT363\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT363.html) Long C(sp3)-C(sp2) Bond C71 - C77 . 1.63 Ang. [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 7.897 Check [PLAT911\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT911.html) Missing FCF Refl Between Thmin & STh/L= 0.600 145 Report [PLAT971\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 1.36A From Hf1 1.99 eA-3

[PLAT971\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 1.00A From Cl5 1.72 eA-3

[PLAT971\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 1.21A From Hf1 1.69 eA-3

[PLAT971\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 1.26A From C77 1.60 eA-3

[PLAT971\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT971.html) Check Calcd Resid. Dens. 1.18A From Hf1 1.54 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 1.09A From Cl1 -1.85 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 1.83A From C23 -1.76 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 1.53A From Cl1 -1.66 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 1.50A From Cl1 -1.55 eA-3

[PLAT972\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT972.html) Check Calcd Resid. Dens. 0.77A From Hf1 -1.51 eA-3

[PLAT977\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT977.html) Check Negative Difference Density on H5 -0.46 eA-3

[PLAT977\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT977.html) Check Negative Difference Density on H44 -0.47 eA-3

[PLAT977\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT977.html) Check Negative Difference Density on H73 -0.31 eA-3

[PLAT977\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT977.html) Check Negative Difference Density on H77B -0.37 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**

[PLAT012\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT012.html) No \_shelx\_res\_checksum Found in CIF ...... Please Check [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 .... 0.70 mm [PLAT083\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT083.html) SHELXL Second Parameter in WGHT Unusually Large 75.67 Why ? [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 [PLAT333\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT333.html) Large Aver C6-Ring C-C Dist C71 -C76 . 1.43 Ang. [PLAT432\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT432.html) Short Inter X...Y Contact Cl3 ..C66 3.15 Ang.

x,3/2-y,1/2+z = 4\_576 Check [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at P1 (Centro SPGR) R Verify [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at P2 (Centro SPGR) S Verify [PLAT794\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT794.html) Tentative Bond Valency for Hf1 (IV) . 3.32 Info [PLAT912\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT912.html) Missing # of FCF Reflections Above STh/L= 0.600 3091 Note [PLAT933\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT933.html) Number of OMIT Records in Embedded .res File ... 3 Note [PLAT951\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT951.html) Calculated (ThMax) and CIF-Reported Kmax Differ 2 Units

[PLAT952\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT952.html) Calculated (ThMax) and CIF-Reported Lmax Differ 5 Units [PLAT957\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT957.html) Calculated (ThMax) and Actual (FCF) Kmax Differ 2 Units [PLAT958\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT958.html) Calculated (ThMax) and Actual (FCF) Lmax Differ 5 Units [PLAT992\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT992.html) Repd & Actual \_reflns\_number\_gt Values Differ by 1 Check

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

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

25 **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

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

29 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

5 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 1239\_0ma\_a ·ellipsoid plot**

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