# 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: PdtmedaCF3NN

```
Bond precision:   C-C = 0.0073 A            Wavelength=0.71075

Cell:             a=13.0204(19)    b=8.1491(10)        c=15.1590(19)
                  alpha=90         beta=91.198(8)      gamma=90
Temperature:      193 K

                  Calculated                 Reported
Volume            1608.1(4)                  1608.1(4)
Space group       P 21/n                     P 1 21/n 1
Hall group        -P 2yn                     -P 2yn
Moiety formula    C10 H16 F6 N4 O2 Pd        C10 H16 F6 N4 O2 Pd
Sum formula       C10 H16 F6 N4 O2 Pd        C10 H16 F6 N4 O2 Pd
Mr                444.67                     444.65
Dx,g cm-3         1.837                      1.836
Z                 4                          4
Mu (mm-1)         1.228                      1.229
F000              880.0                      880.0
F000'             876.60
h,k,lmax          16,10,19                   16,10,19
Nref              3685                       3647
Tmin,Tmax         0.782,0.782                0.674,0.782
Tmin'             0.782

Correction method= # Reported T Limits: Tmin=0.674 Tmax=0.782
AbsCorr = MULTI-SCAN

Data completeness= 0.990           Theta(max)= 27.472

R(reflections)= 0.0417( 3299)      wR2(reflections)= 0.1130( 3647)

S = 1.146                  Npar= 208
```

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

```
PLAT213_ALERT_2_C Atom C5             has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N4 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C5      - C6       .     1.35 Ang.
```

## Alert level G

```
CHEMS02_ALERT_1_G  Please check that you have entered the correct
            _publ_requested_category classification of your compound;
            FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
            FO or CO or EO for organic.
            From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or A
            From the CIF: _chemical_formula_sum :C10 H16 F6 N4 O2 Pd1
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0      0.998 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C1 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C4 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1        (II)        .    2.13 Info
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.3 Low
```

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   0 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 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 26/06/2020; check.def file version of 17/06/2020**