checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: jod1092s_squeezed

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

Cell:          a=13.1905(11)     b=14.4688(11)     c=20.9164(16)
               alpha=71.625(2)   beta=74.668(2)    gamma=73.472(2)
Temperature:   100 K

                  Calculated                  Reported
Volume            3564.2(5)                   3564.2(5)
Space group       P -1                        P -1
Hall group        -P 1                        ?
                  2(C34 H42 Br N3 O2 Pd), C4
Moiety formula                                ?
                  H10 O
Sum formula       C72 H94 Br2 N6 O5 Pd2       C36 H47 Br N3 O2.50 Pd
Mr                1496.13                     748.08
Dx,g cm-3         1.394                       1.394
Z                 2                           4
Mu (mm-1)         1.677                       1.677
F000              1540.0                      1540.0
F000'             1535.35
h,k,lmax          17,19,28                    17,19,28
Nref              18422                       16776
Tmin,Tmax         0.732,0.920                 0.767,0.921
Tmin'             0.708

Correction method= MULTI-SCAN

Data completeness= 0.911          Theta(max)= 28.700

R(reflections)= 0.0322( 14107)    wR2(reflections)= 0.0783( 16776)

S = 1.045                    Npar= 818
```

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
PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density 4.72

Alert level C

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PLAT045_ALERT_1_C Calculated and Reported Z Differ by ............          0.50 Ratio
PLAT220_ALERT_2_C Large Non-Solvent    C    Ueq(max)/Ueq(min) ...          3.35 Ratio
PLAT220_ALERT_2_C Large Non-Solvent    C    Ueq(max)/Ueq(min) ...          3.54 Ratio
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..         5.60 Ratio
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..         6.08 Ratio
PLAT420_ALERT_2_C D-H Without Acceptor        N1    -   H01A   ...            ?
PLAT420_ALERT_2_C D-H Without Acceptor        N4    -   H04B   ...            ?
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Alert level G

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HYDTR01_ALERT_1_G  Extra text has been found in the _refine_ls_hydrogen_treatment fi
           Explanatory text should be in the _publ_section_refinement field.
           Hydrogen treatment given as NH2 free with SADI, rigid methyls, other
           Hydrogen treatment identified as  riding
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        6
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)      200 Deg.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1    -- C18    ..        8.25 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd2    -- Br2    ..        6.94 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd2    -- C68    ..        7.18 su
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        4
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        6
```

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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   7 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 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*, 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 24/03/2011; check.def file version of 16/03/2011