checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hoffmannj200204_0m

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: hoffmannj200204_0m

```
Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:           a=12.6051(9)    b=16.0123(12)       c=18.4340(12)
                alpha=90        beta=104.712(2)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          3598.7(4)                 3598.7(4)
Space group     P 21/n                    P 1 21/n 1
Hall group      -P 2yn                    -P 2yn
Moiety formula  C48 H36 Li2 P2            0.5(C48 H36 Li2 P2)
Sum formula     C48 H36 Li2 P2            C24 H18 Li P
Mr              688.59                    344.29
Dx,g cm-3       1.271                     1.271
Z               4                         8
Mu (mm-1)       0.156                     0.156
F000            1440.0                    1440.0
F000'           1441.28
h,k,lmax        18,22,26                  18,22,26
Nref            10968                     10966
Tmin,Tmax       0.963,0.968               0.716,0.747
Tmin'           0.963

Correction method= # Reported T Limits: Tmin=0.716 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 30.508

R(reflections)= 0.0447( 8967)     wR2(reflections)= 0.1170( 10966)

S = 1.035                  Npar= 469
```

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

```
PLAT220_ALERT_2_C NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range        4.4 Ratio
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C23 Check
PLAT411_ALERT_2_C Short Inter H...H Contact  H38      ..H38      .       2.07 Ang.
                                                 1-x,2-y,1-z  =      3_676 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.873 Check
```

Alert level G

```
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         24 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 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
```

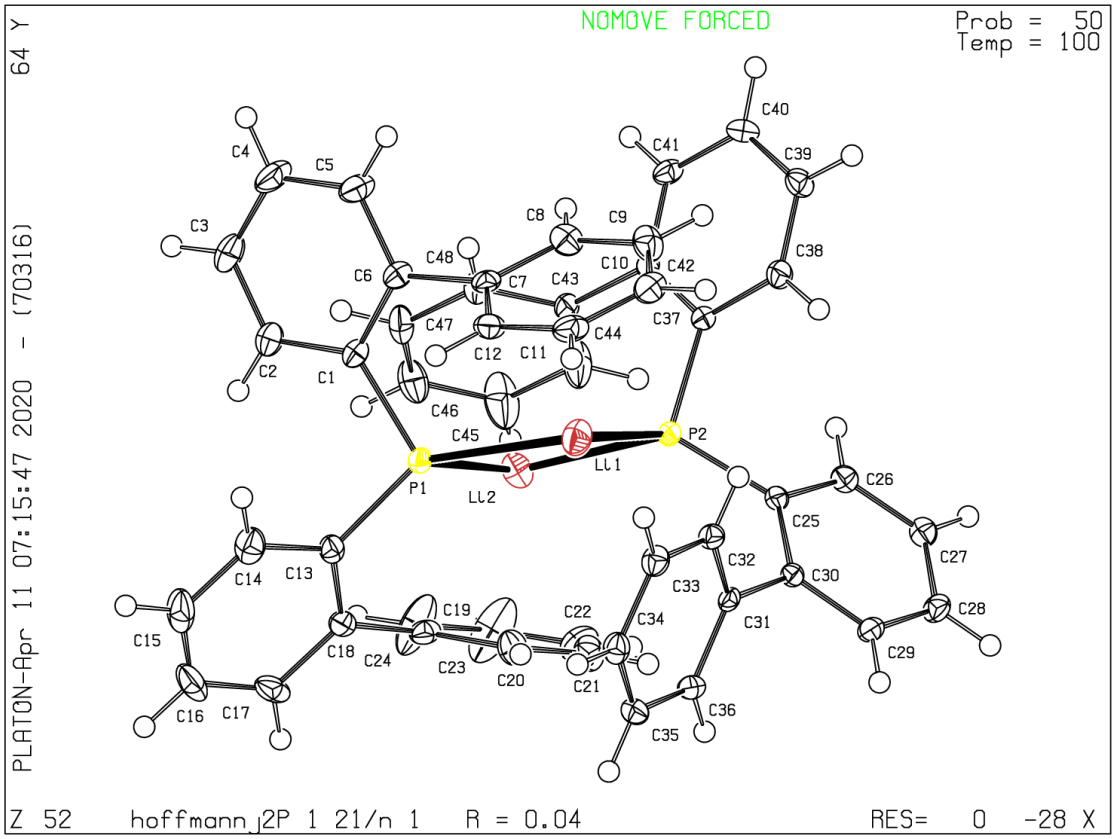
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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* 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 22/12/2019; check.def file version of 13/12/2019

Datablock hoffmannj200204_0m - ellipsoid plot