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: 02487AnaIMatesanz

```
Bond precision:  C-C = 0.0250 A          Wavelength=0.71073

Cell:           a=15.8231(5)    b=9.2474(3)         c=19.9600(6)
                alpha=90        beta=110.006(1)     gamma=90
Temperature:    296 K

                Calculated                Reported
Volume          2744.36(15)               2744.36(15)
Space group     C 2/c                     C 1 2/c 1
Hall group      : -C 2yc                  -C 2yc
Moiety formula  C8 H14 I2 N2 Pt           ?
Sum formula     C8 H14 I2 N2 Pt           C8 H14 I2 N2 Pt
Mr              587.09                    587.10
Dx,g cm-3       2.842                     2.842
Z               8                         8
Mu (mm-1)       14.692                    14.692
F000            2080.0                    2080.0
F000'           2060.85
h,k,lmax        18,11,24                  18,11,24
Nref            2505                      2499
Tmin,Tmax       0.041,0.110               0.130,0.220
Tmin'           0.009

Correction method= # Reported T Limits: Tmin=0.130 Tmax=0.220
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 25.350

R(reflections)= 0.0377( 2259)     wR2(reflections)= 0.1191( 2499)

S = 1.198                 Npar= 120
```

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.025 Ang.

Alert level C

PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.4 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C6 - C7 . 1.37 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N1 --H1A . Please Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H4 ..I1 . 3.30 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H5 ..I1 . 3.31 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H6 ..I2 . 3.32 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1A ..I2 . 3.20 Ang.
PLAT481_ALERT_4_C Long D...A H-Bond Reported N1 ..I2 4.04 Ang.

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 79.21 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Pt1 (II) . 1.07 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
5 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

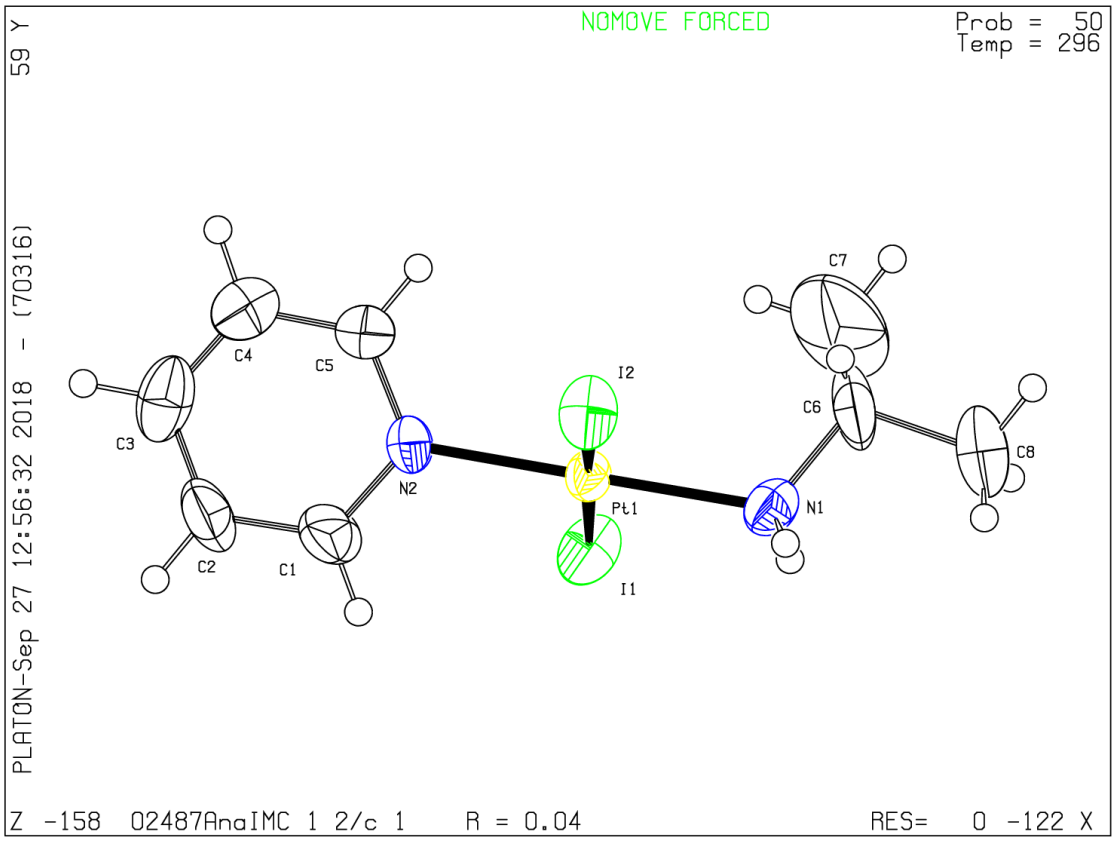
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 26/09/2018; check.def file version of 13/09/2018

Datablock 02487AnaIMatesanz - ellipsoid plot