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: naka171

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Bond precision:    C-C = 0.0064 A            Wavelength=0.71073

Cell:              a=15.9074(6)     b=20.9224(8)      c=22.6113(9)
                   alpha=90         beta=90           gamma=90
Temperature:       103 K

                   Calculated                   Reported
Volume             7525.5(5)                    7525.5(5)
Space group        P b c a                      P b c a
Hall group         -P 2ac 2ab                   -P 2ac 2ab
Moiety formula     C41 H40 P2 Pt Si, C H2 Cl2   C41 H40 P2 Pt Si, C H2 Cl2
Sum formula        C42 H42 Cl2 P2 Pt Si         C42 H42 Cl2 P2 Pt Si
Mr                 902.77                       902.78
Dx,g cm-3          1.594                        1.594
Z                  8                            8
Mu (mm-1)          4.018                        4.018
F000               3600.0                       3600.0
F000'              3592.21
h,k,lmax           19,25,27                     19,25,27
Nref               7015                         7011
Tmin,Tmax          0.594,0.755                  0.389,0.766
Tmin'              0.309

Correction method= # Reported T Limits: Tmin=0.389 Tmax=0.766
AbsCorr = EMPIRICAL

Data completeness= 0.999           Theta(max)= 25.500

R(reflections)= 0.0325( 5562)      wR2(reflections)= 0.0783( 7011)

S = 1.026                  Npar= 448
```

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**
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C42 Check
PLAT420_ALERT_2_C D-H Without Acceptor   Si1   -- H2   ...   Please Check
PLAT420_ALERT_2_C D-H Without Acceptor   Si1   -- H3   ...   Please Check

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⚪ **Alert level G**
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF   Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   24.98 Why ?
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL   2016 Note

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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
   3 **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
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   2 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 13/08/2017; check.def file version of 27/07/2017