checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ao_of_cisdppe_aucl2_1

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: ao_of_cisdppe_aucl2_1

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Bond precision:    C-C = 0.0091 A              Wavelength=0.71073

Cell:              a=13.1726(10)     b=12.8043(10)       c=15.2893(12)
                   alpha=90          beta=100.906(1)     gamma=90
Temperature:       180 K

                   Calculated                 Reported
Volume             2532.2(3)                  2532.2(3)
Space group        C c                        C 1 c 1
Hall group         C -2yc                     C -2yc
Moiety formula     C26 H22 Au2 Cl2 P2         C26 H22 Au2 Cl2 P2
Sum formula        C26 H22 Au2 Cl2 P2         C26 H22 Au2 Cl2 P2
Mr                 861.22                     861.21
Dx,g cm-3          2.259                      2.259
Z                  4                          4
Mu (mm-1)          11.925                     11.925
F000               1600.0                     1600.0
F000'              1587.47
h,k,lmax           16,16,19                   16,16,19
Nref               5662[ 2835]                5477
Tmin,Tmax          0.231,0.303                0.557,0.746
Tmin'              0.195

Correction method= # Reported T Limits: Tmin=0.557 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.93/0.97        Theta(max)= 27.214
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R(reflections)= 0.0149(5298)   wR2(reflections)= 0.0323(5477)

S = 0.715   Npar= 289

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**
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement   Please Check

Author Response: The PArsson Flack parameter is relatively small and no improvement was seen upon twin refinement

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🟡 **Alert level C**
GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
            outside the range 0.80 <> 2.00
            Goodness of fit given =   0.715
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.37 Report
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00908 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   7 Report
            2 0 0,   3 1 0,   2 2 0,   0 0 4, -1 1 4, -2 0 6,
            0 0 6,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....   5 Note
            2 0 0,   1 1 0, -1 1 4, -2 0 6,   0 0 6,

⚪ **Alert level G**
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   1 Note
            Au02
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   1 Note
            1 1 0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   7 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   4.8 Low
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameter Values Zero ....   Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ....   0.70 Note
            Predicted wR2: Based on SigI**2 4.65 or SHELX Weight 4.65
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   1 Info

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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
   5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   7 **ALERT level G** = General information/check it is not something unexpected

   1 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
   5 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 06/01/2024; check.def file version of 05/01/2024