checkCIF/PLATON report

Structure factors have been supplied for datablock(s) G196

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: G196

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Bond precision:   C-C = 0.0056 A           Wavelength=0.71073

Cell:              a=15.916(3)      b=9.2262(11)        c=15.939(3)
                   alpha=90         beta=95.94(2)       gamma=90
Temperature:       297 K

                 Calculated                  Reported
Volume           2328.0(7)                   2328.0(7)
Space group      P 21/n                      P 1 21/n 1
Hall group       -P 2yn                      -P 2yn
Moiety formula   C52 H44 Cu2 I2 N2 P2        C26 H22 Cu I N P
Sum formula      C52 H44 Cu2 I2 N2 P2        C26 H22 Cu I N P
Mr               1139.73                     569.90
Dx,g cm-3        1.626                       1.626
Z                2                           4
Mu (mm-1)        2.346                       2.346
F000             1128.0                      1128.8
F000'            1128.07
h,k,lmax         19,11,19                    19,11,19
Nref             4534                        4505
Tmin,Tmax        0.608,0.829                 0.527,0.826
Tmin'            0.564

Correction method= # Reported T Limits: Tmin=0.527 Tmax=0.826
AbsCorr = ANALYTICAL

Data completeness= 0.994            Theta(max)= 25.910

R(reflections)= 0.0322( 3751)                    wR2(reflections)=
                                                 0.0873( 4505)
S = 0.941                  Npar= 274
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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

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PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C52 H44 Cu2 I2 N2 P2
             Rep.: C26 H22 Cu I N P
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.59 Report
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C23 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C21 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C21      --C26      .      1.37 Ang.
PLAT350_ALERT_3_C Short  C-H (X0.96,N1.08A)  C19      - H19      .      0.82 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         6 Note
               1  1  0,   2  0  0,  -1  0  1,   0  1  1,   1  0  1,   0  0  2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        12 Report
               3  1  0,   4  0  0,   2  2  1,   3  0  1,   1  2  2,   2  1  2,
               3  2  2,  -3  0  3,  -1  0  3,  -4  0  4,  -2  0  4,  -3  0  5,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....        11 Note
               3  1  0,   4  0  0,   1  0  1,   2  2  1,   1  2  2,   2  1  2,
               3  2  2,  -3  0  3,  -4  0  4,  -2  0  4,  -3  0  5,
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Alert level G

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PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I1       --Cu1_a    .      56.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --P1       .       9.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --N1       .       7.0 s.u.
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data     Please Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        10 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.66 Note
             Predicted wR2: Based on SigI**2  1.87 or SHELX Weight  9.58
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         7 Info
PLAT982_ALERT_1_G The Cu-f'=    0.3283 Deviates from  IT-value =       0.3201 Check
PLAT982_ALERT_1_G The  I-f'=   -0.4378 Deviates from  IT-value =      -0.4742 Check
PLAT983_ALERT_1_G The Cu-f"=    1.2708 Deviates from  IT-Value =       1.2651 Check
PLAT983_ALERT_1_G The  I-f"=    1.8209 Deviates from  IT-Value =       1.8119 Check
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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
 10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 14 ALERT level G = General information/check it is not something unexpected

  8 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
  4 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

Datablock G196 - ellipsoid plot