checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

```
Bond precision:   C-C = 0.0036 A           Wavelength=0.71073

Cell:           a=8.7358(18)       b=9.303(2)        c=10.296(2)
                alpha=68.021(3)    beta=86.161(3)    gamma=76.083(3)
Temperature:    296 K

                 Calculated                  Reported
Volume           752.9(3)                    753.0(3)
Space group      P -1                        P -1
Hall group       -P 1                        -P 1
Moiety formula   C13 H11 Cu N2 O6, 2(H2 O)   ?
Sum formula      C13 H15 Cu N2 O8            C13 H15 Cu N2 O8
Mr               390.82                      390.81
Dx,g cm-3        1.724                       1.724
Z                2                           2
Mu (mm-1)        1.498                       1.498
F000             400.0                       400.0
F000'            400.85
h,k,lmax         10,11,12                    10,11,12
Nref             2991                        2963
Tmin,Tmax        0.626,0.706                 0.647,0.723
Tmin'            0.614

Correction method= # Reported T Limits: Tmin=0.647 Tmax=0.723
AbsCorr = ?

Data completeness= 0.991            Theta(max)= 26.104

R(reflections)= 0.0321( 2714)                    wR2(reflections)=
                                                 0.0866( 2963)
S = 1.052                  Npar= 217
```

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

```
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...       1.13 Do !
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)        2.2 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        14 Report
                  1  0  0,  -7  1  0,  -8  2  0,   0  2  0,  -4  8  0,   4 -3  1,
                  5 -3  1,   6 -3  1,  -5  0  1,  -2  0  1,  -1  0  1,  -7  1  1,
                  3  6  2,   0 -7  4,
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          6 Report
              H1A   H1B   H2A   H2B   H3A   H3B
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.16 Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated   and Succeeded by SHELXL     2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         13 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.095 Note
              Predicted wR2: Based on SigI**2  2.80 or SHELX Weight  8.24
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 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
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   5 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 11/11/2024; check.def file version of 11/11/2024

Datablock shelx - ellipsoid plot