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

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Bond precision:   C-C = 0.0053 A            Wavelength=1.54184

Cell:          a=9.3380(5)        b=9.6015(5)        c=11.3991(7)
               alpha=97.334(5)    beta=104.595(5)    gamma=116.924(5)
Temperature:   293 K

                  Calculated                  Reported
Volume            846.52(10)                  846.52(9)
Space group       P -1                        P -1
Hall group        -P 1                        -P 1
Moiety formula    C13 H13 Cu N3 O7 S, H2 O    ?
Sum formula       C13 H15 Cu N3 O8 S          C13 H15 Cu N3 O8 S
Mr                436.89                      436.88
Dx,g cm-3         1.714                       1.714
Z                 2                           2
Mu (mm-1)         3.442                       3.442
F000              446.0                       446.0
F000'             444.10
h,k,lmax          11,11,14                    11,11,14
Nref              3355                        3335
Tmin,Tmax         0.516,0.653                 0.894,1.000
Tmin'             0.334

Correction method= # Reported T Limits: Tmin=0.894 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994          Theta(max)= 72.408

R(reflections)= 0.0449( 2989)      wR2(reflections)= 0.1323( 3335)

S = 1.047                  Npar= 252
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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 B

PLAT230_ALERT_2_B Hirshfeld Test Diff for   C10   --C11   .   9.0 s.u.

Author Response: mainly due to rotational disorder of the thiophene group around the linking C-C bond

PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of   O31 Check

Author Response: mainly due to librational disorder of nitrate NO3 group around the N-atom

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🟡 Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for   S   --C9   .   6.2 s.u.

Author Response: mainly due to rotational disorder of the thiophene group around the linking C-C bond

PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   S Check

Author Response: mainly due to librational disorder of nitrate NO3 group around the N-atom

PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Cu Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   N3 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C9 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2B   ..N3   .   2.65 Ang.

⚪ Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   6 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.005 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   4 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)   293 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu   (II)   .   2.25 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters   1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   6 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   20 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   2.2 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged   Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   2 Info

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

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 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 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
 4 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check
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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 18/09/2020; check.def file version of 20/08/2020