checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bs

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: bs

Bond precision: C-C = 0.0075 A Wavelength=0.71073

Cell: a=11.6920(9) b=17.5555(14) c=15.4921(17)
alpha=90 beta=96.439(2) gamma=90
Temperature: 328 K

	Calculated	Reported
Volume	3159.8(5)	3159.8(5)
Space group	I 2/c	I2/c
Hall group	-I 2yc	-I2yc
Moiety formula	C24 H20 Cu F6 N8 Si [+ solvent]	?
Sum formula	C24 H20 Cu F6 N8 Si [+ solvent]	C48 H40 Cu2 F12 N16 Si2
Mr	626.12	1252.22
Dx,g cm-3	1.316	1.316
Z	4	2
Mu (mm-1)	0.790	0.790
F000	1268.0	1268.0
F000'	1270.21	
h,k,lmax	13,20,18	13,20,18
Nref	2807	2807
Tmin,Tmax	0.888,0.910	
Tmin'	0.888	

Correction method= Not given

Data completeness= 1.000 Theta(max)= 25.098

R(reflections)= 0.0624(2379) wR2(reflections)= 0.1809(2807)

S = 1.082 Npar= 184

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

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PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        Si1 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          2 Check
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ...          ! Note
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Alert level C

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PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         F1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C5 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C4       -C6_b     .       1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0075 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.550 Check
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          2 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      15.25 Why ?
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT432_ALERT_2_G Short Inter X...Y Contact  F4       ..C7       .       2.82 Ang.
                                              x,-y,1/2+z  =      6_556 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        455 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.17 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         24 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         68% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       50.2 Degree
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
   3 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   4 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
   6 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 12/09/2022; check.def file version of 09/08/2022

Datablock bs - ellipsoid plot