checkCIF/PLATON report

Structure factors have been supplied for datablock(s) as

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: as

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

Cell: a=11.7160(5) b=17.4096(9) c=15.4786(8)
alpha=90 beta=96.609(2) gamma=90
Temperature: 198 K

	Calculated	Reported
Volume	3136.2(3)	3136.2(3)
Space group	I 2/a	I 2/a
Hall group	-I 2ya	-I 2ya
Moiety formula	C24 H20 Cu F6 N8 Si [+ solvent]	?
Sum formula	C24 H20 Cu F6 N8 Si [+ solvent]	C24 H20 Cu F6 N8 O0 Si
Mr	626.12	626.11
Dx,g cm-3	1.326	1.326
Z	4	4
Mu (mm-1)	0.796	0.796
F000	1268.0	1268.0
F000'	1270.21	
h,k,lmax	13,20,18	13,20,18
Nref	2648	2648
Tmin,Tmax	0.887,0.909	
Tmin'	0.887	

Correction method= Not given

Data completeness= 1.000 Theta(max)= 24.598

R(reflections)= 0.0591(2401) wR2(reflections)= 0.2619(2648)

S = 1.196 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

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 .. 6 Check
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

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Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5857
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.26 Report
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 C8 Check
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 ..... 4.284 Check

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Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C24 H20 Cu F6 N8 O0 Si
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	96.00	96.00	0.00
H	80.00	80.00	0.00
Cu	4.00	4.00	0.00
F	24.00	24.00	0.00
N	32.00	32.00	0.00
O	4.00	0.00	4.00
Si	4.00	4.00	0.00

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 22 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
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
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0200 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 443 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.19 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 309 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 !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 80% 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

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PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       49.2 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
  21 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
  10 ALERT type 3 Indicator that the structure quality may be low
   6 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 10/05/2023; check.def file version of 10/05/2023

Datablock as - ellipsoid plot