checkCIF/PLATON report

Structure factors have been supplied for datablock(s) b

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: b

Bond precision: C-C = 0.0071 A Wavelength=0.71073

Cell: a=11.6529(7) b=17.5398(10) c=15.5802(9)
alpha=90 beta=96.327(4) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	3165.0(3)	3165.0(3)
Space group	I 2/c	I 2/c
Hall group	-I 2yc	-I 2yc
Moiety formula	C24 H20 Cu F6 N8 Si, 0.668(C3 H8)	?
Sum formula	C26 H25.34 Cu F6 N8 Si	C26 H0 Cu F6 N8 Si
Mr	655.57	655.70
Dx,g cm-3	1.376	1.322
Z	4	4
Mu (mm-1)	0.793	0.790
F000	1337.5	1236.0
F000'	1339.70	
h,k,lmax	13,20,18	13,20,18
Nref	2779	2727
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.981 Theta(max)= 24.997

R(reflections)= 0.0657(2297) wR2(reflections)= 0.2099(2727)

S = 1.054 Npar= 215

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
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Author Response: These alerts are generated because there is disorder in the structure

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Alert level C

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CHEMW01_ALERT_1_C  The ratio of given/expected molecular weight as calculated
            from the _chemical_formula_sum lies outside
            the range 0.99 <> 1.01
            Calculated formula weight =   629.9620
            Formula weight given      =   655.7000
DENSD01_ALERT_1_C  The ratio of the submitted crystal density and that
            calculated from the formula is outside the range 0.99 <> 1.01
            Crystal density given    =      1.322
            Calculated crystal density =      1.376
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT046_ALERT_1_C Reported Z, MW and D(calc) are Inconsistent ....      1.376 Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT213_ALERT_2_C Atom F4              has ADP max/min Ratio .....        3.4 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         F3 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        Cu1 Check
```

Author Response: These alerts are generated because there is disorder in the structure

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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C5 Check
```

Author Response: These alerts are generated because there is disorder in the structure

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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 ..............    0.00712 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         52 Report
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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C26 Cu1 F6 N8 Si1
            Atom count from the _atom_site data:  C26.004 H25.34399 Cu1 F6 N8 Si1
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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  C26 H0 Cu F6 N8 Si
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        104.00    104.02   -0.02
           H          4.00    101.38  -97.38
           Cu         4.00      4.00    0.00
           F         24.00     24.00    0.00
           N         32.00     32.00    0.00
           Si         4.00      4.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        100% Note
PLAT411_ALERT_2_G Short Inter H...H Contact  H2       ..H15B     .       2.14 Ang.
                                          -1/2+x,1/2-y,z  =      8_455 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H3       ..H19A     .       1.93 Ang.
                                        3/2-x,1/2-y,1/2-z  =      7_655 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H8       ..H14C     .       1.76 Ang.
                                           1-x,1-y,1-z  =      5_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F1       ..C14      .       2.48 Ang.
                                           -1+x,-1+y,z  =      1_445 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F1       ..C14      .       2.48 Ang.
                                          1-x,-1+y,1/2-z  =      2_645 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F2       ..C16      .       2.47 Ang.
                                        1/2-x,1/2-y,1/2-z  =      7_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F2       ..C15      .       2.94 Ang.
                                        1/2-x,1/2-y,1/2-z  =      7_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F2       ..C17      .       2.95 Ang.
                                        1/2-x,1/2-y,1/2-z  =      7_555 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C16      -H16C            1_555   1_555 ........     #   43 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.16 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 .............        20 Note
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        69% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         50 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.1 Low
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 ..       50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
31 **ALERT level G** = General information/check it is not something unexpected

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 13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 22 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
  6 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 b - ellipsoid plot