checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelxl

Bond precision: C-C = 0.0225 A Wavelength=0.71073

Cell: a=22.5641(9) b=37.1408(15) c=30.0021(11)
alpha=90 beta=105.686(1) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	24206.8(16)	24206.8(16)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C62 H48 Cu3 N3 O15, C	((C18 H16 O4)2, (Cu 2+)2, (C3 N O H7)2)1.5
Sum formula	C63 H48 Cu3 N3 O15	C63 H69 Cu3 N3 O15
Mr	1277.70	1298.83
Dx,g cm-3	0.701	0.713
Z	8	8
Mu (mm-1)	0.557	0.557
F000	5232.0	5400.0
F000’	5241.90	
h,k,lmax	26,44,35	26,44,35
Nref	21466	21379
Tmin,Tmax	0.783,0.841	
Tmin’	0.783	

Correction method= Not given

Data completeness= 0.996 Theta(max)= 25.070

R(reflections)= 0.0808(12669) wR2(reflections)= 0.2465(21379)

S = 1.030 Npar= 685

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 A
PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) 11

Alert level B

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PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        4.6 Ratio
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for       C111
PLAT341_ALERT_3_B Low Bond Precision on  C-C Bonds ...............     0.0225 Ang
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Alert level C

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CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.99 <> 1.01
           From the CIF: _cell_formula_units_Z                   8
           From the CIF: _chemical_formula_weight          1298.83
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   63.00  756.69
           H         1.01   48.00   48.38
           N        14.01    3.00   42.02
           O        16.00   15.00  239.99
           Cu       63.55    3.00  190.64
           Calculated formula weight            1277.72
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT043_ALERT_1_C Check Reported Molecular Weight .............    1298.83
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          1
PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....        3.2 prola
PLAT213_ALERT_2_C Atom C18             has ADP max/min Ratio .....        4.0 prola
PLAT213_ALERT_2_C Atom C59             has ADP max/min Ratio .....        3.3 prola
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        5.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O10    --  C31     ..       0.18 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C121
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C131
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Cu1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Cu3
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C14
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C56
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C12    -C17          1.37 Ang.
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C63 H69 Cu3 N3 O15
            Atom count from _chemical_formula_moiety:C6039 H14038 Cu2 N2001 O200
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:C63 H69 Cu3 N3 O15
            Atom count from the _atom_site data:  C63 H48 Cu3 N3 O15
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z    8
           From the CIF: _chemical_formula_sum  C63 H69 Cu3 N3 O15
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         504.00    504.00    0.00
           H         552.00    384.00  168.00
           Cu         24.00     24.00    0.00
           N          24.00     24.00    0.00
           O         120.00    120.00    0.00
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HYDTR01_ALERT_1_G  Extra text has been found in the _refine_ls_hydrogen_treatment fi
           Explanatory text should be in the _publ_section_refinement field.
           Hydrogen treatment given as constrained
           Hydrogen treatment identified as  constr
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         6
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .         3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....         ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.      0.15
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....         ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....         ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....         ?
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..       C112
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..       C113
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..       C121
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..       C122
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..       C123
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..       C131
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..       C133
PLAT344_ALERT_2_G Check sp?     Angle Range in Solvent/Ion for ...       C132
PLAT432_ALERT_2_G Short Inter X...Y Contact  N131   ..  C132    ..      1.82 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C131   ..  C132    ..      2.71 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C132   ..  C133    ..      3.16 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         4
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed          !
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
26 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Our explanations to Checkcif Alert level A and B:

Level A

1. PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) 11

The DMF molecules, which are weakly coordinated to the Cu atoms and at least in one case explicitly disordered, have very high anisotropic thermal displacement parameters. Most of atoms comprising these molecules were refined with restricted isotropic thermal displacement parameters.

The SQUEEZE procedure (Platon) was applied to remove the disordered guest molecules of DMF in the large pores of the structure.

Level B

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.6 Ratio

2. This effect is due to the high isotropic parameters of the weakly coordinated DMF molecules (see 1.)

3. PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for C111

C111 is an atom of a weakly coordinated DMF molecule, which neighbors the O-anchor atom which is coordinated to the Cu-atom and has inherently lower U_{eq}.

4. PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds .. 0.0225 Ang

See 1.

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*, 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 15/02/2012; check.def file version of 10/02/2012

Datablock shelxl - ellipsoid plot