Supporting Information

Synthesis and Characterization of Copper(II) Complexes with Tetraazadiphenol Macrocyclic Ligand Having Cyclohexane Rings

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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: complex1

Bond precision: C-C = 0.0028 A Wavelength=0.71073

Cell: a=16.8306(7) b=7.9928(3) c=24.5686(10)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	3305.1(2)	3305.1(2)
Space group	C m c a	Cmca
Hall group	-C 2bc 2	-C 2bc 2
Moiety formula	C30 H34 Cl2 Cu2 N4 O2, 6(H2 O)	C30 H34 Cl2 Cu2 N4 O2, 6(H2 O)
Sum formula	C30 H46 Cl2 Cu2 N4 O8	C30 H46 Cl2 Cu2 N4 O8
Mr	788.71	788.69
Dx,g cm-3	1.585	1.585
Z	4	4
Mu (mm-1)	1.504	1.504
F000	1640.0	1640.0
F000'	1644.30	
h,k,lmax	21,10,31	21,10,31
Nref	1865	1865
Tmin,Tmax	0.588,0.637	0.551,0.661
Tmin'	0.503	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 26.990

R(reflections)= 0.0294(1647) wR2(reflections)= 0.0830(1865)

S = 1.082 Npar= 129

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 G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 5
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 7.32

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PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1    --  Cl1     ..       11.4 su
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................         20 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          9
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.37 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         21
             C7   -N1   -C7'     1.555   1.555   1.555             27.05 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         43
             C7   -C8   -C7'     1.555   1.555   1.555             27.01 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         46
             C9   -C8   -C9'     1.555   1.555   1.555             23.30 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2
             H2 O
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```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 11 ALERT level G = General information/check it is not something unexpected

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

Datablock: complex2

```
Bond precision:  C-C = 0.0033 A          Wavelength=0.71073

Cell:            a=16.8510(7)     b=8.0835(3)     c=24.7963(11)
                 alpha=90         beta=90         gamma=90
Temperature:     173 K
```

	Calculated	Reported
Volume	3377.6(2)	3377.6(2)
Space group	C m c a	Cmca
Hall group	-C 2bc 2	-C 2bc 2
Moiety formula	C30 H34 Br2 Cu2 N4 O2, 6(H2 O)	C30 H34 Br2 Cu2 N4 O2, 6(H2 O)
Sum formula	C30 H46 Br2 Cu2 N4 O8	C30 H46 Br2 Cu2 N4 O8
Mr	877.61	877.61
Dx,g cm-3	1.726	1.726
Z	4	4
Mu (mm-1)	3.680	3.680
F000	1784.0	1784.0
F000'	1784.95	
h,k,lmax	21,10,31	21,10,31
Nref	1908	1905
Tmin,Tmax	0.345,0.692	0.405,0.710
Tmin'	0.319	

```
Correction method= MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.980

R(reflections)= 0.0276( 1625)     wR2(reflections)= 0.0795( 1905)

S = 1.129                  Npar= 129
```

```
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 G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms .............         5
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       7.02
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Br1    --  Cu1     ..      23.7 su
PLAT301_ALERT_3_G Note: Main Residue  Disorder ....................        20 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         9
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.37 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         21
             C7   -N1   -C7'     1.555   1.555   1.555             26.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         44
             C7   -C8   -C7'     1.555   1.555   1.555             26.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         45
             C9   -C8   -C9'     1.555   1.555   1.555             22.00 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2
             H2 O
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
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   6 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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

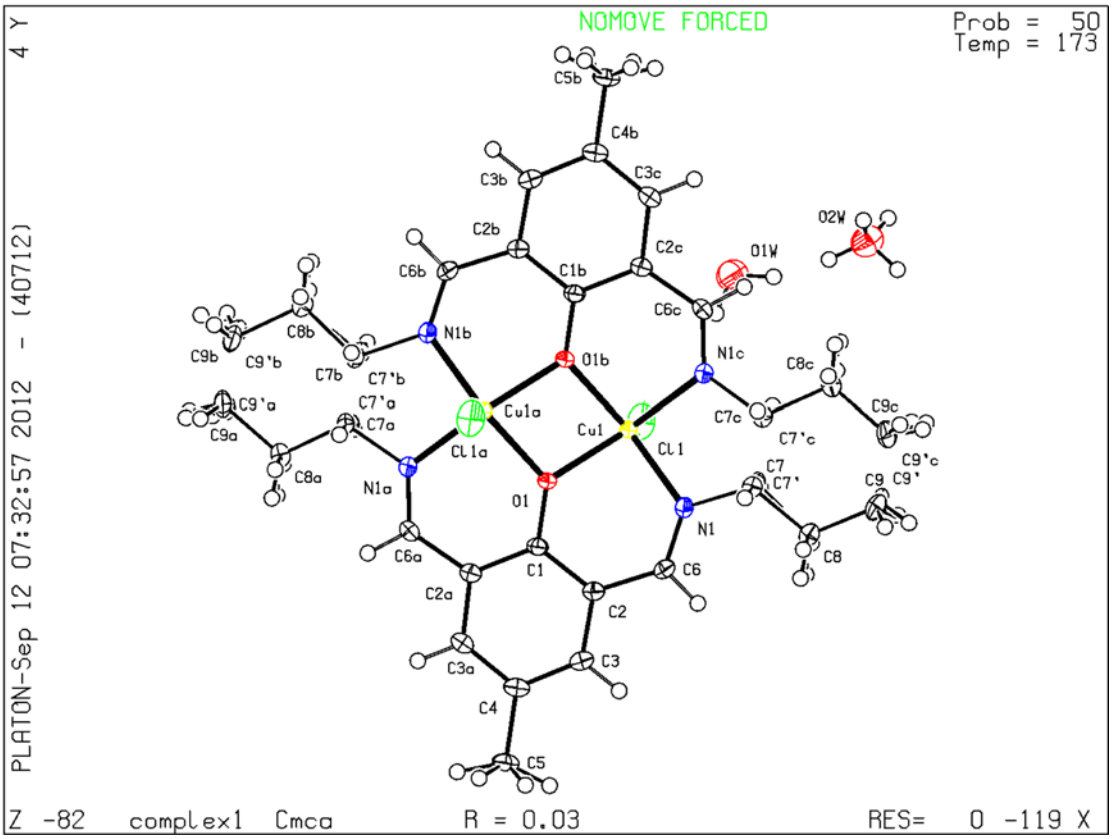
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 04/07/2012; check.def file version of 28/06/2012

Datablock complex1 - ellipsoid plot



Datablock complex2 - ellipsoid plot