Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Four monomeric copper(II) complexes of non-steroidal anti-inflammatory drug Ibuprofen and N-donor ligands: Syntheses, characterization, crystal structures and cytotoxicity studies.

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Table of Contents

Table S1. Hydrogen bonding parameters (Å, °) for complexes **1-4**

	D-H	D....A	H....A	D-H...A
Complex 1				
O1W-H...O4	0.85(4)	2.608(4)	1.78(4)	168(3)
O1W-H...O1^{i}	0.87(3)	2.768(3)	1.91(3)	164(3)
C11-H...O1^{i}	0.93	3.594(3)	2.67	170
Symmetry code: (i) 1-x,-y,-z				
Complex 2				
O1W-H...O2	0.87(3)	2.648(3)	1.83(4)	155(3)
C1-H...O2W	0.93	3.295(4)	2.44	152
O1W-H...O3^{i}	0.84(2)	2.807(2)	1.98(2)	170(2)
C5-H...O3^{i}	0.93	3.485(3)	2.56	170
C10-H...O2W^{ii}	0.93	3.386(4)	2.53	153
Short contacts:				
O4 ...O2W		2.703(5)		
O2W...O1^{iii}		3.014(3)		
Symmetry codes: (i) 1-x,-y,-z; (ii) x+1,y,z; (iii) 1-x,1-y,-z				
Complex 3				
O1W -H ...O2	0.87(3)	2.967(5)	2.10(4)	174(3)
N1-H...O1W ^{i}	0.86(3)	3.102(5)	2.27(3)	162(3)
O1W-H...O2^{ii}	0.85(3)	3.030(5)	2.19(4)	168(3)
C1-H...O1^{iii}	0.97	3.442(4)	2.61	143
Symmetry codes: (i) x,y+1,z; (ii) -x,y-1/2,1/2-z; (iii) -x,1-y,-z				
Complex 4				
C3-H ...O2	0.96	3.417(7)	2.64	138
O1W-H ...O2^{i}	0.83(6)	2.714(4)	1.91(6)	163(6)
N1-H ...O3^{i}	0.86(4)	2.768(6)	1.94(4)	163(4)
N1-H ...O2^{ii}	0.91(6)	2.886(6)	2.07(6)	148(6)
Symmetry codes: (i) 1-x,y+1,1/2-z; (ii) 1-x,y,1/2-z				

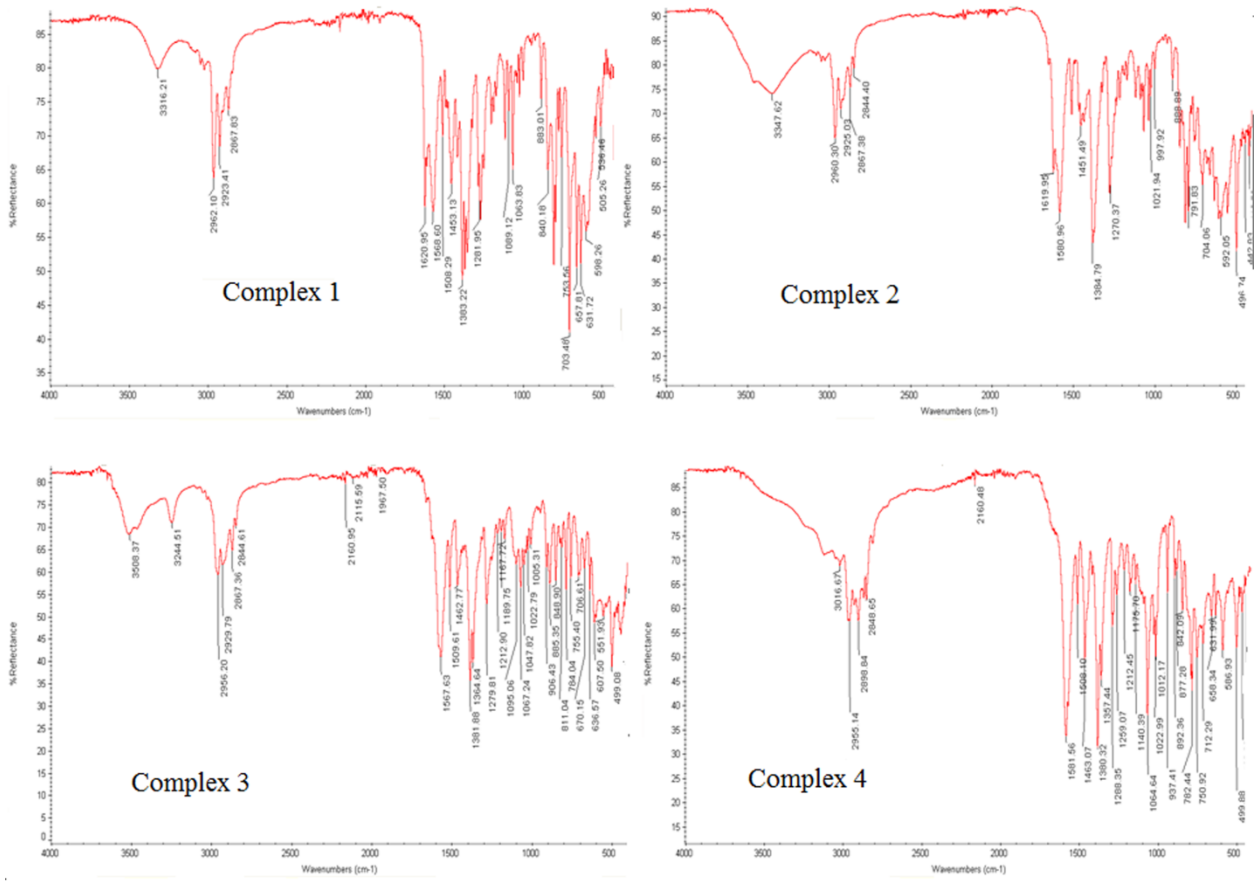

Figure S1. FT-IR spectra of complexes 1-4

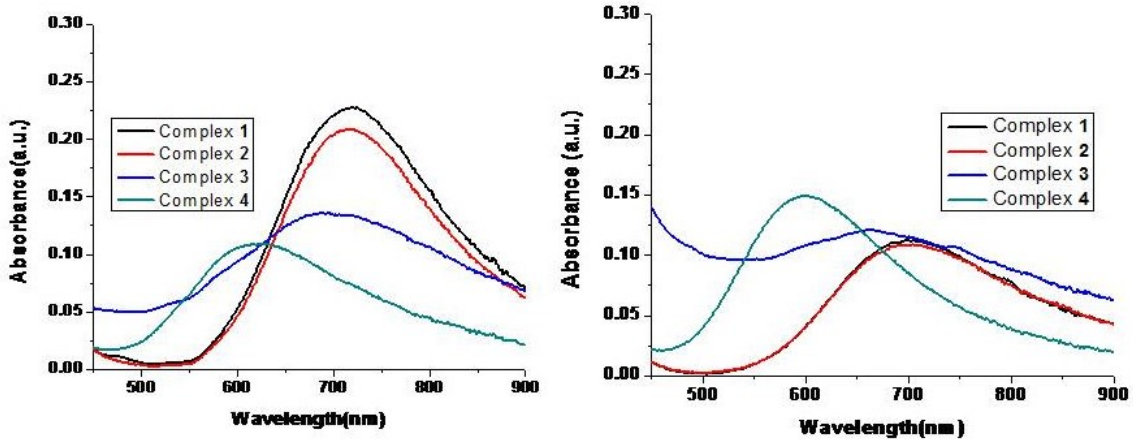

Figure S2. UV-Visible spectra of complexes 1-4 in DMSO and methanol solvent**.**

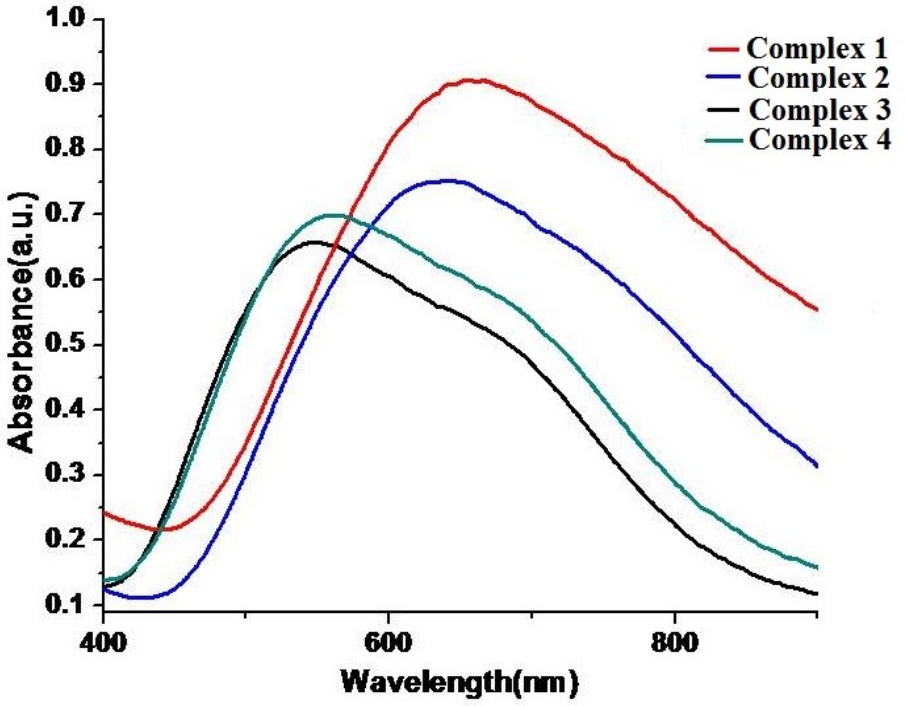

Figure S3. Diffuse Reflectance spectra of complexes **1-4**

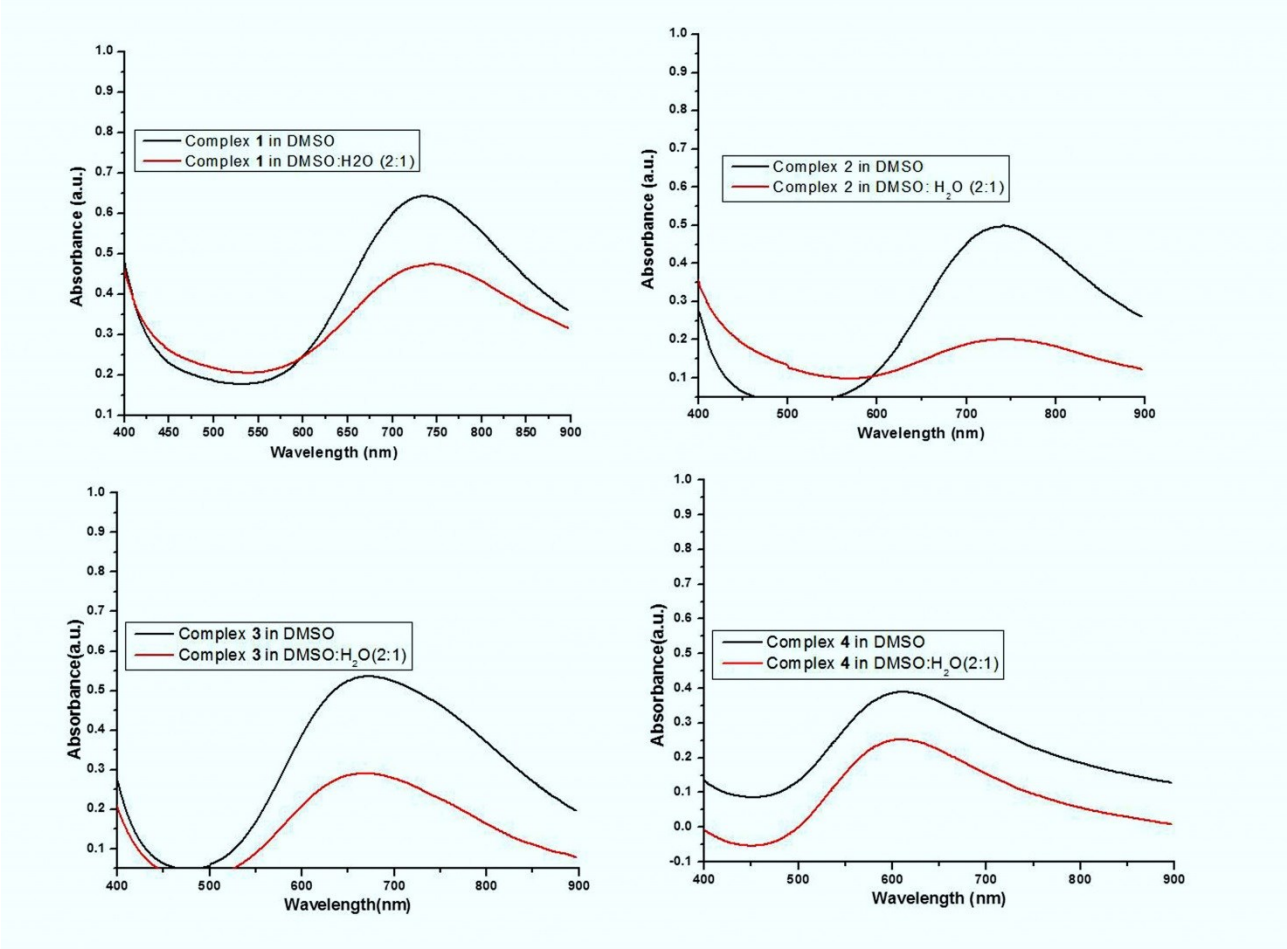

Fig. S4: UV-Visble spectra of complexes 1-4 using DMSO and DMSO-H_2O (2:1) as solvent.

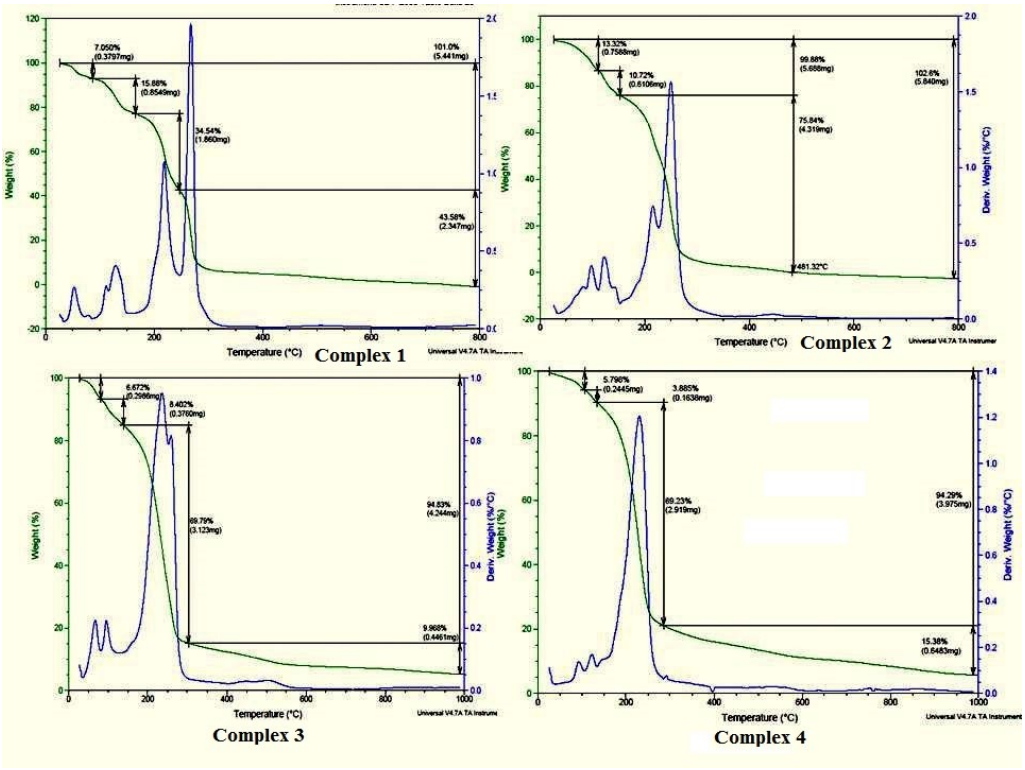

Fig. S5. Combined TGA-DTA plots for complexes 1-4

Datablock: betapic

```
Bond precision:      C-C = 0.0063 A              Wavelength=0.71073
Cell:        a=9.4147(2)     b=11.8811(3)    c=17.5005(4)
             alpha=95.564(1) beta=103.187(1) gamma=103.464(1)
Temperature: 295 K
                    Calculated                      Reported
Volume              1830.12(7)                      1830.12(7)
Space group         P -1                            P -1
Hall group          -P 1                            -P 1
Moiety formula      C38 H50 Cu N2 O5                C38 H50 Cu N2 O5
Sum formula         C38 H50 Cu N2 O5                C38 H50 Cu N2 O5
Mr                  678.35                          678.34
Dx,g cm-3           1.231                           1.231
Z                   2                               2
Mu (mm-1)           0.639                           0.639
F000                722.0                           722.0
F000'               722.90
h,k,lmax            12,15,23                        12,15,23
Nref                8845                            8751
Tmin,Tmax           0.765,0.897                     0.782,0.896
Tmin'               0.741
Correction method= # Reported T Limits: Tmin=0.782
Tmax=0.896 AbsCorr = MULTI-SCAN
Data completeness= 0.989        Theta(max)= 27.998
R(reflections)= 0.0560( 7084)      wR2(reflections)= 0.1690( 8751)
S = 1.079             Npar= 423
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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

PLAT413_ALERT_2_B Short Inter XH3 .. XHn H24B .. H38C .. 1.96 Ang.

Alert level C

PLAT019_ALERT_1_C _diffrn_measured_fraction_theta_full/*_max < 1.0 0.998 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.3 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 6.7 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C23 -- C25 .. 6.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C36 -- C37 .. 6.1 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C22 Check
And 2 other PLAT242 Alerts
More ...
PLAT314_ALERT_2_C Check Small Angle for H2O: Metal-O1W -H1W 78.11 Degree
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00628 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C36 - C37 .. 1.41 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H24A .. H25A .. 1.83 Ang.

Alert level G

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 ... 4 Report

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
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
PLAT793_ALERT_4_G The Model has Chirality at C14 (Centro SPGR) S Verify
PLAT793_ALERT_4_G The Model has Chirality at C27 (Centro SPGR) R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) ..... 2.07 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 28 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note

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Publication of your CIF in IUCr journals

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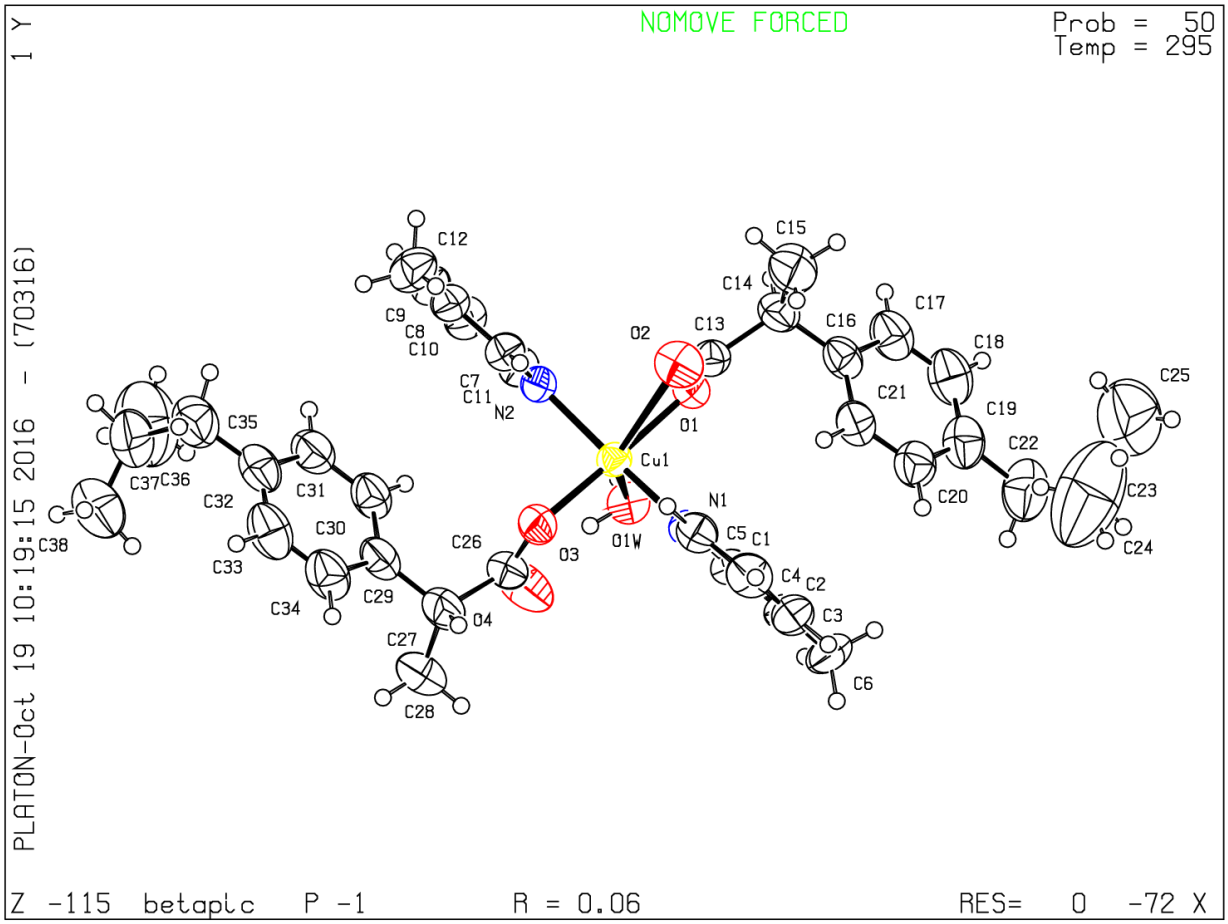
PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock betapic - ellipsoid plot



Complex 2- checkcif

Datablock: Cuibufgamapic

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Bond precision:      C-C = 0.0047 A              Wavelength=0.71073
Cell:        a=10.2706(2)       b=11.8221(3)     c=17.2366(3)
             alpha=104.3850(14) beta=95.6170(14) gamma=109.5680(13)
Temperature: 295 K
                   Calculated                     Reported
Volume             1872.20(7)                     1872.19(7)
Space group        P -1                           P -1
Hall group         -P 1                           -P 1
Moiety formula     C38 H50 Cu N2 O5, O            C38 H50 Cu N2 O5, H2 O
Sum formula        C38 H50 Cu N2 O6               C38 H52 Cu N2 O6
Mr                 694.35                         696.35
Dx,g cm-3          1.232                          1.235
Z                  2                              2
Mu (mm-1)          0.628                          0.629
F000               738.0                          742.0
F000'              738.92
h,k,lmax           13,15,22                       13,15,22
Nref               9057                           8977
Tmin,Tmax          0.773,0.865                    0.646,0.892
Tmin'              0.773
Correction method= # Reported T Limits: Tmin=0.646
Tmax=0.892 AbsCorr = MULTI-SCAN
Data completeness= 0.991       Theta(max)= 27.998
R(reflections)= 0.0490( 7084)      wR2(reflections)= 0.1452( 8977)
S = 1.042             Npar= 432
```

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

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O2W Check
PLAT430_ALERT_2_B Short Inter D...A Contact O2W .. O4 .. 2.70 Ang.

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 2.00 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.0 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 5.7 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C36 Check
PLAT314_ALERT_2_C Check Small Angle for H2O: Metal-O1W -H2W 94.81 Degree
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H24A .. H24A .. 2.09 Ang.

Alert level G

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:C38 H52 Cu1 N2 O6
Atom count from the _atom_site data: C38 H50 Cu1 N2 O6
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 2
From the CIF: _chemical_formula_sum C38 H52 Cu N2 O6
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	76.00	76.00	0.00
H	104.00	100.00	4.00
Cu	2.00	2.00	0.00
N	4.00	4.00	0.00
O	12.00	12.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT793_ALERT_4_G The Model has Chirality at C14 (Centro SPGR) S Verify
PLAT793_ALERT_4_G The Model has Chirality at C27 (Centro SPGR) R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) ..... 2.03 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 2 Note
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES ..... 5 Note

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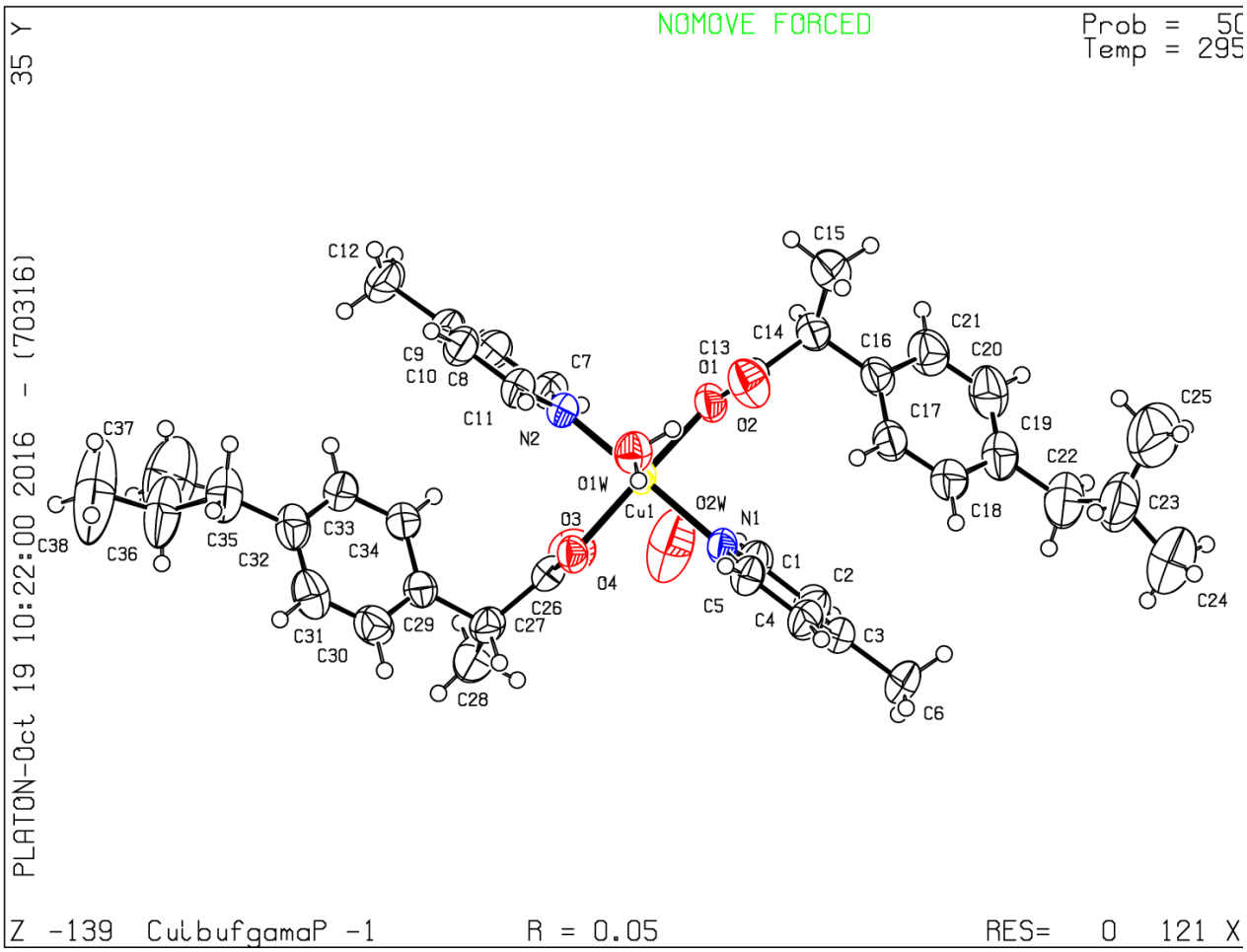
submission.

PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock Cuibufgamapic - ellipsoid plot



Complex 3- checkcif

Datablock: pyrrolidine

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Bond precision:      C-C = 0.0056 A              Wavelength=0.71073
Cell:        a=16.5388(4)   b=6.1918(1)      c=17.4653(4)
             alpha=90       beta=94.8030(14) gamma=90
Temperature: 295 K
                   Calculated                      Reported
Volume             1782.25(7)                      1782.25(7)
Space group        P 21/c                          P 21/c
Hall group         -P 2ybc                         -P 2ybc
Moiety formula     C34 H52 Cu N2 O4, 2(H2 O)       C34 H52 Cu N2 O4, 2(H2 O)
Sum formula        C34 H56 Cu N2 O6                C34 H56 Cu N2 O6
Mr                 652.36                          652.34
Dx,g cm-3          1.216                           1.216
Z                  2                               2
Mu (mm-1)          0.655                           0.655
F000               702.0                           702.0
F000'              702.90
h,k,lmax           21,8,23                         21,8,23
Nref               4303                            4282
Tmin,Tmax          0.855,0.943                     0.848,0.945
Tmin'              0.735
Correction method= # Reported T Limits: Tmin=0.848
Tmax=0.945 AbsCorr = MULTI-SCAN
Data completeness= 0.995       Theta(max)= 28.000
R(reflections)= 0.0548( 3371)      wR2(reflections)= 0.1572( 4282)
S = 1.064             Npar= 235
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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

PLAT230_ALERT_2_B Hirshfeld Test Diff for C8 -- C9 .. 8.0 s.u.

Alert level C

PLAT213_ALERT_2_C Atom C16A has ADP max/min Ratio ..... 3.4 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 4.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C15 -- C17 .. 0.21 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
And 2 other PLAT242 Alerts
More ...
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.6 Note
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C8 -C13 1.37 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C6 - C7 .. 1.38 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of >C15 is Constrained at 0.6 Check
And 23 other PLAT300 Alerts
More ...
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 15 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
H2 O
PLAT793_ALERT_4_G The Model has Chirality at C6 (Centro SPGR) S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 5 Note
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES ..... 4 Note

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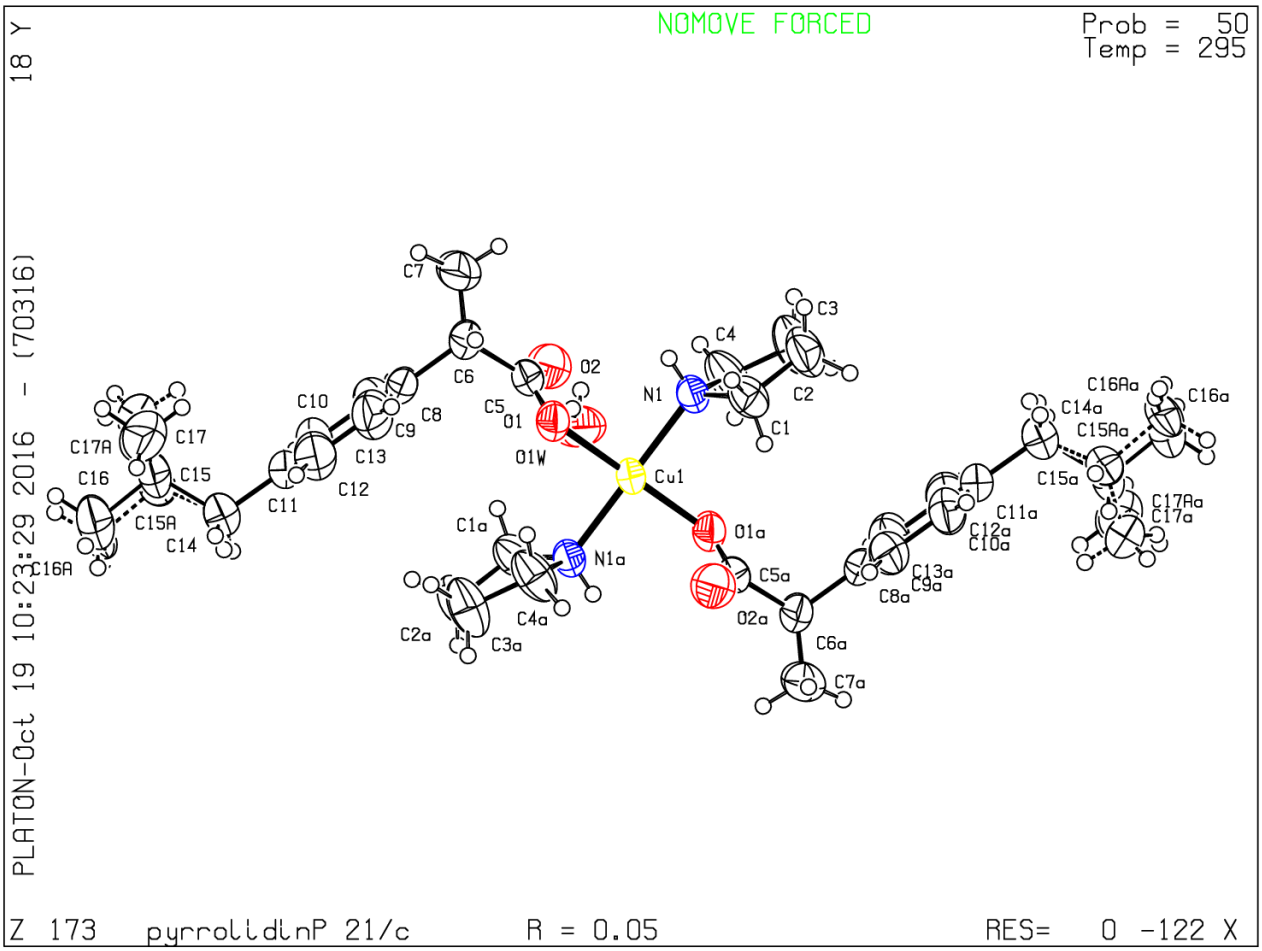
Datablock pyrrolidine - ellipsoid plot



Complex 4- checkcif

Datablock: ibu7

```
Bond precision:      C-C = 0.0081 A              Wavelength=0.71073
Cell:        a=9.6804(8)    b=6.7371(4)    c=29.453(3)
             alpha=90       beta=92.188(3) gamma=90
Temperature: 295 K
```

	Calculated	Reported
Volume	1919.5(3)	1919.5(3)
Space group	P 2/c	P 2/c
Hall group	-P 2yc	-P 2yc
Moiety formula	2(C13 H17 O2), C8 H26 Cu N4 O	2(C13 H17 O2), C8 H26 Cu N4 O
Sum formula	C34 H60 Cu N4 O5	C34 H60 Cu N4 O5
Mr	668.41	668.40
Dx,g cm-3	1.156	1.156
Z	2	2
Mu (mm-1)	0.609	0.609
F000	722.0	722.0
F000'	722.89	
h,k,lmax	11,8,34	11,8,34
Nref	3372	2773
Tmin,Tmax	0.903,0.941	0.621,0.947
Tmin'	0.808	

```
Correction method= # Reported T Limits: Tmin=0.621
Tmax=0.947 AbsCorr = MULTI-SCAN
Data completeness= 0.822       Theta(max)= 24.992
R(reflections)= 0.0640( 2162)      wR2(reflections)= 0.1489( 2773)
S = 1.058             Npar= 230
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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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.822 Note

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Alert level B

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C17 Check

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Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.9 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 6.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C14 -- C15A .. 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C14 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
And 2 other PLAT242 Alerts
More ...
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00809 Ang.
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label O1
CU1 O1
PLAT712_ALERT_1_C ANGLE Unknown or Inconsistent Label O1

N1 CU1 O1
PLAT712_ALERT_1_C ANGLE Unknown or Inconsistent Label O1
N1 CU1 O1
PLAT712_ALERT_1_C ANGLE Unknown or Inconsistent Label O1
N2 CU1 O1
PLAT712_ALERT_1_C ANGLE Unknown or Inconsistent Label O1
N2 CU1 O1

Alert level G

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 ... 4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of >C15A is Constrained at 0.6 Check
And 15 other PLAT300 Alerts
More ...
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 7 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15 -- C16 . 1.72 Ang.
PLAT793_ALERT_4_G The Model has Chirality at C6 (Centro SPGR) S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) ..... 2.12 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 27 Note
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES ..... 3 Note

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
14 **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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
20 ALERT type 4 Improvement, methodology, query or suggestion
1 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* 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 11/08/2016; check.def file version of 04/08/2016

Datablock ibu7 - ellipsoid plot