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

Structure-function correlation of mononuclear nonheme copper(II) compounds based on ligand topology and phenoxazinone synthase activity

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Synthesis and characterization of BQPN

BQPN-H_2 was prepared by modification of a reported procedure [1]. To a stirred THF solution (40 mL) of **BQPN-H_2** (3.8 g, 10.86 mmol), 21.0 mL of aqueous formaldehyde (37%) (6.48 g, 217 mmol) was added. The solution slowly turned dark red after ~5min. To this red mixture, the sodium cyanoborohydride (1.38 g, 22.0 mmol) was added slowly till a yellow colour solution was obtained. The solution was stirred for ~24 h and THF was removed which afforded yellow crude powder. This crude product on recrystallization in hot ethanol resulted in a crystalline solid. Yield = 3.0 g. Anal. Calc. for $C_{23}H_{24}N_4$ **BQPN** (MW = 356.46 g mol^{-1}): C, 77.50; H 6.79; N 15.72; Found: C, 78.35; H, 6.92; N, 15.06. Selected IR bands (KBr, cm−1): 1562 *ν*(C-N); 3134–2746 *ν*(CH).

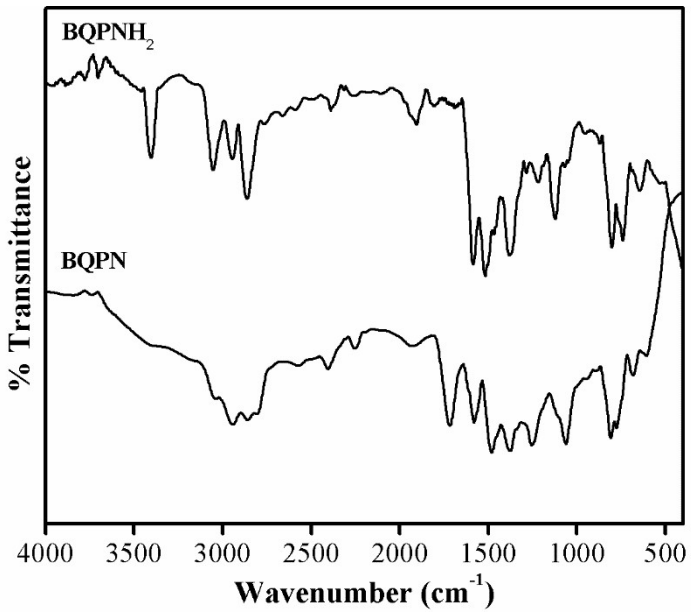

Fig. S1 – Comparative IR spectra's of $BQPNH_2$ and BQPN.

Synthesis of Cu(II) complex [Cu^{II}(BQEN)(CH_3CN)](ClO_4)$_2$ (1)

$CHCl_3$ solution of BQEN (0.43 g / 1.26mmol) was added dropwise to the acetonitrile solution of $Cu(ClO_4)_2.6H_2O$ (0.462 g / 1.26 mmol) resulting in an blue solution. The solution was left for stirring for 12 h and then filtered. Diethyl ether solution was added slowly to yield blue coloured compound. Yield = 0.7g. Crystals suitable for single crystal XRD were grown by slow diffusion of diethyl ether in acetonitrile solution. Anal. Calcd. for $C_{24}H_{25}N_5Cl_2O_8Cu$ **1** (MW = 645.93 g mol^{-1}): C, 44.63; H, 3.90; N, 10.84%. Found: C, 44.90; H, 3.65; N, 10.59%.

IR data (KBr, cm^{-1}): 3184–2777 ν(CH), 1091, 623 $\nu(ClO_4^{-1})$. UV–Vis. λmax(nm) (ε, in L mol^{-1} cm^{-1}) in CH_3CN: 201 (319597), 230 (233240), 301 (60290), 612 (624).

Synthesis of Cu(II) complex $[Cu^{II}(BQPN)(CH_3CN)](ClO_4)_2$ (**2**)

$CHCl_3$ solution of BQPN (0.45 g / 1.26mmol) was added dropwise to the acetonitrile solution of $Cu(ClO_4)_2.6H_2O$ (0.462 g / 1.26 mmol) resulting in an blue solution. The solution was left for stirring for 12 h and then filtered. Diethyl ether solution was added slowly to yield blue coloured compound. Yield = 0.8g. Crystals suitable for single crystal XRD were grown by slow diffusion of diethyl ether in acetonitrile solution. Anal. Calcd. for $C_{25}H_{27}N_5Cl_2O_8Cu$ **2** (MW = 659.96 g mol^{-1}): C, 45.50; H, 4.12; N, 10.61%. Found: C, 45.48; H, 4.28; N, 10.54%. IR data (KBr, cm^{-1}): 3199–2706 ν(CH), 1089, 628 $\nu(ClO_4^{-1})$. UV–Vis. λmax(nm) (ε, in L mol^{-1} cm^{-1}) in CH_3CN: 203 (298203), 227 (182402), 302 (46819), 495 (610).

Phenoxazinone synthase activity

The catalytic oxidation of H_2AP was studied by addition of $1x10^{-5}$ M solution of Cu(II) complex with 100 equiv. of 2-aminophenol (H_2AP, $1x10^{-3}$M) in MeOH under aerobic conditions at room temperature. The catalysed conversion of H_2AP to 2- aminophenoxazine-3-one (2-APX) was monitored at a wavelength of 434 nm (time scan) [2-8] in MeOH. The oxidized product was extracted as 2-aminophenoxazinone species through column chromatography. Neutral alumina was used as a solid support in column and benzene-ethyl acetate solvent mixture was employed as an eluent mixture in the chromatographic separation. The purity of oxidative dimerization product of H_2AP was examined by 1H NMR spectral analysis as well as to identify the final product. 1H NMR data for 2-amino-3H-phenoxazine-3-one (APX), ($CDCl_3$, 400 MHz,) dH: 7.61 (m, 1H), 7.44 (m, 3H), 6.47 (s, 1H), 6.35 (s, 1H), 6.24 (s, 1H).

References

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2. P. K. Mudi, N. Bandopadhyay, M. Joshi, M. Shit, S. Paul, A.R. Choudhury, B. Biswas, *Inorg. Chim. Acta*., 2020, **505,** 119468.
3. N. C. Jana, M. Patra, P. Brand~ao, A. Panja, *Inorg. Chim. Acta*., 2019, **490**, 163.
4. S. S. Massoud, T. Junk, F.A. Mautner, *RSC Adv*,. 2015, **5**, 87139.
5. K. Ghosh, M.G.B. Drew, S. Chattopadhyay, *Inorg. Chim. Acta*., 2018, **482**, 23.
6. S. Thakur, S. Banerjee, S. Das, S. Chattopadhyay, *New J. Chem*., 2019, **43**, 18747.

7. (a) S. Pal, B. Chowdhury, M. Patra, M. Maji, B. Biswas, *Spectrochim. Acta Part A: Mol. Biomol. Spectros*., 2015, **144**, 148; (b) A. De, D. Dey, H.R. Yadav, M. Maji, V. Rane, R.M. kadam, A.R. Choudhury, B. Biswas, *J. Chem. Sci*., 2016, **128**, 1775.
8. C. K. Pal, S. Mahato, H.R. Yadav, A.R. Choudhury, B. Biswas, *Polyhedron*, 2019, **174**, 114156.

Table S1. Selected bond lengths, angles and Hydrogen bonding Parameters for **1**.

Bond lengths [Å]					
Cu(1)-N(1)	2.004(2)	1.997	Cu(1)-N(2)	2.275(3)	2.236
Cu(1)-N(3)	2.126(2)	2.239	Cu(1)-N(4)	1.973(2)	1.997
Co(1)-N(5)	2.036(3)	2.078			
Bond angles [°]					
N(1)-Cu(1)-N(2)	80.30(10)	81.41	N(1)-Cu(1)-N(3)	94.62(9)	96.64
N(1)-Cu(1)-N(4)	177.15(10)	177.29	N(1)-Cu(1)-N(5)	89.11(11)	91.41
N(2)-Cu(1)-N(3)	83.27(9)	84.56	N(2)-Cu(1)-N(4)	101.32(10)	96.53
N(2)-Cu(1)-N(5)	101.70(12)	138.10	N(3)-Cu(1)-N(4)	83.28(10)	81.37
N(3)-Cu(1)-N(5)	174.25(11)	137.33	N(4)-Cu(1)-N(5)	92.84(11)	91.30

Table S2 – Hydrogen bonding Parameters (Å, °) for **1**.

Compound **1**				
D-H···A	D-H/Å	H···A/Å	D···A/Å	D-H···A/°
C1-H1··· O3	0.930	2.336	3.050	133.33
C13-H13B··· O1	0.960	2.652	3.509	149.01
C13-H13B··· O3	0.960	2.621	3.174	116.96
C21-H21··· N5	0.930	2.495	3.032	116.93
C10-H10B··· O1^{i}	0.960	2.452	3.308	148.40
C24-H24A··· O2^{i}	0.960	2.650	3.266	122.28
C15-H15··· O7^{ii}	0.930	2.488	3.416	175.98
C24-H24C··· O2^{iii}	0.960	2.632	3.238	121.49
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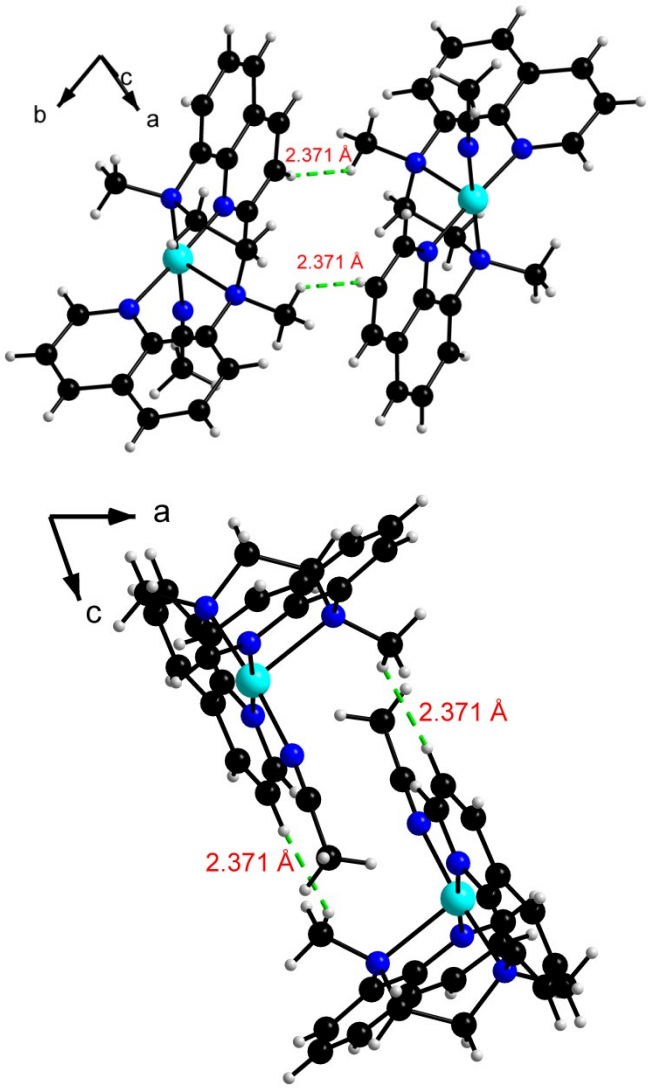
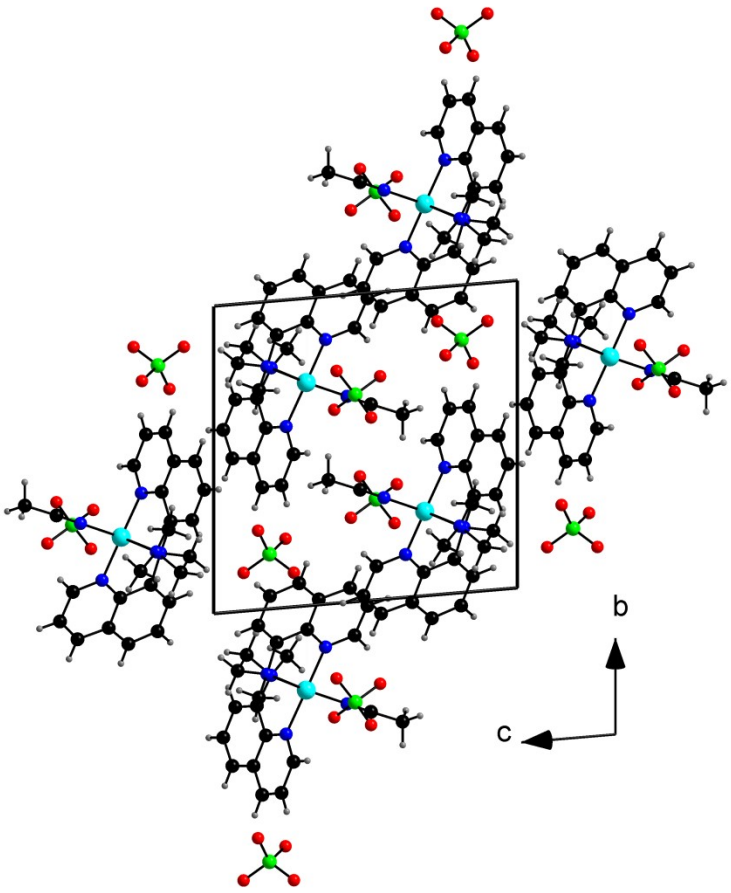


Fig. S2 – C-H···H-C interactions in **1**.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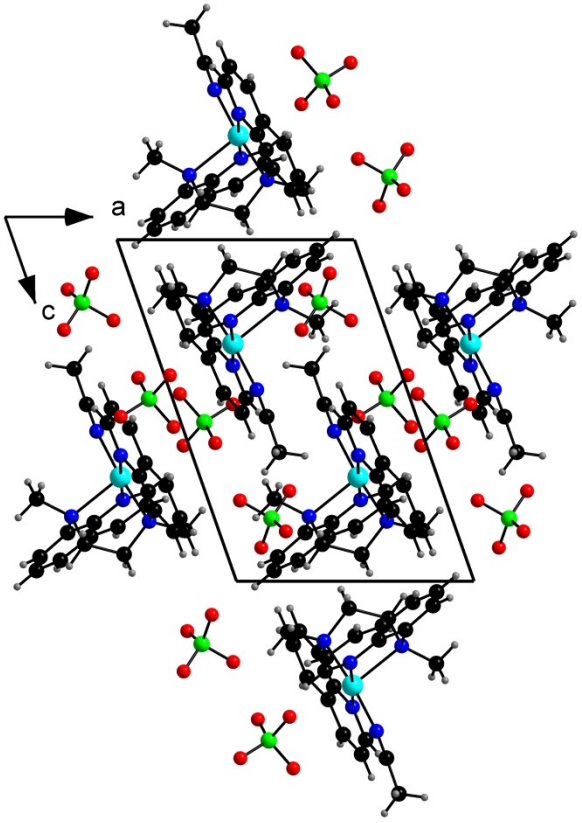
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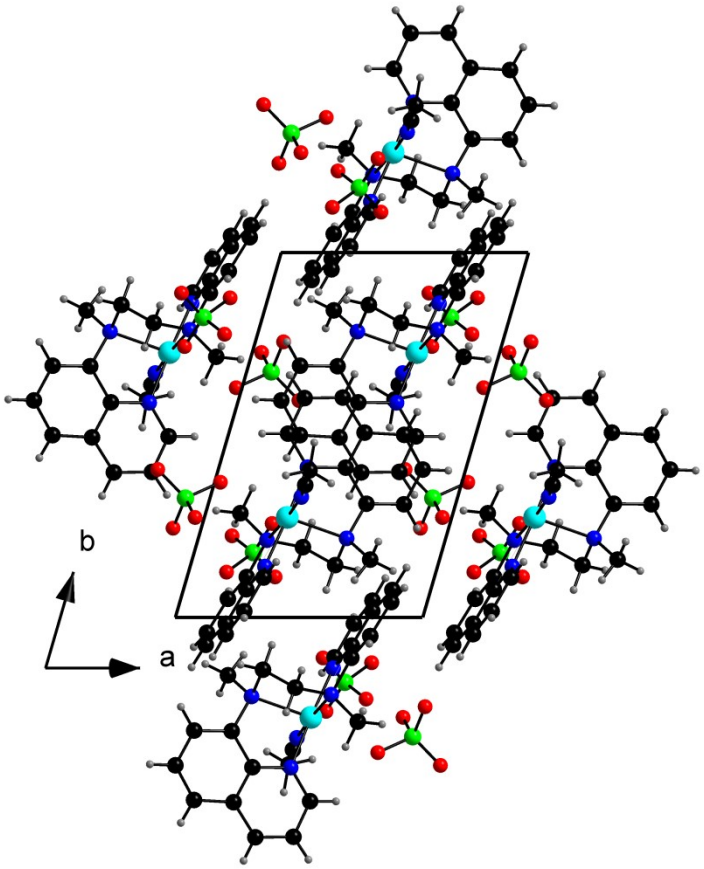


Fig. S3 – Packing diagram in **1** along crystallographic *a*, *b* and *c* axis**.**

Table S3. Selected bond lengths] and angles [°] for **2**.

Bond lengths [Å]					
Cu(1)-N(1)	1.994(3)	2.012	Cu(1)-N(2)	2.096(2)	2.173
Cu(1)-N(3)	2.053(3)	2.067	Cu(1)-N(4)	2.024(2)	2.109
Co(1)-N(5)	2.283(3)	2.274			
Bond angles [°]					
N(1)-Cu(1)-N(2)	81.99(11)	81.67	N(1)-Cu(1)-N(3)	176.81(11)	177.85
N(1)-Cu(1)-N(4)	98.90(11)	97.00	N(1)-Cu(1)-N(5)	87.25(11)	89.03
N(2)-Cu(1)-N(3)	96.16(11)	97.84	N(2)-Cu(1)-N(4)	149.07(10)	139.74
N(2)-Cu(1)-N(5)	118.72(11)	112.89	N(3)-Cu(1)-N(4)	84.03(11)	82.01
N(3)-Cu(1)-N(5)	91.39(11)	93.08	N(4)-Cu(1)-N(5)	92.16(11)	107.31

Table S4– Hydrogen bonding Parameters (Å, °) for **2**.

Compound **2**				
D-H···A	D-H/Å	H···A/Å	D···A/Å	D-H···A/°
C13-H13B··· O6	0.970	2.469	3.379	155.97
C1-H1··· O2^{i}	0.930	2.588	3.441	152.78
C11-H11B··· O4^{ii}	0.970	2.633	3.446	141.59
C14-H14B··· O7^{ii}	0.960	2.551	3.457	157.41
C16-H16··· O8^{ii}	0.930	2.541	3.427	159.34
C14-H14A··· O1^{iii}	0.960	2.531	3.446	159.24
C25-H25C··· O3^{iii}	0.960	2.647	3.429	138.96
C25-H25B··· O4^{iv}	0.960	2.599	3.455	148.56
i = [-x+1/2, y-1/2, -z+1/2], ii = [x+1, y, z], iii = [-x+3/2, y-1/2, -z+1/2], iv = [x+1/2, -y+3/2, z-1/2]				

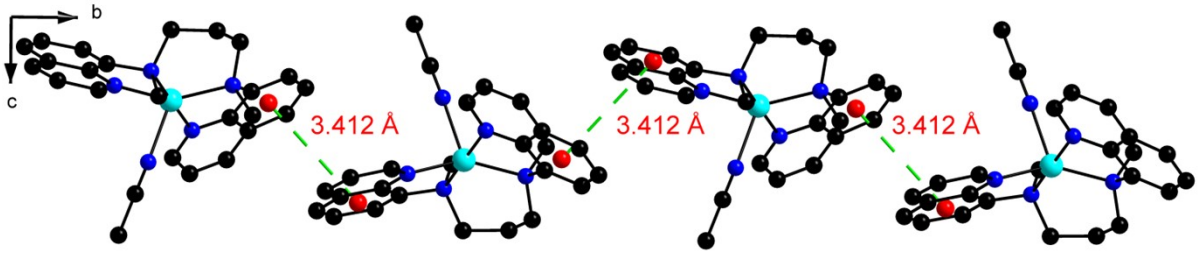
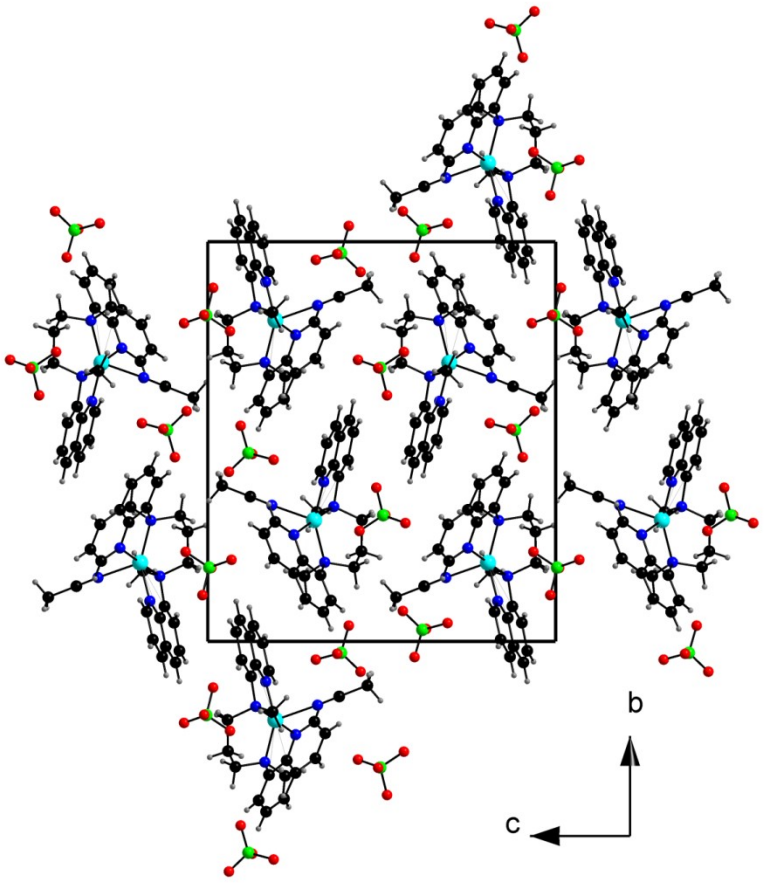


Fig. S4 – π···π interactions in **2**.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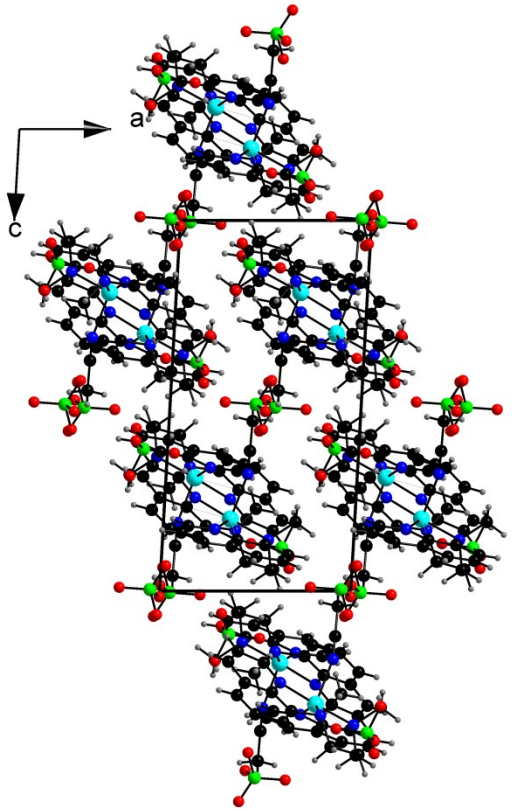
c


a
c

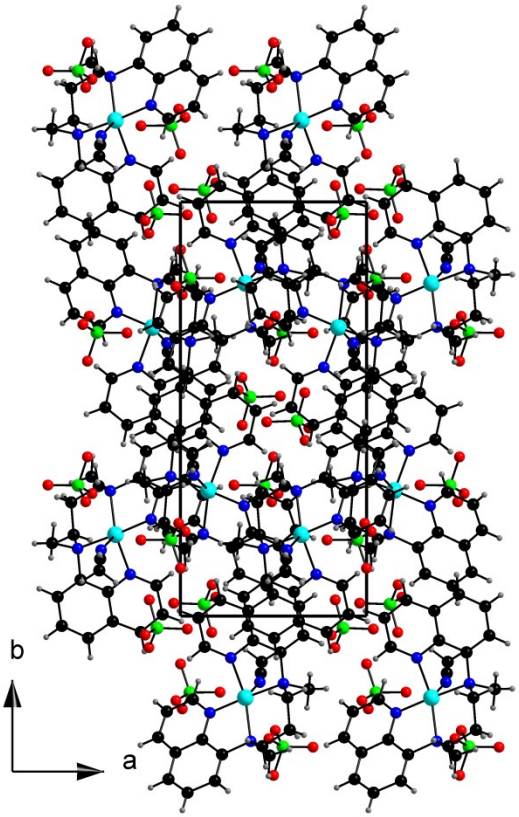


Fig. S5 – Packing diagram in **2** along crystallographic *a*, *b* and *c* axis**.**

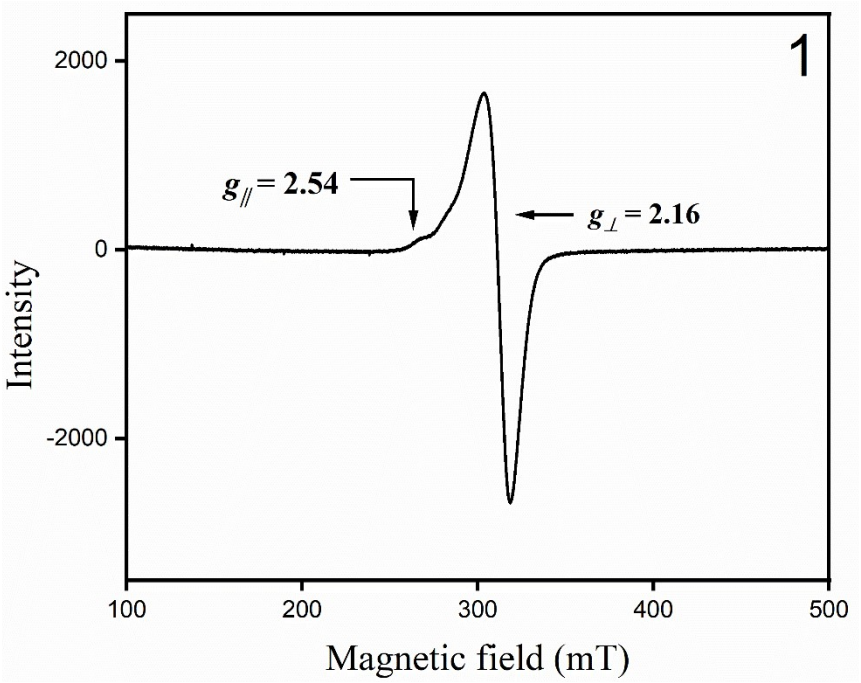


Fig. S6 – X-band EPR spectra of **1** recorded at 77 K in CH_3CN.

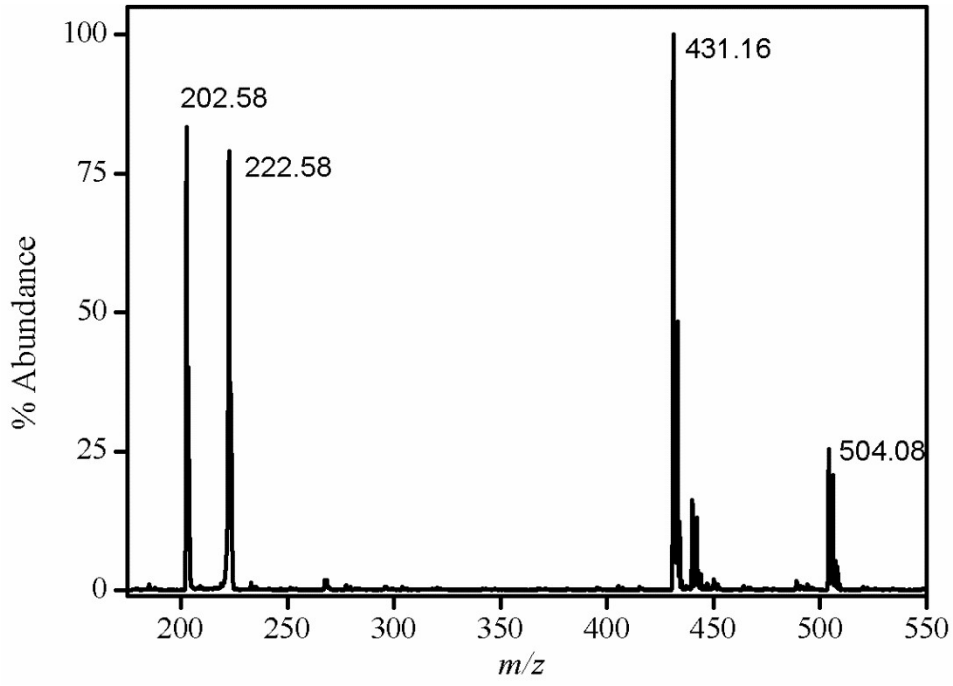


Fig. S7 – ESI-MS spectra of **1**.

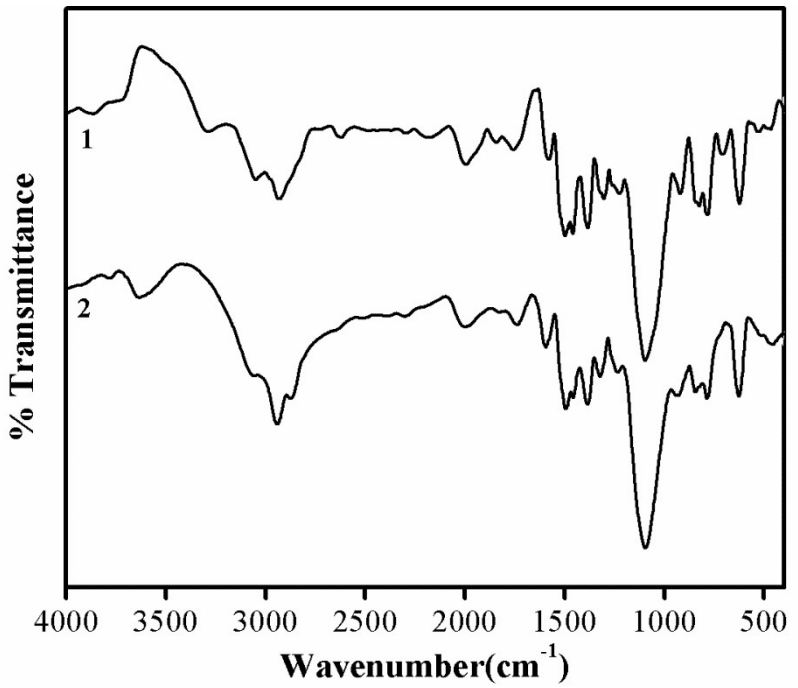


Fig. S8 – Comparative IR spectra's of **1** and **2**.

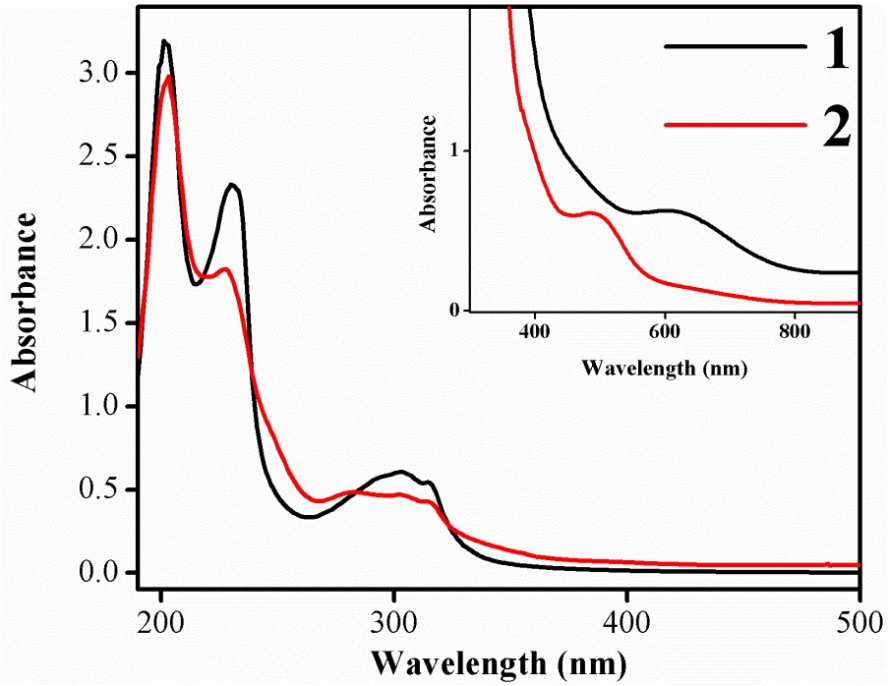


Fig. S9 – Comparative UV-visible spectrum of **1** and **2**.

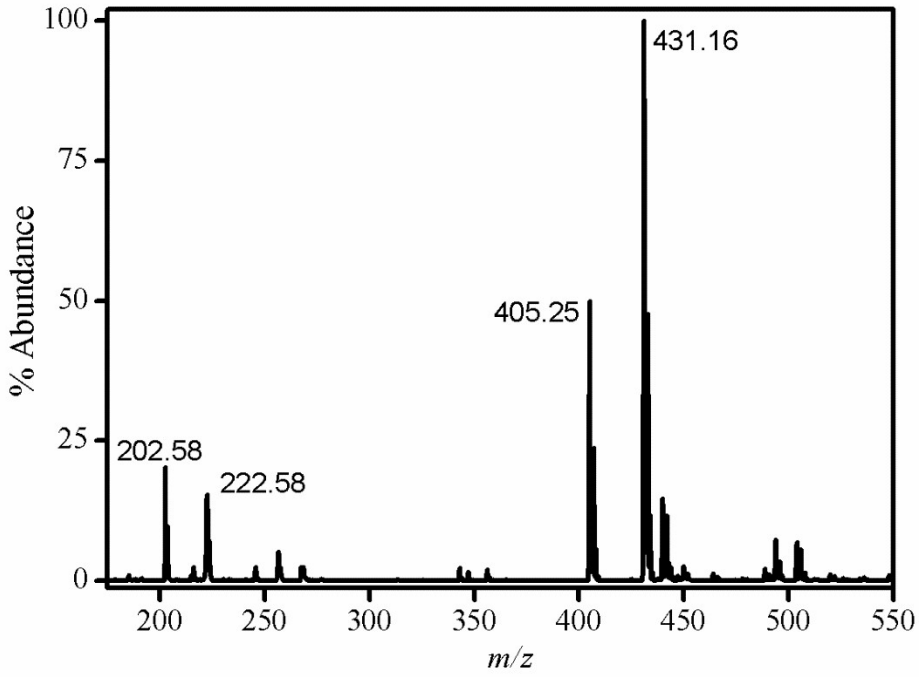


Fig. S10. ESI-MS spectra of **1** with 5 eq. H_2AP

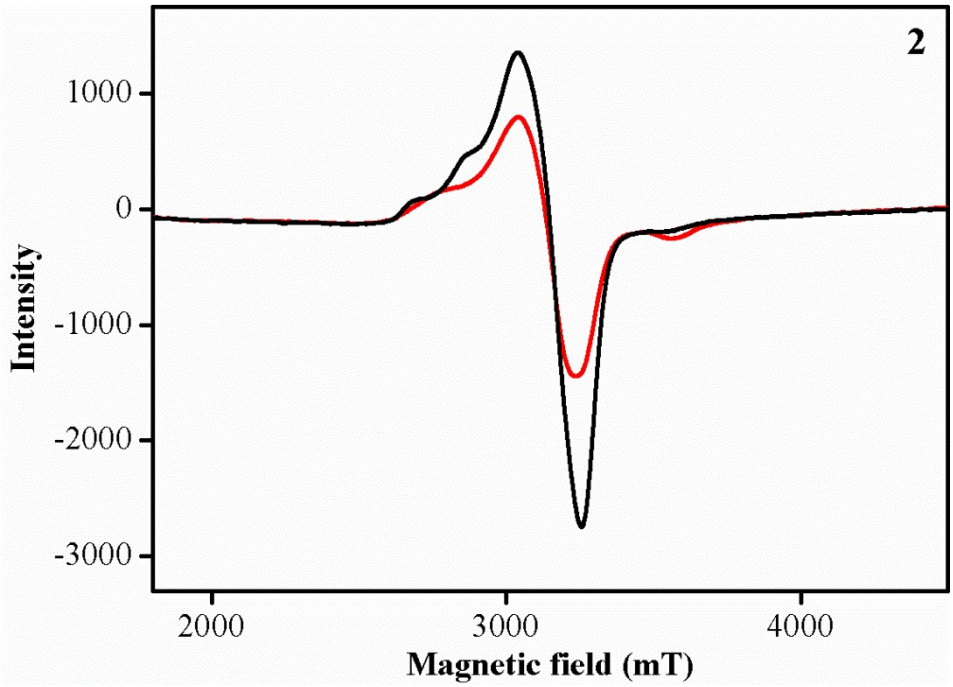


Fig. 9. X-band EPR spectra of **2** with 5 eq. H_2AP recorded at 77 K CH_3CN.

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Structure factors have been supplied for datablock(s) shelx

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No syntax errors found. CIF dictionary Interpreting this report

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Temperature:   296 K
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Hall group	-P 1	-P 1
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Sum formula	C24 H25 Cl2 Cu N5 O8	C24 H25 Cl2 Cu N5 O8
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Dx,g cm-3	1.569	1.569
Z	2	2
Mu (mm-1)	1.051	1.051
F000	662.0	662.0
F000'	663.50	
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The following ALERTS were generated. Each ALERT has the format
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Click on the hyperlinks for more details of the test.

Alert level C

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C23 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       C12      0.169 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          6 Note
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Alert level G

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PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --O3       .       25.0 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        C12 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2       ..C23            3.00 Ang.
                                          -x,1-y,1-z  =      2_566 Check
PLAT793_ALERT_4_G Model has Chirality at N2          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N3          (Centro SPGR)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.21 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         12 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.8 Low
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
  0 ALERT level B = A potentially serious problem, consider carefully
  4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 12 ALERT level G = General information/check it is not something unexpected

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

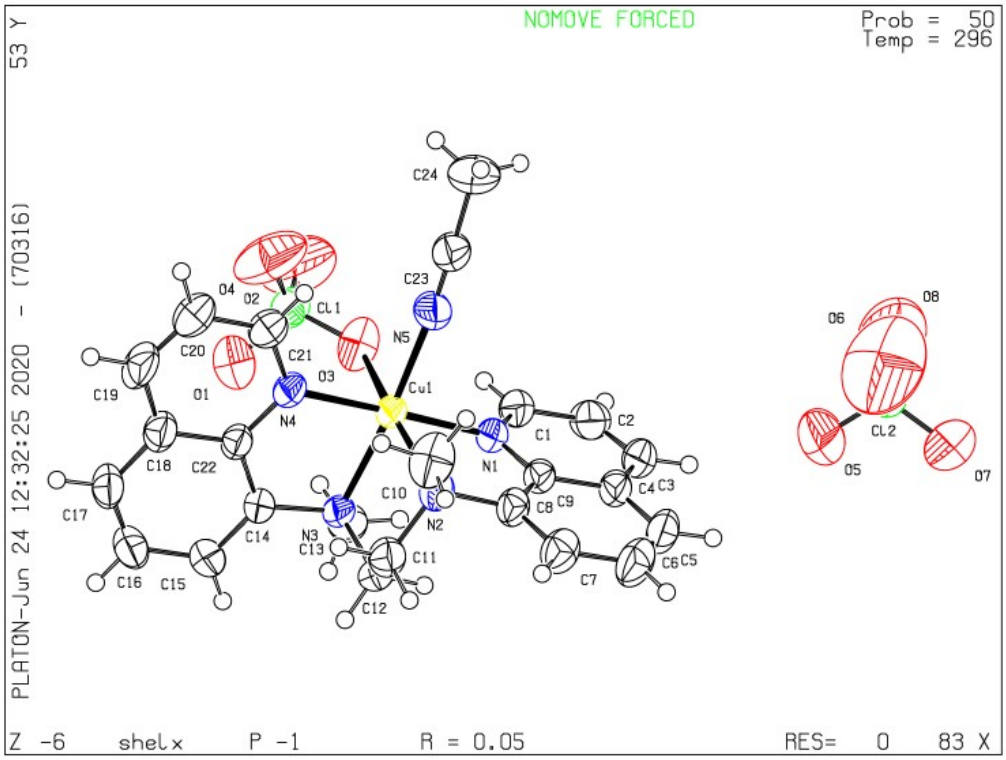
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 04/06/2020; check.def file version of 02/06/2020

Datablock shelx - ellipsoid plot



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Structure factors have been supplied for datablock(s) shelx

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

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Temperature:     296 K
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Hall group	-P 2yn	-P 2yn
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Sum formula	C25 H27 C12 Cu N5 O8	C25 H27 C12 Cu N5 O8
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Dx,g cm-3	1.591	1.591
Z	4	4
Mu (mm-1)	1.045	1.045
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F000'	1359.01	
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Click on the hyperlinks for more details of the test.

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PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl1       0.142 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl3       0.142 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H11B     ..O4       .        2.63 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H25B     ..O4       .        2.65 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          4 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.94A   From O6              -0.44 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.85A   From O2              -0.40 eA-3
```

Alert level G

```
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        Cl1 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        Cl3 Check
PLAT793_ALERT_4_G Model has Chirality at N2          (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at N3          (Centro SPGR)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)       .       2.07 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          9 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 10 ALERT level G = General information/check it is not something unexpected

  1 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
  3 ALERT type 3 Indicator that the structure quality may be low
  7 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

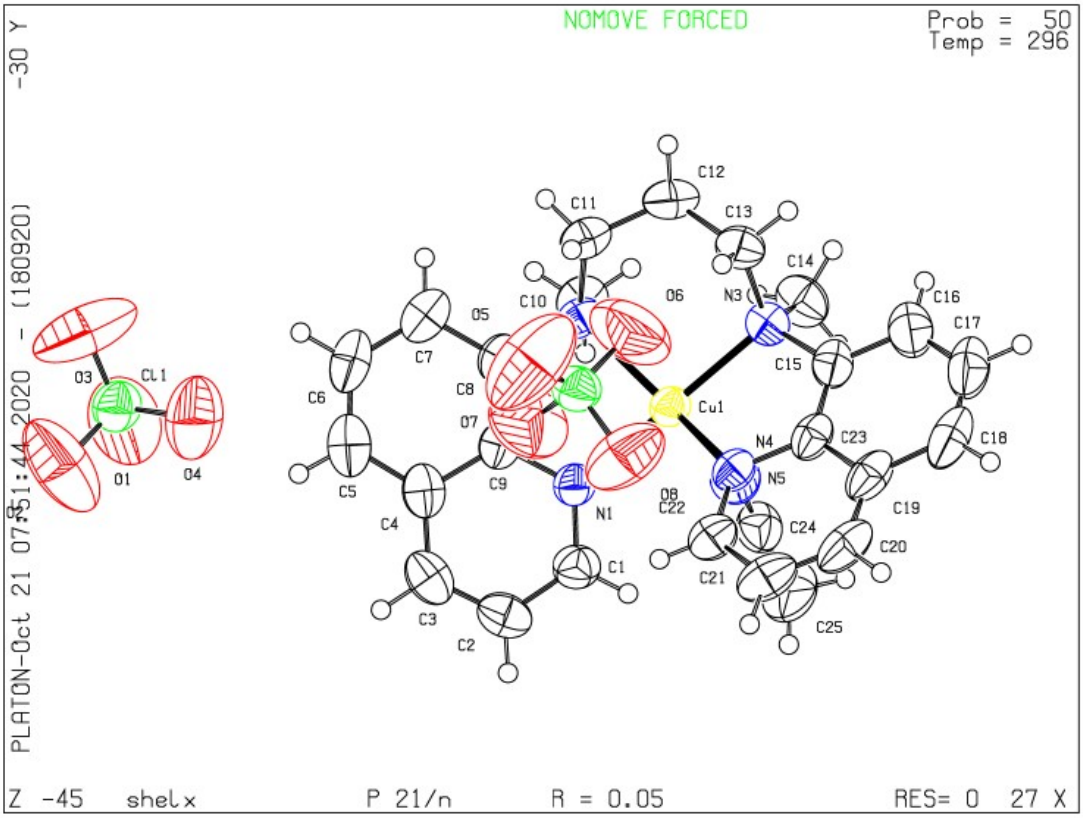
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 18/09/2020; check.def file version of 20/08/2020

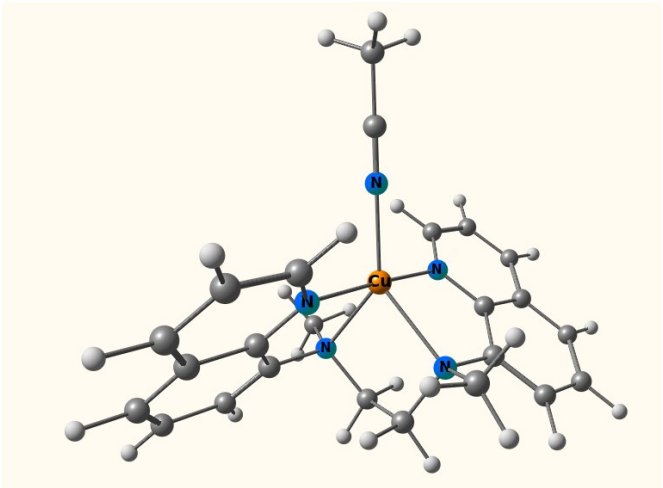
Datablock shelx - ellipsoid plot



Cartesian coordinates and total energies for the geometry optimizations.

1. $[Cu(BQEN)(CH_3CN)]^{2+}$ (**1**) zero point corrected energy=-2842.906094 a.u.

Cu	0.00000	0.00000	0.00000
N	0.32259	1.95803	0.22699
C	-0.63369	2.86842	0.39436
H	-1.65761	2.50945	0.36577
N	2.22852	0.00000	-0.21204
C	-0.36267	4.23256	0.60723
N	0.00000	0.00000	-2.23633
C	0.95112	4.65021	0.66186

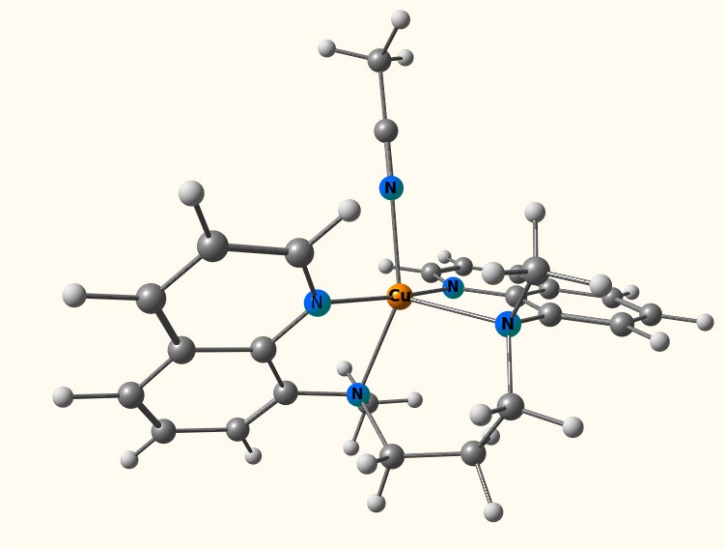


H	1.19386	5.69455	0.83583
C	1.99882	3.71124	0.48929
N	-0.26048	-1.95745	-0.29828
C	3.37300	4.06484	0.53487
H	3.64689	5.09944	0.71655
C	4.34108	3.10263	0.35054
H	5.39189	3.36949	0.38687
C	3.97877	1.75594	0.10586
H	4.76676	1.02508	-0.04579
C	2.65188	1.37182	0.05819
C	1.64012	2.34616	0.25869
C	2.92028	-0.98202	0.66772
H	2.46950	-1.96551	0.52564
H	2.80515	-0.67711	1.70926
H	3.98882	-1.05884	0.43755
C	2.41430	-0.35806	-1.65345
H	2.29511	-1.44153	-1.73889
H	3.43306	-0.11580	-1.98032
C	1.41681	0.35946	-2.55912
H	1.51232	1.44291	-2.44801
H	1.64448	0.11803	-3.60469
C	-0.94292	0.98118	-2.84082
H	-1.96836	0.67569	-2.62596

H	-0.81647	1.05702	-3.92657
H	-0.75872	1.96509	-2.40662
C	-0.30851	-1.37192	-2.63298
C	-0.47886	-1.75590	-3.94978
H	-0.40042	-1.02518	-4.74852
C	-0.75663	-3.10251	-4.28768
C	-0.85123	-4.06452	-3.30653
H	-1.05816	-5.09902	-3.56232
C	-0.67840	-3.71089	-1.94252
C	-0.75366	-4.64955	-0.88308
H	-0.95028	-5.69380	-1.10830
C	-0.57685	-4.23164	0.41980
H	-0.62431	-4.92613	1.25079
C	-0.33859	-2.86763	0.66953
H	-0.21432	-2.50846	1.68616
C	-0.41476	-2.34596	-1.60699
N	-1.38781	0.00103	1.54695
H	-1.18555	4.92733	0.73100
H	-0.89011	-3.36946	-5.33059
C	-2.16201	0.00605	2.40784
C	-3.13643	0.01275	3.48941
H	-3.09353	0.96732	4.02226
H	-2.91691	-0.79743	4.19131

H -4.14227 -0.12868 3.08247

2. $[Cu(BQPN)(CH_3CN)]^{2+}$ **(2)** zero point corrected energy=-2882.187576 a.u.



Cu 0.00000 0.00000 0.00000

C -2.78468 0.91511 0.63135

H -2.28211 1.65455 1.24711

N -2.01177 0.01351 0.03422

C -4.18471 0.93734 0.47902

H -4.76570 1.69412 0.99393

N -0.34252 -1.97284 -0.84523

N 0.25472 1.95706 -0.61489

C -3.99226 -0.98668 -0.97865

C -4.78311 0.00299 -0.34219

H -5.85781 0.01119 -0.49977

N 2.10591 0.00000 -0.11349

C -4.52329 -1.99399 -1.82646

H -5.58975 -2.01023 -2.02839

N 0.00000 0.00000 2.27362

C -3.68843 -2.94065 -2.37774

H -4.09016 -3.71178 -3.02635

C -2.30172 -2.94324 -2.08515

H -1.68900 -3.73548 -2.50161

C -1.74935 -1.97203 -1.27287

C	-2.58535	-0.96406	-0.73348
C	-0.18183	-3.03886	0.19564
H	-0.86811	-2.84189	1.01987
H	0.83777	-3.04518	0.57783
H	-0.40410	-4.02462	-0.22751
C	0.57149	-2.20887	-2.01249
H	0.24929	-1.53263	-2.81016
H	0.43144	-3.23431	-2.37474
C	2.05930	-2.00512	-1.72671
H	2.41650	-2.68673	-0.94893
H	2.58542	-2.31766	-2.63641
C	2.50419	-0.56861	-1.45802
H	3.59722	-0.51204	-1.52705
H	2.09661	0.10197	-2.22050
C	2.74588	-0.76788	0.99603
H	2.63755	-0.21016	1.92382
H	3.80773	-0.93933	0.79298
H	2.26043	-1.73441	1.11120
C	2.52406	1.41034	-0.08841
C	3.82239	1.81231	0.15674
H	4.59052	1.09084	0.41251
C	4.18588	3.17835	0.06035
H	5.21182	3.46521	0.26493

C	3.26131	4.12726	-0.31568
H	3.54677	5.16968	-0.41712
C	1.91965	3.74656	-0.58110
C	0.91643	4.65508	-1.00402
H	1.16631	5.70341	-1.13945
C	-0.36011	4.19632	-1.25148
H	-1.14403	4.86006	-1.59814
C	-0.65232	2.83580	-1.03047
H	-1.65655	2.46125	-1.19526
C	1.54607	2.37708	-0.42902
C	-0.10864	0.01833	3.42787
C	-0.24038	0.04017	4.87937
H	-1.24501	-0.28246	5.16784
H	-0.06872	1.05377	5.25334