Supplementary Material

D,L-Citrullinato-Bipyridine copper complex: Experimental and theoretical characterization

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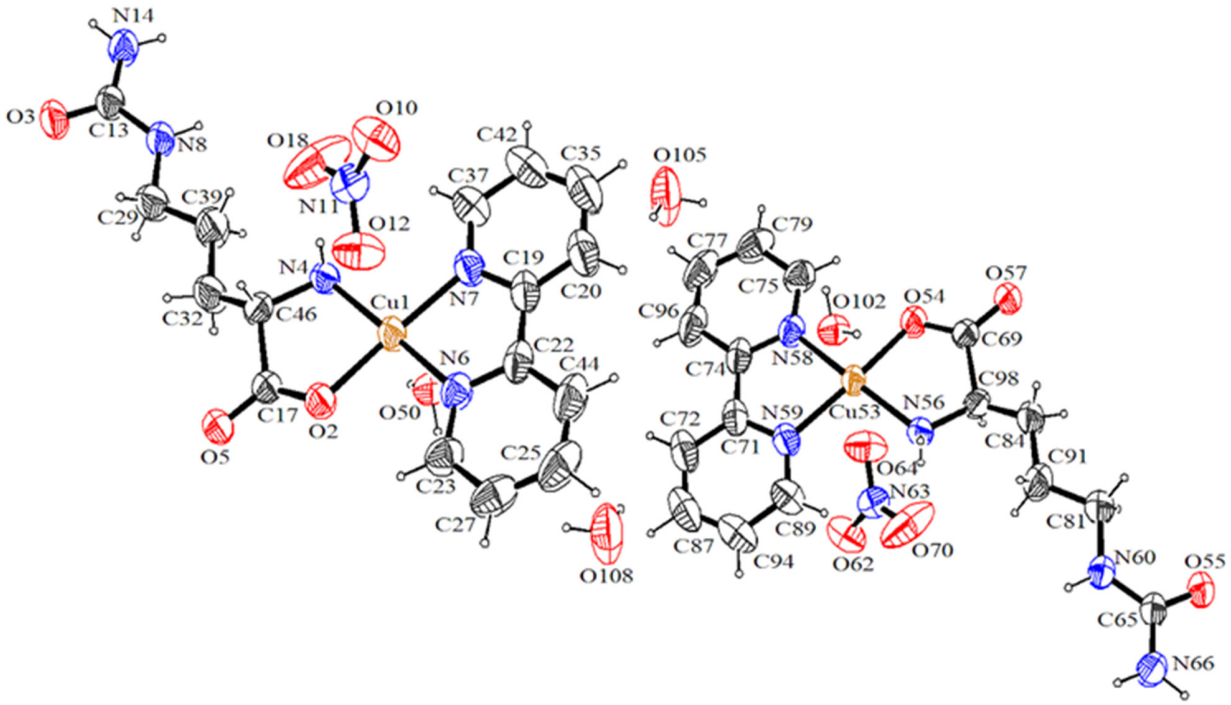

Figure S1. ORTEP diagram of D, L pairs of the [Cu($C_6H_{12}N_3O_3$)($C_{10}H_{10}N_2$)(NO_3)H_2O] complex. Ellipsoids are drawn at the 50% probability level.

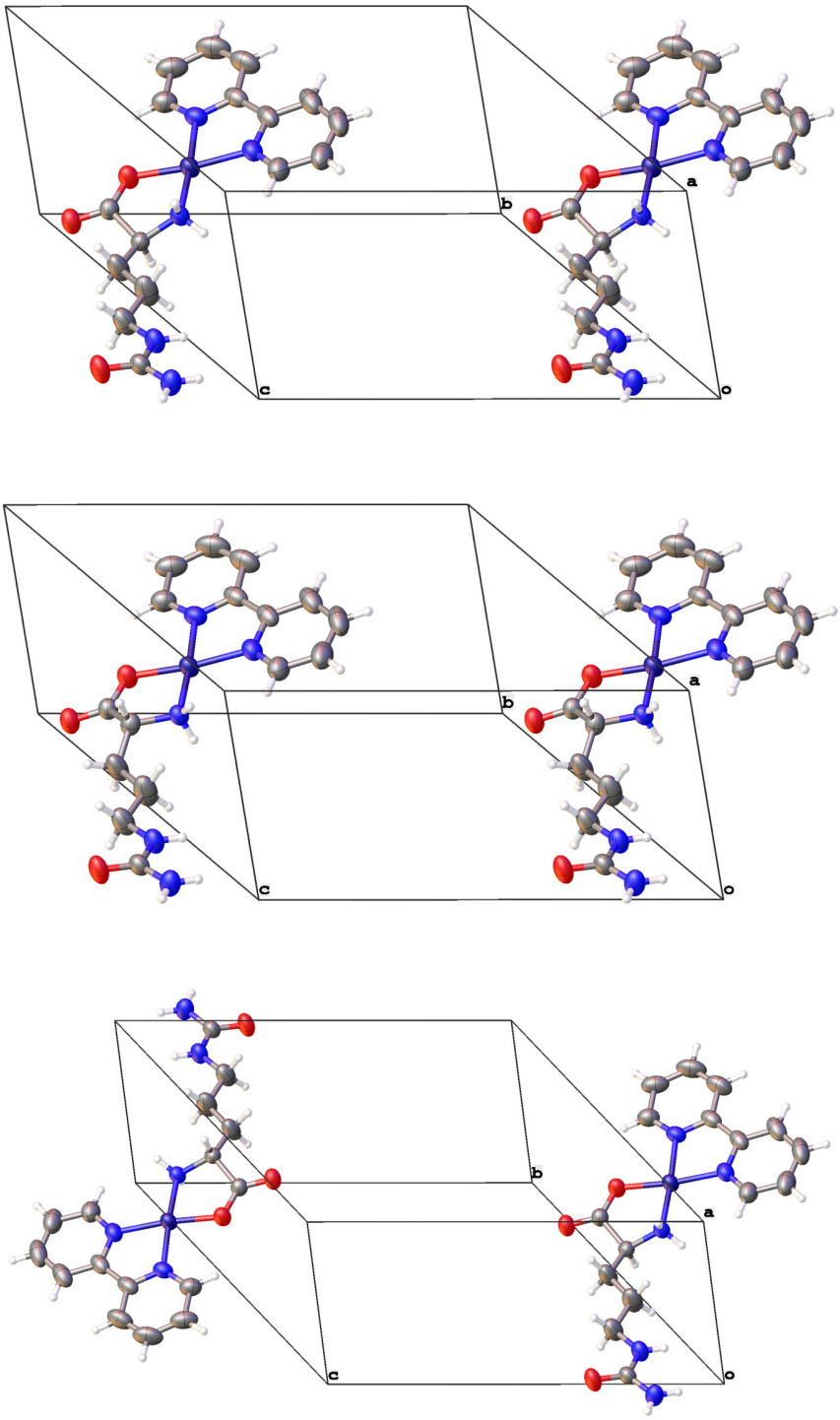

Figure S2. Enantiomers L, L, D, D and D, L

Table S1. *Crystal data*

$C_{16}H_{20}CuN_5O_3 \cdot 2(H_2O) \cdot NO_3$	$Z = 2$
$M_r = 491.95$	$F(000) = 510$
Triclinic, $P\bar{1}$	$D_x = 1.476$ Mg m^{-3}
$a = 7.2136$ (3) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 12.2497$ (6) Å	Cell parameters from 13926 reflections
$c = 14.1356$ (6) Å	$\theta = 3.2–28.5°$
$\alpha = 65.430$ (4)°	$\mu = 1.04$ mm^{-1}
$\beta = 77.331$ (3)°	$T = 293$ K
$\gamma = 82.046$ (3)°	Block, blue
$V = 1106.75$ (9) Å^3	0.32 × 0.25 × 0.20 mm

Xcalibur, Atlas, Gemini diffractometer	6762 independent reflections
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source	5370 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.038$
Detector resolution: 10.5564 pixels mm^{-1}	$\theta_{max} = 30.5°$, $\theta_{min} = 2.9°$
ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan *CrysAlis PRO* 1.171.42.49 (Rigaku Oxford Diffraction, 2022) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	$k = -17 \rightarrow 17$
$T_{min} = 0.959$, $T_{max} = 1.000$	$l = -20 \rightarrow 20$
42723 measured reflections	

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.8436P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
6762 reflections	$\Delta\rangle_{max} = 0.49$ e Å^{-3}
304 parameters	$\Delta\rangle_{min} = -0.39$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Computing details

Data collection: *CrysAlis PRO* 1.171.42.49 (Rigaku OD, 2022); cell refinement: *CrysAlis PRO* 1.171.42.49 (Rigaku OD, 2022); data reduction: *CrysAlis PRO* 1.171.42.49 (Rigaku OD, 2022); program(s) used to refine structure: *SHELXL* 2018/3 (Sheldrick, 2015); molecular graphics: Olex2 1.5 (Dolomanov *et al.*, 2009); software used to prepare material for publication: Olex2 1.5 (Dolomanov *et al.*, 2009).

Table S2. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (a61322_mo)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.19614 (4)	0.65013 (2)	1.07596 (2)	0.04356 (10)	
O11	0.2862 (3)	0.60138 (15)	0.95971 (13)	0.0505 (4)	
O2	0.5532 (3)	1.33849 (17)	0.52786 (14)	0.0620 (5)	
N12	0.2853 (3)	0.80974 (18)	0.97170 (16)	0.0413 (4)	
O10	0.4487 (3)	0.65695 (16)	0.79722 (13)	0.0522 (4)	
O14	0.5020 (3)	0.59127 (16)	1.14234 (15)	0.0511 (4)	
H14A	0.600615	0.631678	1.111859	0.077*	
H14B	0.531058	0.517727	1.153910	0.077*	
N15	0.0940 (3)	0.49149 (18)	1.17244 (16)	0.0457 (4)	
O27	0.5479 (6)	0.7889 (3)	0.5769 (2)	0.1113 (12)	
H27A	0.506549	0.751043	0.547994	0.167*	
H27B	0.535250	0.747538	0.643246	0.167*	
N21	0.0795 (3)	0.6903 (2)	1.20118 (16)	0.0468 (4)	
N4	0.5181 (4)	1.22531 (19)	0.70318 (16)	0.0513 (5)	
H4	0.502412	1.223687	0.765841	0.062*	
O31	-0.3854 (3)	0.8548 (2)	1.0485 (2)	0.0730 (6)	
N29	-0.2171 (3)	0.8374 (2)	1.00933 (18)	0.0504 (5)	
O28	-0.1572 (3)	0.7333 (2)	1.0208 (2)	0.0730 (6)	
C3	0.5368 (4)	1.3314 (2)	0.61963 (18)	0.0460 (5)	

N13	0.5375 (4)	1.42915 (19)	0.63971 (17)	0.0557 (6)	
H13A	0.549507	1.498839	0.588466	0.067*	
H13B	0.525987	1.422137	0.703811	0.067*	
C9	0.3730 (4)	0.6777 (2)	0.87544 (18)	0.0419 (5)	
O30	-0.1117 (4)	0.9197 (2)	0.9616 (3)	0.1193 (13)	
C22	0.0002 (4)	0.5959 (3)	1.28571 (19)	0.0505 (6)	
C23	-0.0821 (4)	0.6072 (4)	1.3794 (2)	0.0672 (8)	
H23	-0.137270	0.541946	1.437039	0.081*	
C16	0.0076 (3)	0.4842 (3)	1.26917 (19)	0.0502 (6)	
C20	0.1089 (4)	0.3954 (2)	1.1488 (2)	0.0554 (6)	
H20	0.167162	0.402104	1.081170	0.067*	
C18	-0.0469 (5)	0.2782 (3)	1.3218 (3)	0.0794 (11)	
H18	-0.092689	0.205418	1.372704	0.095*	
C19	0.0406 (5)	0.2872 (3)	1.2214 (3)	0.0680 (8)	
H19	0.052754	0.221115	1.203648	0.082*	
C5	0.5238 (5)	1.1134 (3)	0.6902 (2)	0.0663 (8)	
H5A	0.441302	1.122685	0.641305	0.080*	
H5B	0.652418	1.095367	0.659802	0.080*	
C7	0.4590 (6)	0.8954 (3)	0.7856 (2)	0.0674 (9)	
H7BC	0.432023	0.909834	0.717003	0.081*	0.488 (14)
H7BD	0.586097	0.857478	0.788662	0.081*	0.488 (14)
H7AA	0.360275	0.901290	0.746640	0.081*	0.512 (14)
H7AB	0.579077	0.880228	0.744987	0.081*	0.512 (14)
C24	-0.0818 (5)	0.7163 (4)	1.3869 (3)	0.0764 (10)	
H24	-0.135162	0.724940	1.449743	0.092*	
C26	0.0766 (4)	0.7948 (3)	1.2086 (2)	0.0592 (7)	
H26	0.129364	0.859748	1.149639	0.071*	
C6	0.4646 (7)	1.0148 (3)	0.7890 (2)	0.0777 (11)	
H6A	0.338371	1.036086	0.819767	0.093*	
H6B	0.549475	1.006342	0.836460	0.093*	
C25	-0.0017 (5)	0.8111 (4)	1.3006 (3)	0.0714 (9)	
H25	-0.000065	0.885317	1.303648	0.086*	
C17	-0.0651 (5)	0.3761 (3)	1.3451 (3)	0.0710 (9)	
H17	-0.126043	0.371291	1.411834	0.085*	
C8B	0.3289 (14)	0.8092 (4)	0.8641 (4)	0.0424 (17)	0.488 (14)
H8B	0.207673	0.832671	0.838555	0.051*	0.488 (14)
C8A	0.4262 (11)	0.7915 (5)	0.8843 (4)	0.0392 (15)	0.512 (14)
H8A	0.548100	0.769938	0.909148	0.047*	0.512 (14)
H12A	0.372 (5)	0.838 (3)	0.986 (3)	0.062 (9)*	
H12B	0.189 (6)	0.851 (4)	0.964 (3)	0.081 (12)*	

Table S3. Atomic displacement parameters (Å^2) for (a61322_mo)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.05292 (18)	0.03860 (16)	0.03474 (15)	-0.01065 (12)	0.00253 (11)	-0.01291 (11)
O11	0.0705 (12)	0.0383 (8)	0.0394 (8)	-0.0133 (8)	0.0023 (8)	-0.0151 (7)
O2	0.0949 (15)	0.0500 (10)	0.0337 (8)	-0.0101 (10)	0.0041 (9)	-0.0152 (7)
N12	0.0473 (11)	0.0364 (9)	0.0375 (10)	-0.0063 (9)	0.0006 (8)	-0.0149 (8)
O10	0.0729 (12)	0.0436 (9)	0.0388 (8)	-0.0052 (8)	-0.0012 (8)	-0.0190 (7)
O14	0.0612 (11)	0.0415 (9)	0.0511 (10)	-0.0001 (8)	-0.0098 (8)	-0.0198 (8)
N15	0.0432 (10)	0.0435 (10)	0.0420 (10)	-0.0090 (8)	-0.0022 (8)	-0.0095 (8)
O27	0.189 (3)	0.103 (2)	0.0446 (12)	-0.067 (2)	0.0018 (17)	-0.0253 (13)
N21	0.0444 (11)	0.0538 (12)	0.0399 (10)	-0.0025 (9)	-0.0023 (8)	-0.0190 (9)
N4	0.0725 (15)	0.0412 (10)	0.0341 (9)	-0.0075 (10)	-0.0021 (9)	-0.0114 (8)
O31	0.0590 (13)	0.0928 (17)	0.0845 (16)	0.0068 (11)	-0.0113 (11)	-0.0564 (14)
N29	0.0505 (12)	0.0487 (12)	0.0564 (12)	-0.0035 (9)	-0.0166 (10)	-0.0215 (10)
O28	0.0631 (13)	0.0605 (13)	0.1078 (19)	0.0016 (10)	-0.0152 (12)	-0.0473 (13)
C3	0.0526 (13)	0.0437 (12)	0.0359 (11)	-0.0084 (10)	0.0006 (9)	-0.0127 (9)
N13	0.0840 (17)	0.0409 (11)	0.0406 (11)	-0.0103 (11)	-0.0110 (10)	-0.0128 (9)
C9	0.0508 (13)	0.0362 (10)	0.0374 (10)	-0.0039 (9)	-0.0063 (9)	-0.0139 (9)
O30	0.0683 (16)	0.0537 (14)	0.184 (3)	-0.0098 (12)	-0.0324 (19)	0.0098 (17)
C22	0.0393 (12)	0.0685 (16)	0.0348 (11)	0.0002 (11)	-0.0057 (9)	-0.0134 (11)
C23	0.0530 (16)	0.098 (2)	0.0421 (14)	0.0020 (15)	-0.0020 (11)	-0.0242 (15)
C16	0.0397 (12)	0.0594 (15)	0.0373 (11)	-0.0063 (10)	-0.0044 (9)	-0.0056 (10)
C20	0.0558 (15)	0.0453 (13)	0.0598 (16)	-0.0104 (11)	-0.0059 (12)	-0.0155 (12)
C18	0.072 (2)	0.0530 (17)	0.081 (2)	-0.0212 (15)	-0.0062 (17)	0.0068 (16)
C19	0.0583 (17)	0.0435 (14)	0.091 (2)	-0.0120 (12)	-0.0135 (16)	-0.0126 (14)
C5	0.093 (2)	0.0462 (14)	0.0508 (15)	-0.0107 (14)	0.0117 (15)	-0.0205 (12)
C7	0.099 (2)	0.0457 (14)	0.0474 (14)	-0.0201 (15)	0.0186 (15)	-0.0197 (12)
C24	0.0625 (19)	0.122 (3)	0.0550 (17)	0.0111 (19)	-0.0086 (14)	-0.051 (2)
C26	0.0569 (16)	0.0682 (18)	0.0605 (16)	-0.0043 (13)	-0.0049 (13)	-0.0359 (14)
C6	0.129 (3)	0.0440 (15)	0.0498 (16)	-0.0240 (17)	0.0089 (17)	-0.0146 (12)
C25	0.0601 (18)	0.097 (3)	0.079 (2)	0.0051 (17)	-0.0102 (16)	-0.060 (2)
C17	0.0643 (18)	0.067 (2)	0.0528 (16)	-0.0150 (15)	0.0016 (13)	0.0019 (14)
C8B	0.056 (4)	0.034 (2)	0.037 (2)	-0.003 (2)	-0.012 (2)	-0.0114 (18)
C8A	0.042 (3)	0.040 (2)	0.036 (2)	-0.009 (2)	-0.004 (2)	-0.0150 (18)

Document origin: *publCIF* [Westrip, S. P. (2010). *J. Apply. Cryst.*, **43**, 920-925]

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a61322_mo

No syntax errors found. CIF dictionary Interpreting this report

Datablock: a61322_mo

Bond precision: C-C = 0.0046 A Wavelength=0.71073

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alpha=65.430(4) beta=77.331(3) gamma=82.046(3)

Temperature: 293 K

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Hall group	-P 1	-P 1
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Sum formula	C16 H24 Cu N6 O8 [+ solvent]	C16 H24 Cu N6 O8
Mr	491.96	491.95
Dx,g cm-3	1.476	1.476
Z	2	2
Mu (mm-1)	1.040	1.040
F000	510.0	510.0
F000'	510.87	
h,k,lmax	11,19,22	11,19,22
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Data completeness= 0.953 Theta(max)= 35.242

R(reflections)= 0.0547(6079) wR2(reflections)=

0.1484(9456)

S = 1.017 Npar= 304

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 C

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O28 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N29 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O27 0.111 Check

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Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 7 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 3% Note
PLAT414_ALERT_2_G Short Intra D-H..H-X H8A ..H12A . 1.83 Ang.
x,y,z = 1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X H12B ..H8B . 1.87 Ang.
x,y,z = 1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 71 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note
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). 3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 462 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

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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.

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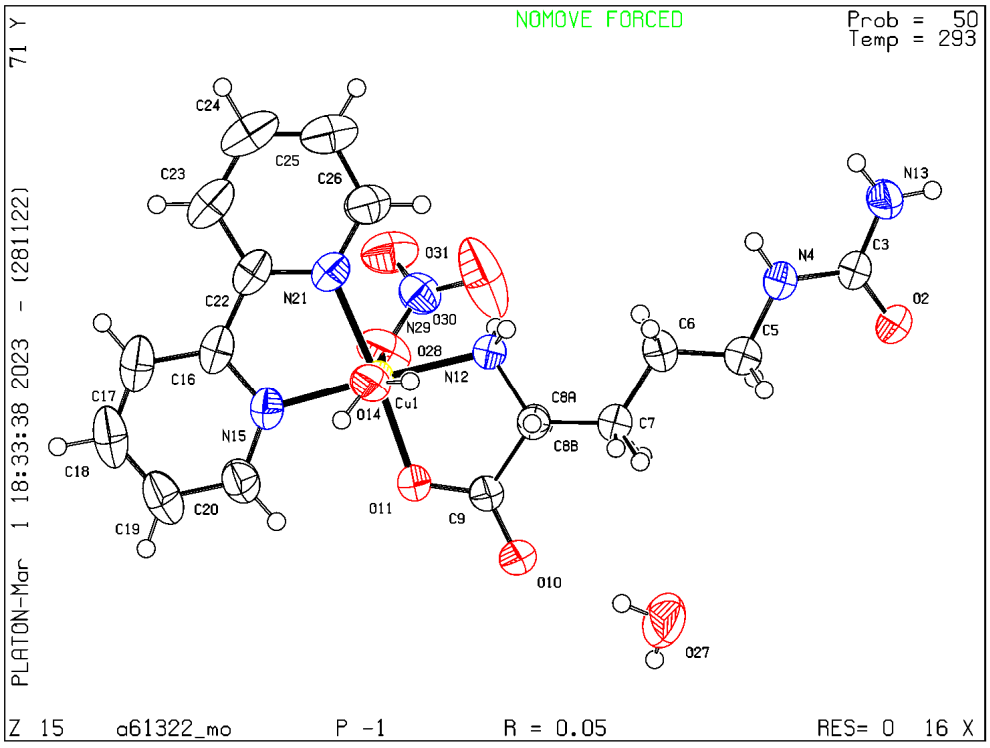

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