Crystal structure for new coordination polymer obtained via solvothermal synthesis in Berghof autoclave

Andrzej Kochel[a]*, Kamil Twaróg[a], Małgorzata Hołyńska[b]*

[a] Department of Chemistry, Wrocław University, F. Joliot Curie 14, 50 383 Wrocław, Poland
[b]Fachbereich Chemie and Wissenschaftliches Zentrum für Materialwissenschaften, Philipps-Universität Marburg, Hans-Meerwein-Straße, D-35043 Marburg, Germany
E-mail:andrzej.kochel@chem.uni.wroc.pl (A. Kochel)
holynska@chemie.uni-marburg.de (M. Hołyńska)

Coordination polymer *[Cu(2,3-pdc)H$_2$O]$_n$* was obtained by solvothermal synthesis in a Berghof BF100 pressure reactor using QUIN (quinolinic Acid) and $Cu(HSO_3)_2$ as substrates. The resulting compound crystallizes in triclinic system, in a space group of $P\bar{1}$, with a = 7.434(3) Å, b = 7.523(4) Å, c = 7.881(3) Å, α = 62.68(5)°, β = 79.02(5)°, γ = 78.90(5)°, V = 381.5(3) Å^3, Z = 2.

The coordination sphere of the Cu^{2+} ion is filled by three symmetry-dependent 2,3-pdc ligands through 3 oxygen atoms derived from the ligand carboxyl groups (O1, O1^{ii} and O3^{i}), a nitrogen atom (N1^{i}) derived from the ligand aromatic ring, and a water molecule. The resulting environment of the Cu^{2+} ion adopts the shape of a distorted tetragonal pyramid. This polymer forms one-dimensional chains extending along [100], and the occurrence of hydrogen bonds (Table 1) stabilizes the crystal structure.

Table 1: Hydrogen bonding parameters for *[Cu(2,3-pdc)H$_2$O]$_n$* [Å], symmetry codes: (i) -x+1, -y, -z+1, z+1/2; (ii) x, y+1, z.

D-H···A	D-H, [Å]	H···A, [Å]	D···A, [Å]	D-H···A, [°]
O(1W)-H(1W)···O(4)^{i}	0.84	1.84(5)	2.64(2)	158
O(1W)-H(2W)···O(2)^{ii}	0.84	1.90(4)	2.68(2)	154

The figure below shows the copper(II) coordination polymer structure (II).

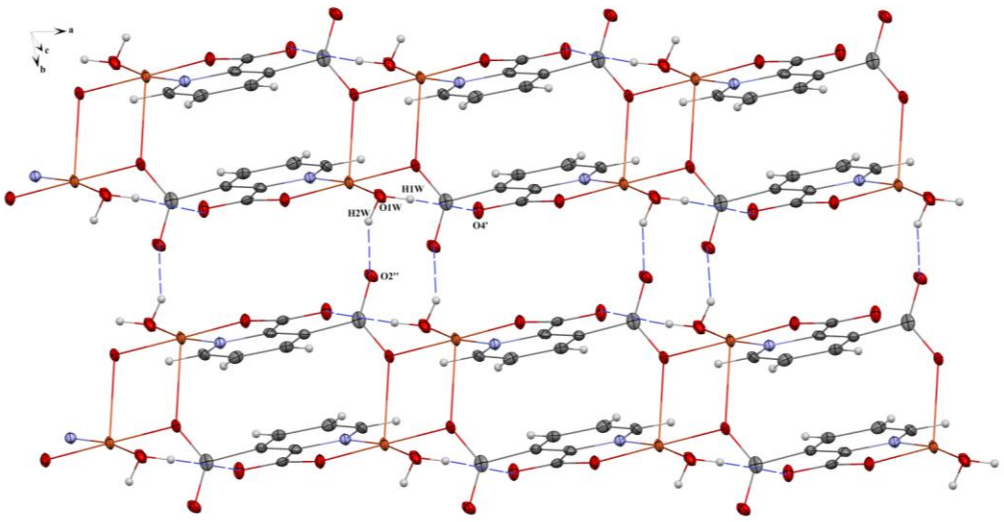

Figure 1: Copper(II) coordination polymer structure (1D).