



STRUCTURAL
CHEMISTRY

Volume 78 (2022)

Supporting information for article:

A new mixed-valence Cu^I/Cu^{II} three-dimensional coordination polymer constructed with an *N,O*-donor ligand generated *via* solvothermal synthesis: structural features and magnetic properties

Andrzej Kochel, Małgorzata Hołyńska, Kamil Twaróg, Aneta Jezierska, Jarosław Panek and Jacek Wojaczyński

NMR spectra

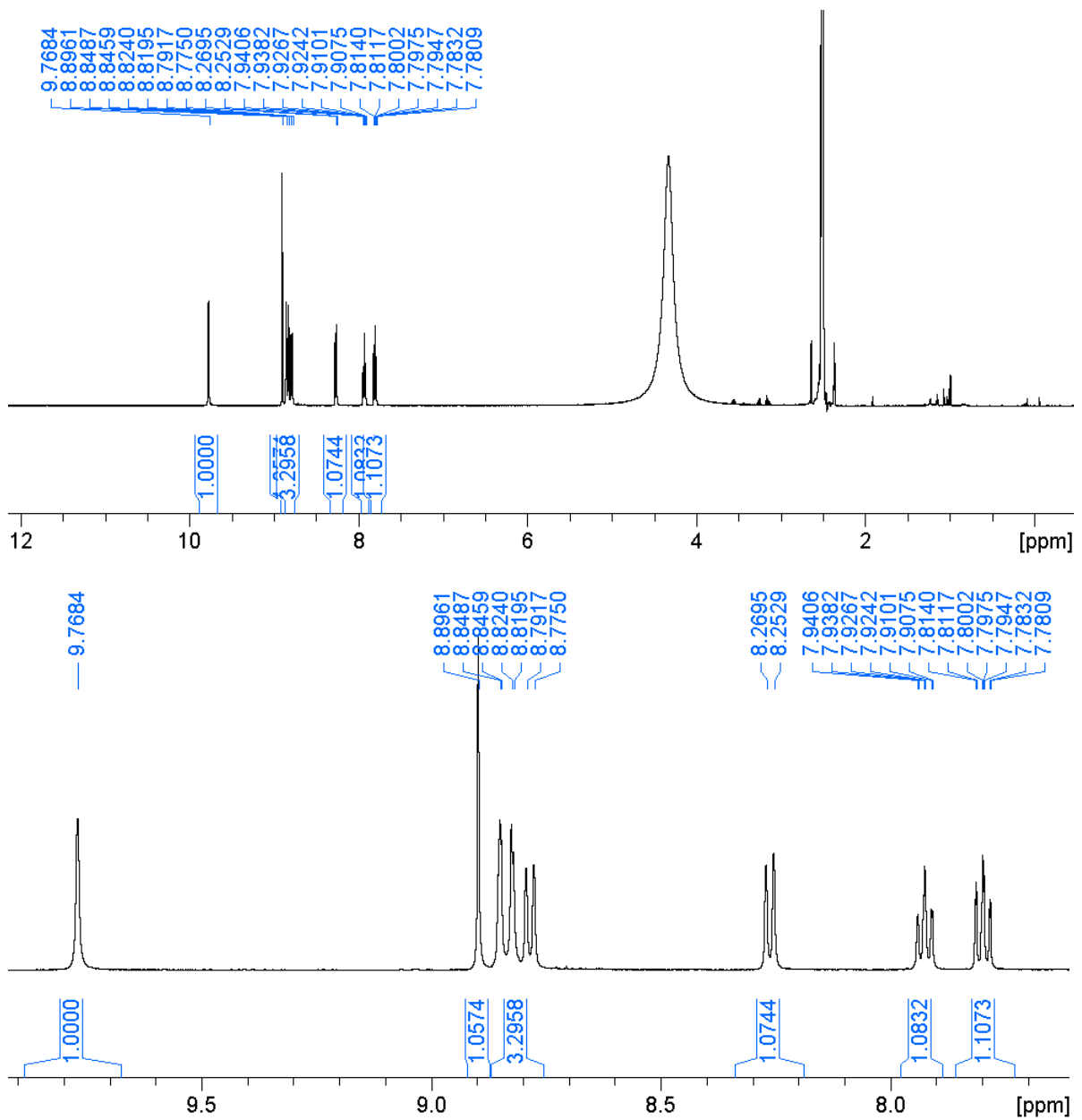


Figure S1 ¹H NMR spectrum of $C_{14}H_{10}N_3O_2^+Cl^- \cdot 2H_2O$ (500 MHz, DMSO-*d*₆) – the entire range (top figure) and the downfield part

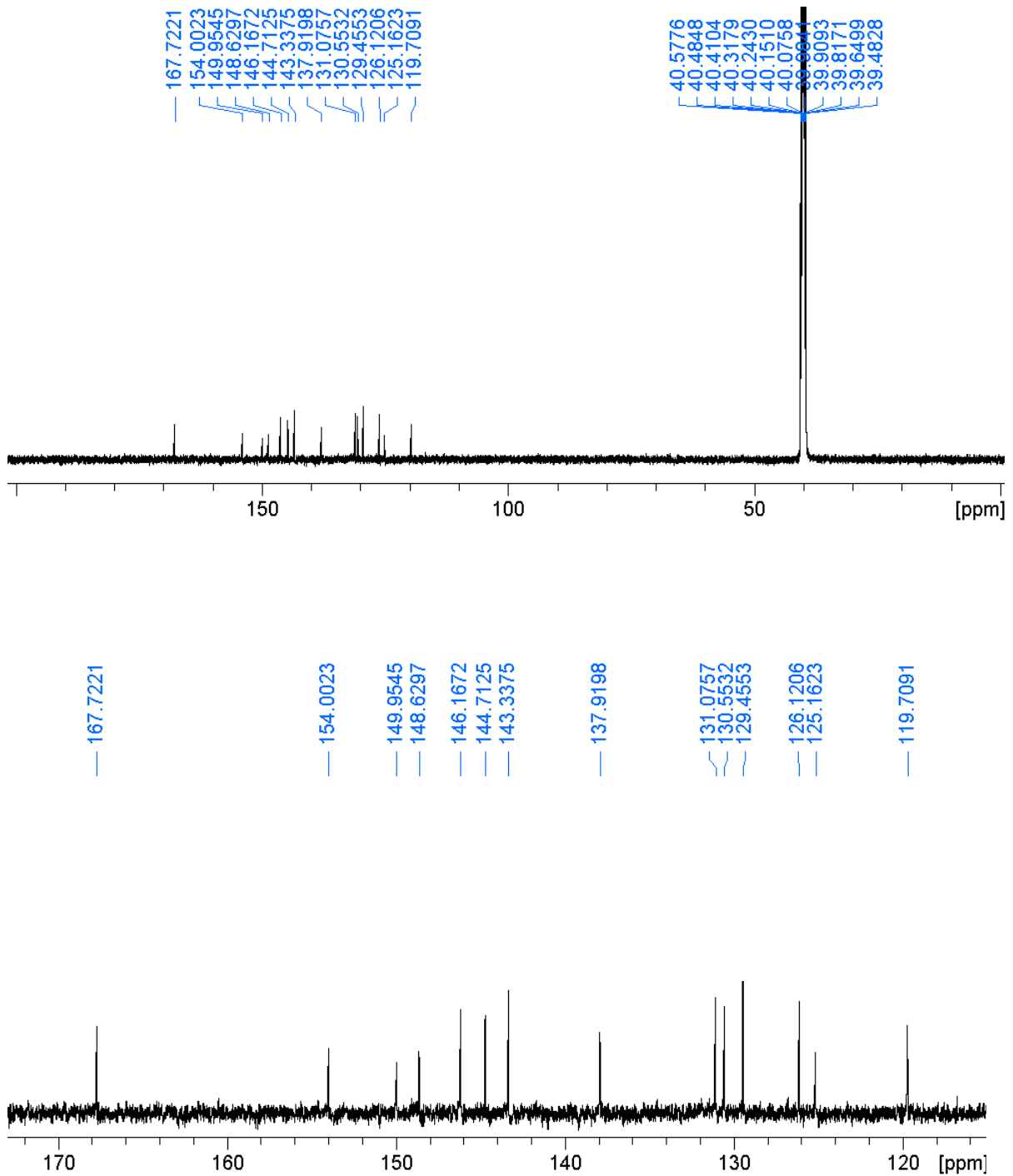


Figure S2 ^{13}C NMR spectrum of $\text{C}_{14}\text{H}_{10}\text{N}_3\text{O}_2^+\text{Cl}^- \cdot 2\text{H}_2\text{O}$ (125 MHz, $\text{DMSO-}d_6$) – the entire range (top figure) and the downfield region

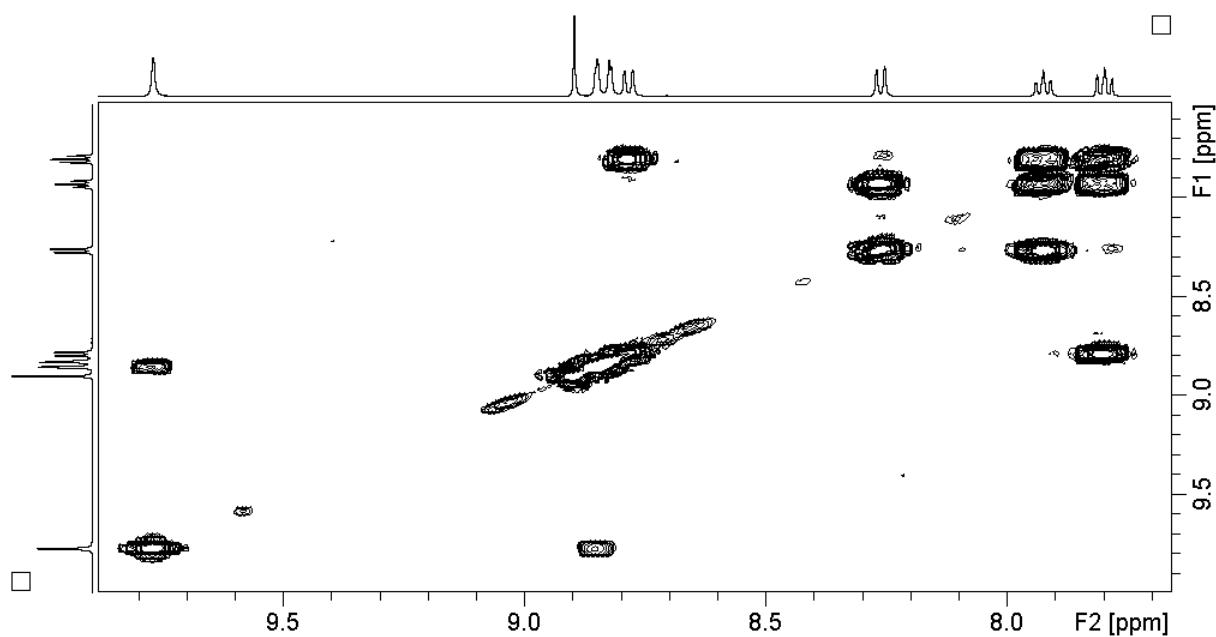


Figure S3 ^1H - ^1H COSY spectrum of $\text{C}_{14}\text{H}_{10}\text{N}_3\text{O}_2^+\text{Cl}^- \cdot 2\text{H}_2\text{O}$

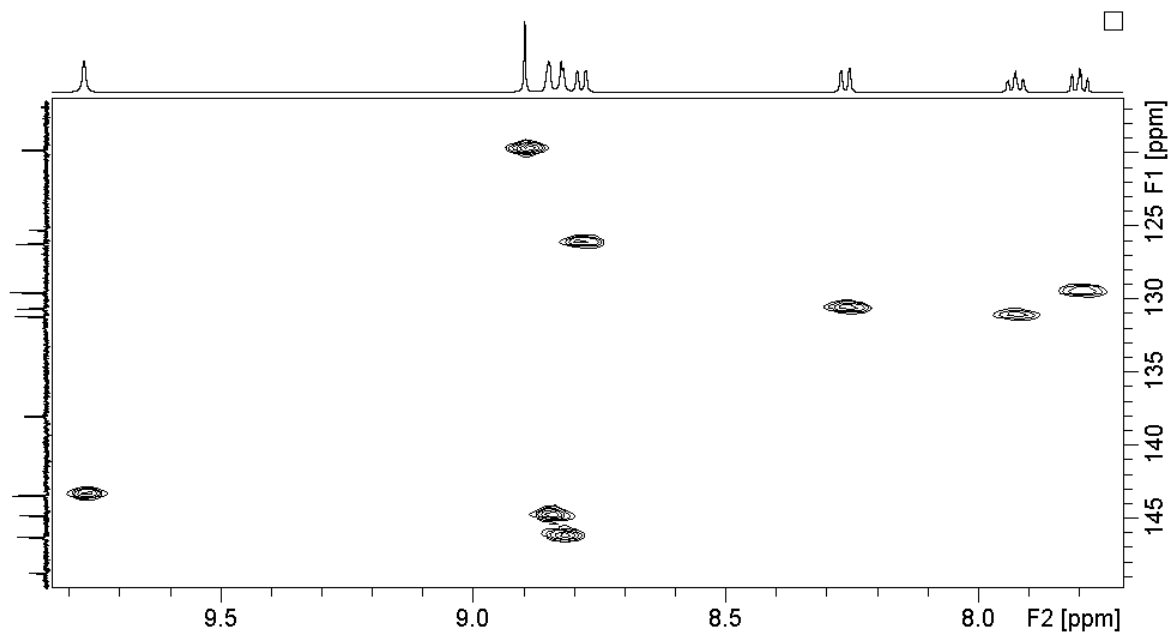


Figure S4 ^1H - ^{13}C HMQC spectrum of $\text{C}_{14}\text{H}_{10}\text{N}_3\text{O}_2^+\text{Cl}^- \cdot 2\text{H}_2\text{O}$

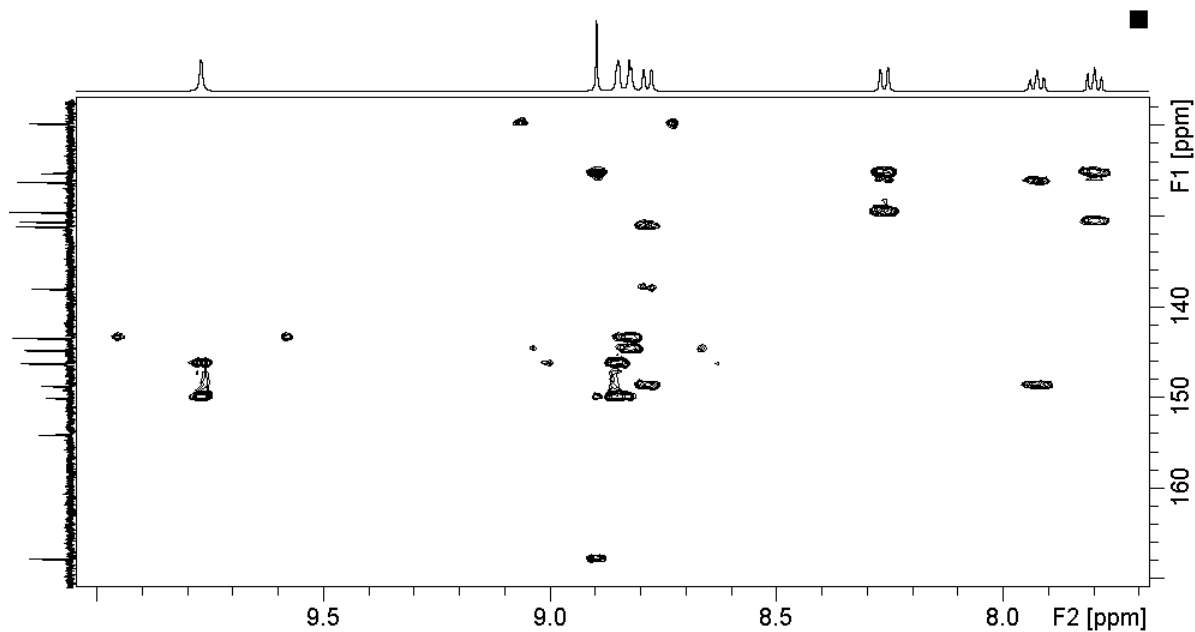
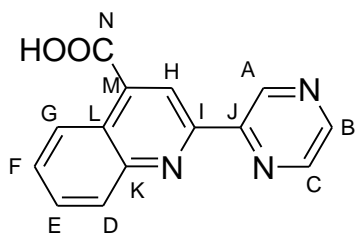


Figure S5 ^1H - ^{13}C HMBC NMR spectrum of $\text{C}_{14}\text{H}_{10}\text{N}_3\text{O}_2^+\text{Cl}^- \cdot 2\text{H}_2\text{O}$

Table S14 Interpretation of the recorded NMR spectra.



Signal assignment:

Position	$\delta(^1\text{H})/\text{ppm}$	$\delta(^{13}\text{C})/\text{ppm}$
A	9,77	143,3
B	8,83	146,2
C	8,83	144,7
D	8,26	130,6
E	7,93	131,1
F	7,80	129,5
G	8,78	126,1
H	8,90	119,7
I	-	150,0
J	-	154,0
K	-	148,6
L	-	125,2
M	-	137,9

N * 167,7

*The COOH signal in ^1H NMR spectrum has not been identified, either it is very broad or (more likely) an averaged signal of this group and water is seen.