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Electronic supplementary information

From mononuclear to linear one-dimensional coordination species of copper(II)-chloranilate: design and characterization

Marijana Jurić, Krešimir Molčanov*, Dijana Žilić and Biserka Kojić-Prodić

Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia.

Table S1 Geometric parameters of copper(II) coordination spheres (Å, °) in compounds **1**–**6**. Symmetry operators: *i*) –*x*, –*y*, 1–*z*; *ii*) –1–*x*, –*y*, 1–*z*; *iii*) 1+*x*, *y*, *z*; *iv*)1–*x*, *y*, 1/2–*z*; *v*) *x*, 1+*y*, *z*; *vi*) 1–*x*, 1+*y*, 1/2–*z*; *vii*) -1+*x*, *y*, *z*; *viii*) 1–*x*, –*y*, 1–*z*; *ix*) 1–*x*, *y*, 1/2–*z*; *x*) 1–*x*, 1+*y*, 1/2–*z*; *xi*) 1/2–*x*, 3/2–*y*, –*z*.

1		**2**		**3**	
Cu1–O1	1.9999(17)	Cu1–O1	1.9673(17)	Cu1–O1	1.956(2)
Cu1–O1^{viii}	1.9999(17)	Cu1–O2	1.9652(16)	Cu1–O2	1.963(2)
Cu1–O2	1.9444(19)	Cu1–O3	1.9333(17)	Cu1–O3^{vii}	1.953(3)
Cu1–O2^{viii}	1.9444(19)	Cu1–O4	1.9453(18)	Cu1–O4^{vii}	1.955(2)
Cu1–O5	2.418(2)	Cu1–O7	2.2799(18)	Cu1–N1	2.203(4)
O2^{viii}–Cu1–O2	180	O2–Cu1–O1	82.69(7)	O1–Cu1–O2	83.30(10)
O2^{viii}–Cu1–O1^{viii}	83.23(7)	O3–Cu1–O1	96.66(7)	O3^{vii}–Cu1–O1	167.57(11)
O2^{viii}–Cu1–O1	96.77(7)	O4–Cu1–O1	169.92(7)	O3^{vii}–Cu1–O2	95.63(10)
O2^{viii}–Cu1–O5^{viii}	91.85(9)	O1–Cu1–O7	91.03(7)	O4^{vii}–Cu1–O1	95.44(10)
O2^{viii}–Cu1–O5	88.15(9)	O3–Cu1–O2	172.01(7)	O4^{vii}–Cu1–O2	169.91(11)
O2–Cu1–O1^{viii}	96.77(7)	O4–Cu1–O2	94.62(7)	O3^{vii}–Cu1–O4^{vii}	83.44(10)
O2–Cu1–O1	83.23(7)	O2–Cu1–O7	97.19(7)	O1–Cu1–N1	99.46(14)
O2–Cu1–O5^{viii}	88.15(9)	O3–Cu1–O4	84.65(7)	O2–Cu1–N1	95.18(14)
O2–Cu1–O5	91.85(9)	O3–Cu1–O7	90.78(7)	O3^{vii}–Cu1–N1	92.97(14)
O1^{viii}–Cu1–O1	180	O4–Cu1–O7	98.95(7)	O4^{vii}–Cu1–N1	94.91(14)
O1^{viii}–Cu1–O5^{viii}	89.51(8)				
O1^{viii}–Cu1–O5	90.49(8)				
O1–Cu1–O5^{viii}	90.49(8)				
O1–Cu1–O5	89.51(8)				
O5^{viii}–Cu1–O5	180				

4		**5**	
Cu1–O1	2.281(5)	Cu1–O1	1.978(2)
Cu1–O1^{i}	2.281(5)	Cu1–O1^{iv}	1.978(2)
Cu1–O2^{ii}	2.048(5)	Cu1–O2^{v}	1.979(2)
Cu1–O2^{iii}	2.048(5)	Cu1–O2^{vi}	1.979(2)
Cu1–O3	2.024(7)	Cu1–O3	2.314(4)
Cu1–O3^{i}	2.024(7)	Cu1– O3^{iv}	2.314(4)
O3–Cu1–O3^{i}	179.9(4)	O1–Cu1–O1^{iv}	82.85(9)
O3–Cu1–O2^{ii}	90.0(3)	O1–Cu1–O2^{v}	97.24(9)
O3–Cu1–O2^{iii}	90.0(3)	O1–Cu1–O2^{vi}	179.36(11)
O3–Cu1–O1	88.7(2)	O1–Cu1–O3	89.97(12)

O3–Cu1–O1^{i}	91.3(2)	O1–Cu1–O3^{iv}	90.22(12)
O3^{i}–Cu1–O2^{ii}	90.0(3)	O1^{iv}–Cu1–O2^{v}	179.36(11)
O3^{i}–Cu1–O2^{iii}	90.0(3)	O1^{iv}–Cu1–O2^{vi}	97.24(9)
O3^{i}–Cu1–O1	91.3(2)	O1^{iv}–Cu1–O3	90.22(12)
O3^{i}–Cu1–O1^{i}	88.7(2)	O1^{iv}–Cu1–O3^{iv}	89.97(12)
O2^{ii}–Cu1–O2^{iii}	180.0(3)	O2^{v}–Cu1–O2^{vi}	
O2^{ii}–Cu1–O1	75.8(2)	O2^{v}–Cu1–O3	89.15(12)
O2^{ii}–Cu1–O1^{i}	104.2(2)	O2^{v}–Cu1–O3^{iv}	90.67(12)
O2^{iii}–Cu1–O1	104.2(2)	O2^{vi}–Cu1–O3	90.67(12)
O2^{iii}–Cu1–O1^{i}	75.8(2)	O2^{vi}–Cu1–O3^{iv}	89.15(12)
O1–Cu1–O1^{i}	180.0(2)	O3–Cu1–O3^{iv}	179.76(14)
6a		**6b**	
Cu1a–O1a	2.1654(14)	Cu1b–O1b	2.0469(13)
Cu1a–O1a^{ix}	2.1654(14)	Cu1b–O1b^{xi}	2.0469(13)
Cu1a–O2a^{v}	2.1703(14)	Cu1b–O2b	2.2995(13)
Cu1a–O2a^{x}	2.1703(14)	Cu1b–O2b^{xi}	2.2995(13)
Cu1a–N1a	2.000(2)	Cu1b–N1b	2.004(2)
Cu1a–N1a^{xi}	2.000(2)	Cu1b–N1b^{ix}	2.004(2)
N1a^{ix}–Cu1a–N1a	177.70(7)	N1b–Cu1b–N1b^{xi}	180
N1a^{ix}–Cu1a–O1a	89.17(7)	N1b–Cu1b–O1b	88.51(6)
N1a^{ix}–Cu1a–O1a^{ix}	92.65(7)	N1b–Cu1b–O1b^{xi}	91.49(6)
N1a^{ix}–Cu1a–O2a^{v}	86.58(7)	N1b–Cu1b–O2b^{xi}	87.09(6)
N1a^{ix}–Cu1a–O2a^{x}	91.59(7)	N1b–Cu1b–O2b	92.91(6)
N1a–Cu1a–O1a	92.65(7)	N1b^{xi}–Cu1b–O1b	91.49(6)
N1a–Cu1a–O1a^{ix}	89.17(7)	N1b^{xi}–Cu1b–O1b^{xi}	88.51(6)
N1a–Cu1a–O2a^{v}	91.59(7)	N1b^{xi}–Cu1b–O2b^{xi}	92.91(6)
N1a–Cu1a–O2a^{x}	86.58(7)	N1b^{xi}–Cu1b–O2b	87.09(6)
O1a–Cu1a–O1a^{ix}	75.84(6)	O1b–Cu1b–O1b^{xi}	180
O1a–Cu1a–O2a^{v}	104.48(5)	O1b–Cu1b–O2b^{x}	104.82(5)
O1a–Cu1a–O2a^{x}	179.16(6)	O1b–Cu1b–O2b	75.18(5)
O1a^{ix}–Cu1a–O2a^{v}	179.16(6)	O1b^{xi}–Cu1b–O2b^{xi}	75.18(5)
O1a^{ix}–Cu1a–O2a^{x}	104.48(5)	O1b^{xi}–Cu1b–O2b	104.82(5)
O2a^{v}–Cu1a–O2a^{x}	75.22(6)	O2b^{xi}–Cu1b–O2b	180

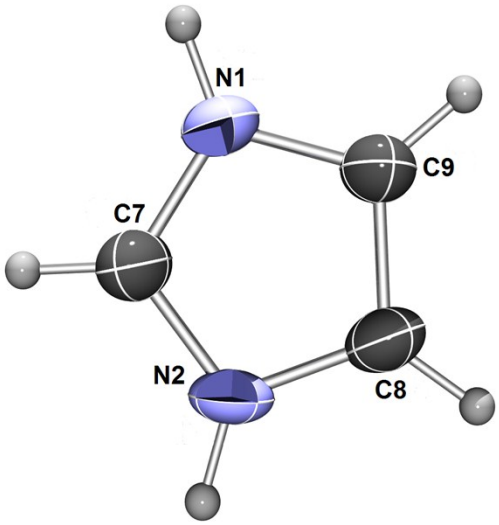

Fig. S1 ORTEP-3 drawing of the imidazolium cation in **1**. Displacement ellipsoids are drawn at the probability of 50% and hydrogen atoms are shown as spheres of arbitrary radii.

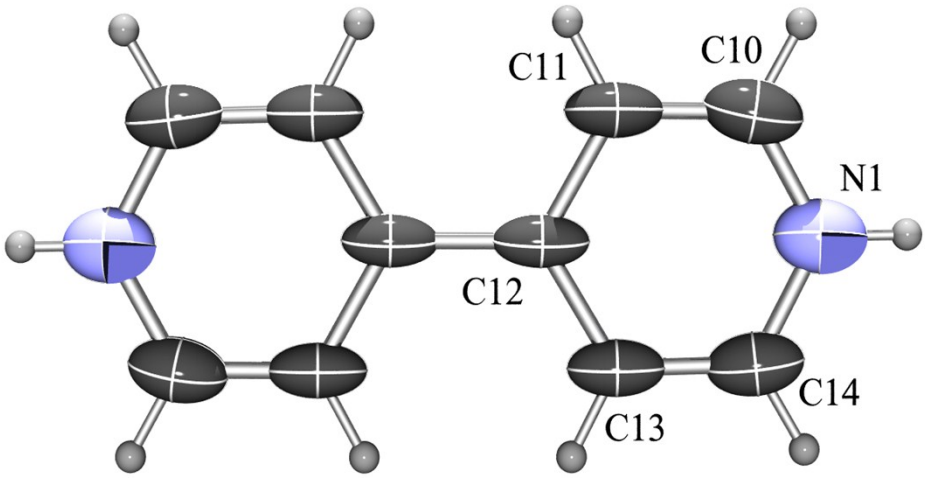

Fig. S2 ORTEP-3 drawing of the 4,4'-bipyridinium cation in **2**. Displacement ellipsoids are drawn at the probability of 50% and hydrogen atoms are shown as spheres of arbitrary radii.