Supplementary Information

Discrete Trinuclear Copper(II) Compounds as Building Blocks: Influence of the Peripheral Substituents on the Magnetic Coupling in Oxamato-Bridged Complexes

Wdeson P. Barros,^a Beatriz C. da Silva,^a Natália V. Reis,^a Cynthia L. M. Pereira,^{a,*} Antônio C. Doriguetto,^b Joan Cano,^{c,d,*} Kleber R. Pirota,^e Emerson F. Pedroso,^f Miguel Julve,^c and Humberto O. Stumpf,^{a,*}

^aDepartamento de Química, ICEx, Universidade Federal de Minas Gerais, 31270-901, Belo Horizonte, MG, Brazil

^bInstituto de Química, Universidade Federal de Alfenas, Alfenas, 37130-000, MG, Brazil

^cInstituto de Ciencia Molecular (ICMol), Paterna (Valencia), 46980, Spain

^dFundació General de la Universitat de València (FGUV)

eInstituto de Física Gleb Wataghin, Universidade Estadual de Campinas, 13083-970, SP, Brazil

^fCentro Federal de Educação Tecnológica de Minas Gerais, 30489-000, Belo Horizonte, MG,

Brazil

*Corresponding author. fax: +55 31 34095700

e-mail address: cynthialopes@ufmg.br (C.L.M.P.); stumpf@ufmg.br (H.O.S.); joan.cano@uv.es (J.C.).



Figure S1. Experimental and calculated X-ray powder diffraction pattern (XPD) for $(Bu_4N)_2[Cu(dmso)_2\{Cu(dnopba)\}_2](dmso)_4(1)$.



Figure S2. Experimental and calculated X-ray powder diffraction pattern (XPD) for $(Bu_4N)_2[Cu(dmso)_2\{Cu(dcopba)\}_2(dmso)_2]$ (2)

	1	2
Cu1–O7	2.300(2)	2.343(2)
Cu1–O4	2.043(2)	2.034(2)
Cu1–N2	1.940(2)	1.941(2)
Cu1–N1	1.913(2)	1.909(2)
Cu1–O3	1.942(1)	1.941(2)
Cu2–O8	2.323(2)	2.367(2)
Cu2–O6	1.996(1)	1.981(1)
Cu2–O5	1.967(1)	1.984(2)
O3–Cu1–O7	92.91(6)	91.20(7)
N1–Cu1–O7	94.54(6)	97.06(8)
N2-Cu1-O7	95.90(6)	95.10(8)
O4–Cu1–O7	99.03(6)	96.99(7)
O3–Cu1–N2	163.88(7)	166.22(8)
N1–Cu1–O4	159.93(7)	160.55(8)
O3–Cu1–N1	83.97(7)	84.50(8)
N1–Cu1–N2	81.90(7)	82.58(9)
N2-Cu1-O4	82.06(7)	82.83(8)
O4–Cu1–O3	109.87(6)	108.58(7)
O6–Cu2–O8	97.57(6)	97.67(7)
O6–Cu2–O(8) ⁱ	82.43(6)	82.33(7)
O5–Cu2–O8	93.02(6)	91.80(7)
O5-Cu2-O(8) ⁱ	86.98(6)	88.20(7)

Table S1. Selected bonds lengths (Å) and angles (°) for compounds 1 and $2^{a,b}$

O6–Cu2–O5	85.19(6)	85.12(7)
O5–Cu2–O(6) ⁱ	94.81(6)	94.88(7)
C1–O2	1.216(3)	1.209(3)
C201	1.228(3)	1.236(3)
С9–Об	1.256(3)	1.249(3)
C10–O5	1.260(2)	1.266(2)
C1–C2	1.563(2)	1.565(3)
C9–C10	1.539(2)	1.545(3)

^a Estimated standard deviations are given in parentheses. ^b Symmetry code: (i) = 2-x, 2-y, -z.