SUPPORTING INFORMATION

Ferromagnetic coupling in a dicopper(II) oxamate complex bridged by carboxylate groups

Tamyris T. da Cunha,[a,b] Cleverton O. C. da Silveira,[a] Vitor M. M. Barbosa,[a] Willian X. C. Oliveira,[a] Eufrânio N. da Silva Júnior,[a] Fabio F. Ferreira,[c] Emerson F. Pedroso,[c] Cynthia L. M. Pereira*[a]

[a]Departamento de Química, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais. Av. Antônio Carlos 6627, Pampulha, Belo Horizonte, Minas Gerais, 31270-901 Brazil. e-mail: cynthialopes@ufmg.br

[b]Instituto Federal de Educação, Ciência e Tecnologia de Minas Gerais, Campus Avançado Itabirito. R. José Benedito, 139, Santa Efigênia, Itabirito, MG, 35450-000, Brazil.

[c]Centro de Ciências Naturais e Humanas (CCNH), Universidade Federal do ABC (UFABC), Av. dos Estados 5001, Santo André, SP, 09210-580, Brazil.

[d]Centro Federal de Educação Tecnológica de Minas Gerais, Av. Amazonas 5523, Belo Horizonte

Table S1. Summary of the crystal data and refinement parameters for **1** and **2**.

Compound	**1**	**2**
Chemical Formulae	$C_{32}H_{32}N_4O_{20}Cu_2$	$C_{16}H_{16}N_2O_{10}Zn$
*F*w / g mol^{-1}	919.52	461.68
λ / Å	0.71073	0.71073
Crystal Size / mm^3	0.21 × 0.17 × 0.13	0.16 × 0.14 × 0.13
Crystal System	Triclinic	Monoclinic
Space Group	$P\bar{1}$	$C2/c$
a / Å	8.7512(6)	12.3838(6)
b / Å	9.7054(6)	7.2105(3)
c / Å	12.4718(9)	20.8942(9)
α / º	67.684(6)	90
β / º	74.454(6)	105.847(5)
γ / º	65.499(6)	90
Volume / Å^3	883.98(12)	1794.81(14)
T / K	150(2)	150(2)
Z	1	4
F(000)	470	944
hkl range	$-10 \le h \le 10$	$-15 \le h \le 10$
	$-12 \le k \le 12$	$-8 \le k \le 8$
	$-15 \le l \le 15$	$-23 \le l \le 26$
ρ_{calc} / g cm^{-3}	1.728	1.709
μ / mm^{-1}	1.298	1.430
Collected reflections	10811	6623
Independent Reflections	3615	1822
Reflections with $I \ge 2\sigma(I)$	1011	1450
R_{int}	0.0390	0.0292
R^a; wR^b [$I \ge 2\sigma(I)$]	0.0333; 0.0768	0.0250; 0.0630
R^a; wR^b (all data)	0.0431; 0.0824	0.0276; 0.0645
Goodness-of-fit on F^2 (S^c)	1.056	1.124
Larg. diff. peak and hole/e Å^{-3}	+0.461; –0.436	+0.266; –0.417
CCDC	1868480	1868481

[a] $R = \sum ||F_o| - |F_c|| / \sum |F_o|$. [b] $wR = [\sum w(|F_o|^2 - |F_c|^2)^2 / \sum w|F_o|^2]^{1/2}$. [c] $S = [\sum w(|F_o|^2 - |F_c|^2)^2 / (N_o - N_p)]^{1/2}$ where *w* is proportional to σ^{-1} whereas N_o and N_p are the number of observed and refined parameters, respectively

Table S2. Crystal data and details of the structure determination for **1a**.

Formula	$C_{16}H_{12}CuN_2O_8$
Molecular weight / g mol^{-1}	423.82
Crystal system	Monoclinic
Space group	$P2_1/c$ (nr. 14)
a/ Å	9.3282(5)
b / Å	9.0226(5)
c / Å	9.2963(5)
β / °	95.931(6)
V / Å^3	778.23(7)
Z, Z'	2, 1
ρ_{calc} / g cm^{-3}	1.8086(2)
R_{exp} / %	1.853
R_{wp} / %	4.951
R_{Bragg} / %	1.457
GOF	2.674
CCDC	2056455

Table S3. The geometry of hydrogen bonds present in the crystal packing of **1**.

		Distance / Å		**Angle / °**
D—H···A	D—H	H···A	D···A	D—H···A
N2^{i}—H2 ^{i}···O1	0.88	2.04	2.86(0)	153
O4—H4A···O10^{ii}	0.84	1.79	2.62(7)	170
O8^{iii}—H8A^{iii} ···O4	0.84	1.89	2.72(6)	172
O10—H10B···O6	0.84	2.00	2.83(9)	142
O10^{iv}—H10A^{iv} ···O8	0.84	2.14	2.90(0)	150

Symmetry codes: (i) -1+x, 1+y, z; (ii) 2-x, 2-y, -z; (iii) x, 2+y, -1+z; (iv) x, -1+y, +z.

Table S4. Final coordinates and equivalent isotropic displacement parameters of the non-hydrogen atoms for **1a**.

Atom	x	y	z	Uiso (Å^2)
Cu1	1/2	1/2	1/2	0.0516
O3	0.3335(5)	0.3879(4)	0.5335(3)	0.0516
O2	0.5457(5)	0.2430(6)	0.8311(4)	0.0516
O1	0.6016(4)	0.4065(4)	0.6675(5)	0.0516
O4	-0.3069(3)	0.0863(3)	0.5422(2)	0.0516
N1	0.2729(2)	0.2113(2)	0.6916(2)	0.0516
C2	0.3623(2)	0.3148(3)	0.6462(3)	0.0516
C1	0.5181(2)	0.3116(3)	0.7187(3)	0.0516
C3	0.12611(19)	0.18827(15)	0.64737(13)	0.0516
C4	0.0422(2)	0.2759(2)	0.54768(16)	0.0516
C8	0.0653(2)	0.06661(16)	0.71152(16)	0.0516
C5	-0.1041(2)	0.24331(19)	0.51073(16)	0.0516
C7	-0.0804(2)	0.0313(2)	0.67680(16)	0.0516
C6	-0.16550(19)	0.12027(17)	0.57575(14)	0.0516
H8	0.0844(2)	0.3602(2)	0.50508(16)	0.0619
H7	-0.1620(2)	0.30321(19)	0.44193(16)	0.0619
H4	0.1245(2)	0.00701(16)	0.77953(16)	0.0619
H1	0.3108(2)	0.1533(2)	0.7600(2)	0.0619
H4A	-0.3241(3)	0.0663(3)	0.4368(2)	0.0619
H5	-0.1219(2)	-0.0527(2)	0.72050(16)	0.0619

Table S5. Some selected bond distances for **1a**.

Bonds	Distances (Å)	Bonds	Distances (Å)
Cu1-O3	1.906(4)	O4-H4A	0.993(3)
Cu1-O1	1.931(4)	C2-C1	1.538(3)
Cu1-C2	2.579(3)	N1-H1	0.870(3)
O2-C1	1.219(5)	C3-C8	1.397(2)
O1-C1	1.282(5)	C3-C4	1.395(2)
O4-C6	1.359(3)	C4-C5	1.404(3)
N1-C2	1.349(3)	C8-C7	1.401(3)
N1-C3	1.404(3)	C5-C6	1.413(2)
O3-C2	1.244(4)	C7-C6	1.415(2)
C8-H8	0.961(3)	C5-H5	0.960(2)
C4-H4	0.960(2)	C7-H7	0.960(2)
N1-C3	1.404(3)		

Table S6. Some selected bond angles for **1a**.

Bonds	Angles (°)	Bonds	Angles (°)
O3-Cu1-O1	88.67(15)	C3-C4-C5	120.56(16)
O3-Cu1-C2	27.29(11)	C3-C8-C7	120.49(15)
Cu1-O1-C1	109.0(3)	C4-C5-C6	119.12(15)
C2-N1-C3	128.82(18)	C8-C7-C6	119.23(15)
Cu1-C2-O3	44.6(2)	O4-C6-C5	120.38(16)
Cu1-C2-C1	75.14(13)	O4-C6-C7	119.28(17)
O1-Cu1-C2	61.42(12)	C5-C6-C7	120.34(16)
N1-C2-C1	115.9(2)	C6-O4-H4A	108.8(3)
O3-C2-C1	119.4(3)	C2-N1-H1	115.3(2)
N1-C2-C1	115.9(2)	C3-N1-H1	115.8(2)
Cu1-C2-N1	166.29(19)	C3-C8-H8	119.3(2)
O1-C1-C2	114.1(3)	C7-C8-H8	120.18(19)
O2-C1-C2	119.5(3)	C4-C5-H5	120.7(2)
O2-C1-O1	125.1(3)	C3-C4-H4	119.8(2)
N1-C3-C4	125.02(15)	C5-C4-H4	119.64(19)
Cu1-O3-C2	108.1(3)	C6-C5-H5	120.2(2)
N1-C3-C8	114.71(14)	C8-C7-H7	120.40(19)
C4-C3-C8	120.27(16)	C6-C7-H7	120.4(2)

Table S7. Intermolecular hydrogen bonds for **1a**. D and A stand for hydrogen donors and acceptors, respectively.

D–H ···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
N1–H1···O2[a]	0.870(3)	2.365(5)	2.749(5)	107.1(2)
N1–H1···O1[b]	0.870(3)	2.443(4)	3.214(4)	148.1(2)
N1–H1···O3[c]	0.870(3)	2.557(3)	3.294(3)	143.1(2)
O4–H4A···O2[d]	0.993(3)	2.270(6)	2.749(5)	108.3(3)
O4–H4A···O1[d]	0.993(3)	2.540(5)	3.500(5)	162.8(3)
C4–H4···O3[a]	0.961(3)	2.325(5)	2.915(5)	119.06(19)

Symmetry code: [a]*x*, *y*, *z*; [b]1-*x*, -½+*y*, 3/2-*z*; [c]*x*, ½-*y*, ½+*z*; [d]-1+x, ½-y,-½+z

Table S8. Geometry of hydrogen bonds present in the crystal packing of **2**.

		Distance / Å		**Angle / °**
D—H···A	D—H	H···A	D···A	D—H···A
O9^{i}—H9B ^{i}···O1	0.91	1.87	2.77(6)	162
O4^{ii}—H4^{ii}···O2	0.82	1.86	2.66(4)	163
O10^{iii}—H10A^{iii} ···O4	0.81	1.97	2.77(5)	165
O10^{iv} —H10B ^{iv} ···O5	0.96	1.88	2.82(0)	162
O8^{v}—H8^{v} ···O6	0.82	1.85	2.62(0)	154
O9^{vi}—H9^{vi}···O8	0.83	1.98	2.78(0)	158

Symmetry codes: (i) ½ +x, -½ +y, z; (ii) ½ +x, -½ +y, ½ +z; (iii) -½ +x, ½ -y, -½ +z ; (iv) -½ +x, -½ +y, z ; (v) -½ +x, -½ -y, -½ +z, (vi) ½ +x, ½ -y, ½ +z ;