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Supporting Information: Antisymmetric Magnetic Interactions in oxo-bridged Copper (II) Bimetallic Systems

Rémi Maurice,[†,‡] Muizz Pradipto,[¶] Nathalie Guihéry,[*,†] Ria Broer,[¶] and Coen de Graaf[*,§,‡]

Laboratoire de Chimie et Physique Quantiques, Université de Toulouse 3, 118, route de Narbonne, 31062 Toulouse France, Departament de Química Física i Inorgànica, Universitat Rovira i Virgili, Marcel·lí Domingo s/n, 43007 Tarragona, Spain, Zernike Institute for Advanced Materials, University of Groningen, Groningen 9747AG, The Netherlands, and Institució Catalana de Recerca i Estudis Avançats (ICREA), Passeig Lluis Companys 23, 08010, Barcelona, Spain

E-mail: nathalie.guihery@irsamc.ups-tlse.fr; coen.degraaf@urv.cat

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- Expression of the magnetic orbitals in the $\vartheta_1 = \vartheta_2 = 40^\circ$ model structure.
- Values of the atomic spin-orbit constant used in the estimation of the spin-orbit coupling listed in Table 5.

[†]Université de Toulouse 3
[‡]Universitat Rovira i Virgili
[¶]University of Groningen
[§]ICREA

- Expression of the magnetic orbitals in the $\vartheta_1 = \vartheta_2 = 40^\circ$ model structure:

$$\phi_s = 0.2260(d^l_{xy} - d^r_{xy}) + 0.5941(d^l_{z^2} + d^r_{z^2}) - 0.3023(d^l_{x^2-y^2} + d^r_{x^2-y^2}) - 0.0952p_y \quad (1)$$

$$\phi_a = -0.2285(d^l_{xy} + d^r_{xy}) - 0.5868(d^l_{z^2} - d^r_{z^2}) + 0.2898(d^l_{x^2-y^2} - d^r_{x^2-y^2}) - 0.1973p_x \quad (2)$$

$$\phi'_s = 0.2313(d^l_{xy} - d^r_{xy}) + 0.5939(d^l_{z^2} + d^r_{z^2}) - 0.2992(d^l_{x^2-y^2} + d^r_{x^2-y^2}) - 0.0919p_y \quad (3)$$

$$\phi'_a = -0.2327(d^l_{xy} + d^r_{xy}) - 0.5860(d^l_{z^2} - d^r_{z^2}) + 0.2872(d^l_{x^2-y^2} - d^r_{x^2-y^2}) - 0.2001p_x \quad (4)$$

- Values of the atomic spin-orbit constant used in the estimation of the spin-orbit coupling listed in Table 5:

$$\zeta_1 = 829 \text{ cm}^{-1} \quad (5)$$

$$\zeta_2 = 931 \text{ cm}^{-1} \quad (6)$$

$$\zeta_3 = 158 \text{ cm}^{-1} \quad (7)$$

$$\zeta_4 = 158 \text{ cm}^{-1} \quad (8)$$

The ζ_4 atomic spin-orbit coupling constant of the O^- ion cannot be determined experimentally in the same way as the others. Hence, considering that this constant should have the same order of magnitude than the one of the O atom, ζ_4 has been set equal to ζ_3.