

Electronic Supplementary Information (ESI)

Molecular squares of Ni^{II} and Cu^{II}: ferromagnetic exchange interaction mediated by syn-anti carboxylate-bridging

Himanshu Arora, Francesc Lloret and Rabindranath Mukherjee*

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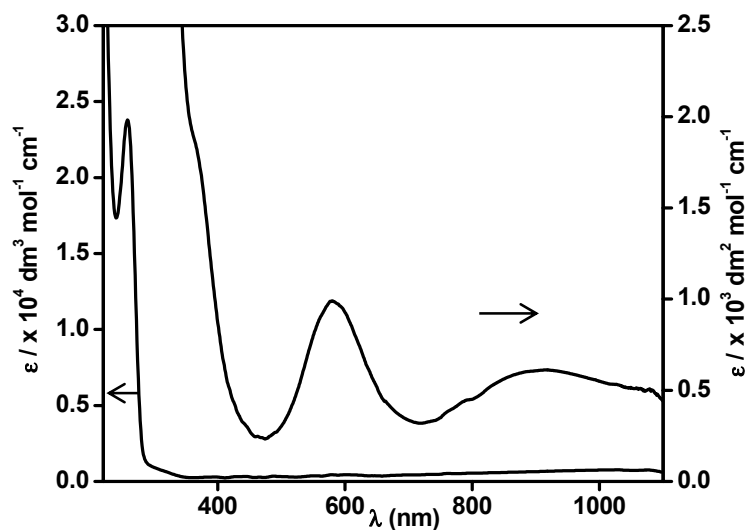


Fig. S1 UV-vis spectra of {[Ni^{II}(L²)]}[ClO₄]₄·MeCN (**1**) in MeCN.

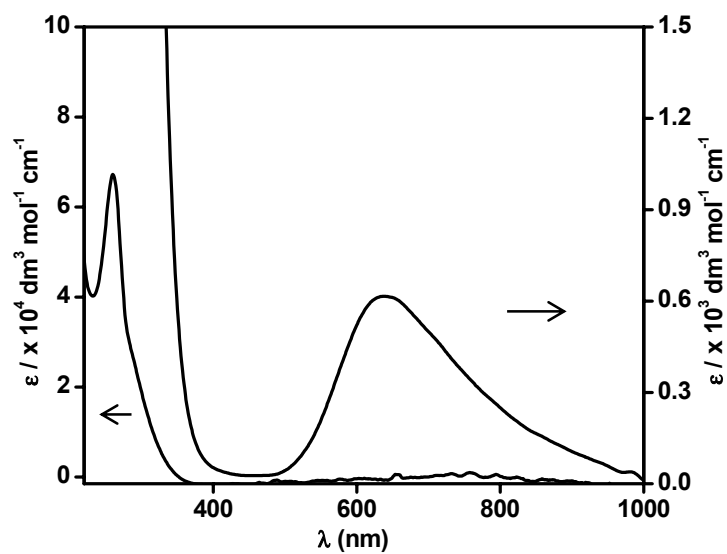


Fig. S2 UV-vis spectra of $\{[\text{Cu}^{\text{II}}(\text{L}^1)(\text{O}_3\text{SCF}_3)]\}_4\cdot\text{H}_2\text{O}$ (**2**) in MeCN.

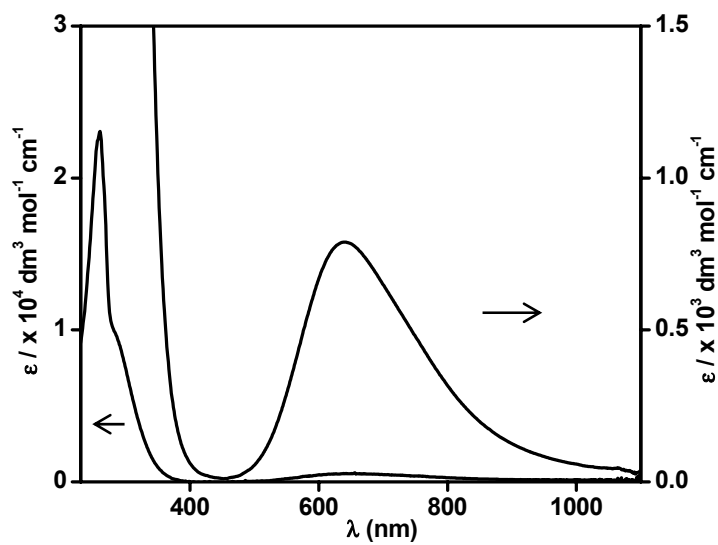


Fig. S3 UV-vis spectra of $\{[\text{Cu}^{\text{II}}(\text{L}^3)(\text{OCIO}_3)]\}_4\cdot\text{MeCN}$ (**3**) in MeCN.

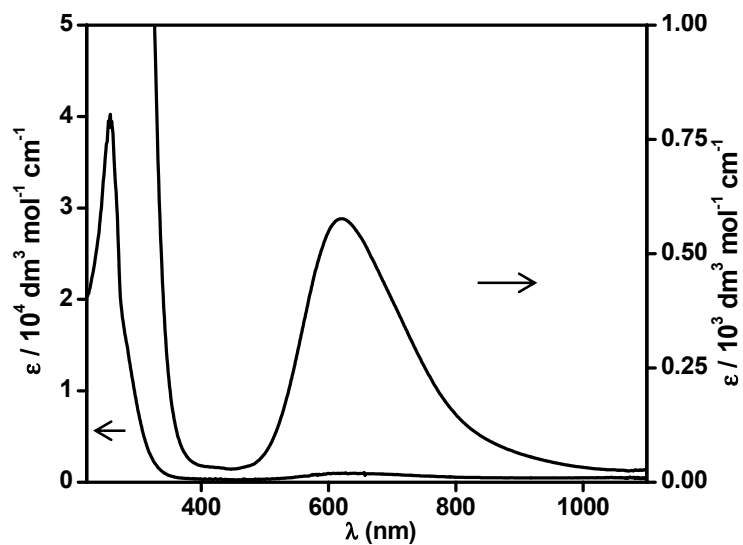


Fig. S4 UV-vis spectra of $\{[\text{Cu}^{\text{II}}(\text{L}^4)][\text{ClO}_4]\}_4 \cdot 3\text{MeCN} \cdot 4\text{H}_2\text{O}$ (**4**) in MeCN.

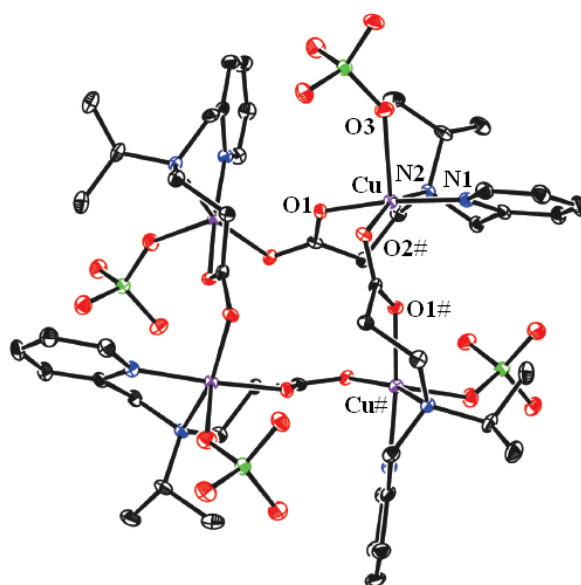


Fig. S5 View of the metal coordination environment in the crystals of $\{[\text{Cu}^{\text{II}}(\text{L}^3)(\text{OCIO}_3)]\}_4 \cdot \text{MeCN}$ (**3**) at 30 % thermal ellipsoids probability. Hydrogen atoms are omitted for clarity.

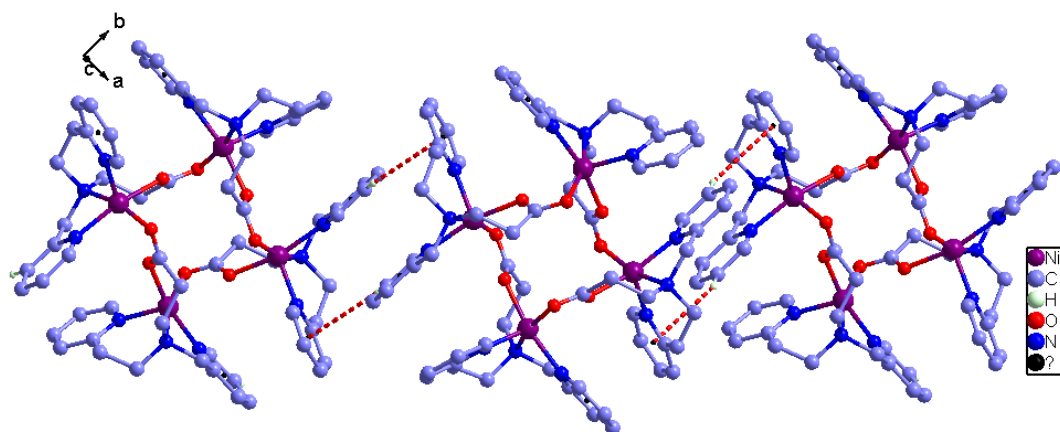


Fig. S6 C-H... π interactions in $\{[\text{Ni}^{\text{II}}(\text{L}^2)][\text{ClO}_4]\}_4\text{MeCN}$ (1).

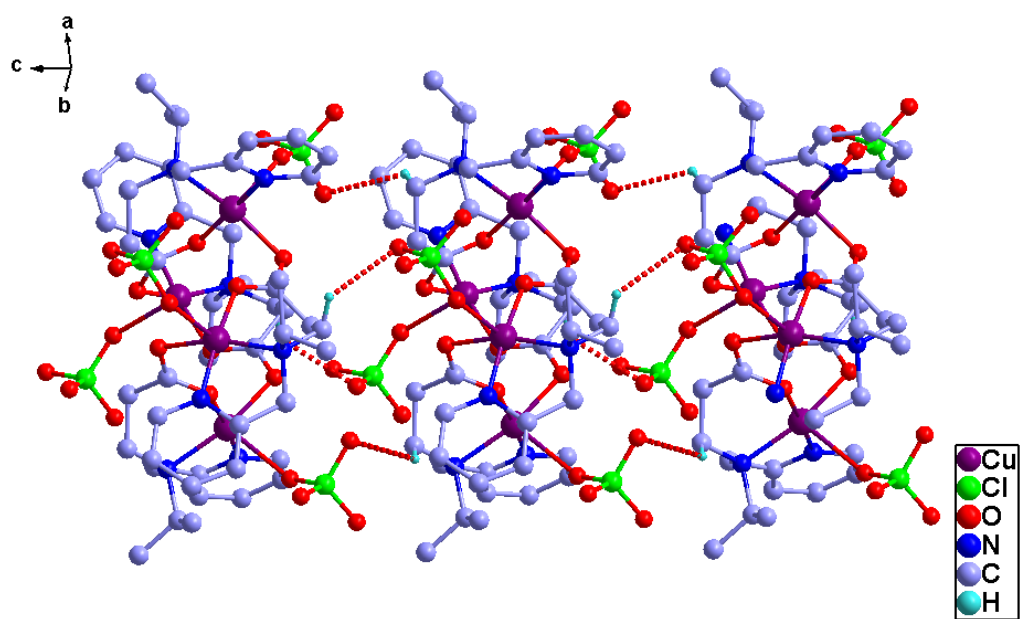


Fig. S7 C-H...O interactions in $\{[\text{Cu}^{\text{II}}(\text{L}^3)(\text{OCIO}_3)]\}_4\text{MeCN}$ (3)

Table S1 C–H \cdots π and C–H \cdots O parameters for **1**, **2** and **3**.

Complex	D–H \cdots A	H \cdots A, Å	D \cdots A, Å	D–H \cdots A
1	C12–H12 \cdots π	3.403	4.1733(10)	141.781 ^o [ⁱ]
2	C8–H8A \cdots O5	2.377 ^[ii]	3.4468(3) ^[ii]	170.163 ^o [ⁱⁱⁱ]
3	C10–H10A \cdots O4	2.635 ^[ii]	3.4163(9) ^[ii]	128.572 ^o [ⁱⁱⁱ]

(i) $0.5 + x, -0.5 + y, 2 - z$. (ii) $x, y, -1 + z$. (iii) $x, y, 1 + z$.