

## Supporting Information

### **Self assembled tetranuclear Cu<sub>4</sub>(II), Ni<sub>4</sub>(II) [2x2] square grids and a dicopper(II) complex of heterocycle based polytopic ligands - Magnetic studies<sup>†</sup>**

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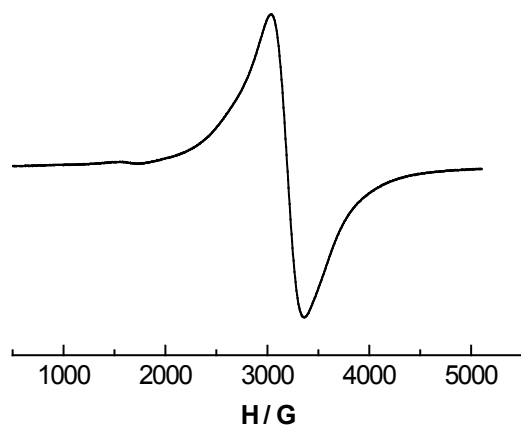
**Table-S1**

Selected hydrogen bond distances (Å) and angles (°) of **1-4**.

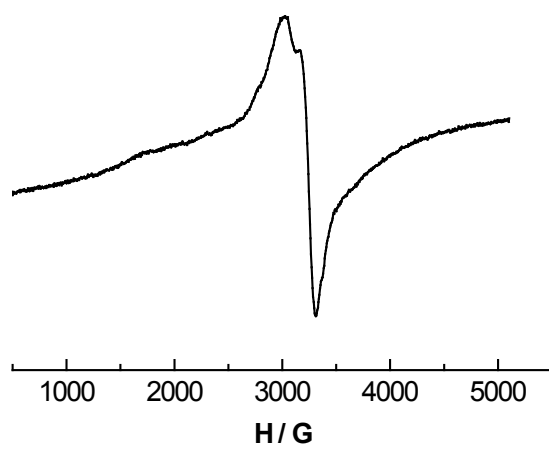
Complex	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
<b>1</b>	N7-H7A..... O100	0.86	2.43	2.931(17)	118
	N7-H7B..... O102	0.86	1.92	2.505(14)	124
	N7-H7B..... O201	0.86	2.11	2.49(2)	107
<b>2</b>	N6-H6N ....O17	0.86	1.95	2.79(2)	164
	N8-H8A ....N10	0.86	2.53	2.80(11)	100
	N14-H14B ....O5	0.86	2.12	2.969(15)	169
	N18-H18N ....O13	0.86	2.24	2.85(3)	128
	N20-H20A ....N22	0.86	2.55	2.831(6)	100
	N20-H20B ....O11	0.86	2.16	3.00(15)	164
	N24-H24 ....O12	0.86	2.05	2.900(11)	169
<b>3</b>	O1W-H2W1 .....N3	0.85	2.17	2.988(9)	163
	N7- H7A..... O1W	0.86	2.17	3.033(9)	176
	N7-H7A..... N3	0.86	2.46	2.737(5)	100
	N7-H7B..... O101	0.86	2.07	2.915(10)	168
<b>4</b>	O3W-H3W1 ....O11A	0.875(17)	1.886(18)	2.758(7)	174(3)
	N3A-H3AB ....O3W	0.88	2.00	2.793(2)	149.7
	N3B-H3BB ....O2W	0.88	2.06	2.914(2)	162.7

### EPR spectra of **2** and **4**:

The X-band EPR spectra of **2** and **4** at different temperatures are very similar. The EPR spectrum of **2** at 200 K (Figure S1) shows an isotropic band centred at  $g = 2.11$  (3183 G for  $\nu = 9.4311$  GHz) which corresponds to the transition  $\Delta M_S = \pm 1$ . The band assigned to half filled transition ( $\Delta M_S = \pm 2$ , much less intense) is observed at  $g = 4.2$  (1605 G for  $\nu = 9.4311$  GHz). The polycrystalline EPR spectrum of **4** (Figure S2) at room temperature gives three very asymmetric three picks, corresponding to the three components of the tensor  $g$ , located at  $g_1=2.23$ ,  $g_2=2.14$  and  $g_3=2.03$  (3017 G, 3144 G and 3310 G, respectively for  $\nu = 9.4287$ ). The band assigned to half filled transition ( $\Delta M_S = \pm 2$ ) is hardly distinguished at  $g_{1/2} = 4.0$  (1683 G for  $\nu = 9.4287$ ).



**Fig. S1:** EPR spectra of **2** at 200 K.



**Fig. S2:** EPR spectra of **4** at room temperature.