Electronic Supplementary Information

For

More surprising difference between two closely similar compartmental ligand families and another dinuclear synthon to stabilize dinuclear-mononuclear cocrystals

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Table S1 Structural parameters (distances in Å and angles in º) in the coordination environment of the copper(II) centers in **1** and **2**

	1	**2**
Cu1–N1	1.964(2)	1.958(2)
Cu1–N2	1.974(2)	1.971(2)
Cu1–O1	1.9528(18)	1.9585(17)
Cu1–O2	1.9376(17)	1.9323(17)
N1–Cu1–O2	169.69(8)	169.72(8)
O1–Cu1–N2	169.93(8)	169.61(8)
O1–Cu1–N1	92.44(9)	93.06(8)
O1–Cu1–O2	77.35(7)	76.81(7)
O2–Cu1–N2	92.59(8)	92.83(8)
N1–Cu1–N2	97.60(9)	97.27(9)
d_{Cu} [a]	0.019	0.023
$d_{N/O}$ [a]	0.0068	0.0074

[a] d_{Cu} is the displacement of the copper center and $d_{N/O}$ is the deviation of the constituent atoms from the corresponding least-squares $N(imine)_2O(phenoxo)_2$ basal plane.

Table S2 Structural parameters (distances in Å and angles in º) in the coordination environment of the copper(II) centers in **3** and **4**

	3	**4**		**3**	**4**
Cu1–N1	1.907(3)	1.913(2)	O1–Cu1–N2	178.05(10)	177.75(9)
Cu1–N2	1.924(3)	1.933(2)	N1–Cu1–O2	178.19(11)	178.19(10)
Cu1–O1	1.894(2)	1.9019(19)	O1–Cu1–N1	96.18(10)	96.35(9)
Cu1–O2	1.880(2)	1.8847(19)	O1–Cu1–O2	82.85(9)	82.41(8)
			O2–Cu1–N2	95.29(10)	95.48(9)
			N1–Cu2–N2	85.70(11)	85.78(10)
d_{Cu}[a]	0.008	0.004			
$d_{N/O}$[a]	0.0168	0.017			
Cu2–N3	1.949(3)	1.953(3)	O8–Cu2–N4	176.99(12)	177.01(11)
Cu2–N4	1.940(3)	1.949(3)	N3–Cu2–O9	176.67(12)	176.75(11)
Cu2–O8	1.911(2)	1.917(2)	O8–Cu2–N3	93.66(12)	93.61(11)
Cu2–O9	1.907(3)	1.911(2)	O8–Cu2–O9	89.13(12)	89.13(10)
			O9–Cu2–N4	93.83(12)	93.86(11)
			N3–Cu2–N4	83.40(13)	83.40(12)
d_{Cu}[a]	0.010	0.014			
$d_{N/O}$[a]	0.020	0.015			
Cu3–N5	1.936(3)	1.945(3)	O12–Cu3–N6	177.68(11)	177.45(10)
Cu3–N6	1.943(3)	1.948(3)	N5–Cu3–O13	176.20(10)	176.42(10)
Cu3–O12	1.897(2)	1.901(2)	O12–Cu3–N5	94.64(11)	94.46(10)
Cu3–O13	1.890(2)	1.896(2)	O12–Cu3–O13	86.62(9)	86.65(9)
			O13–Cu3–N6	94.51(11)	94.53(10)
			N5–Cu3–N6	84.11(13)	84.23(12)
d_{Cu}[a]	0.046	0.047			
$d_{N/O}$[a]	0.020	0.009			

[a] d_{Cu} is the displacement of the copper center and $d_{N/O}$ is the deviation of the constituent atoms from the corresponding least-squares $N(imine)_2O(phenoxo)_2$ basal plane.

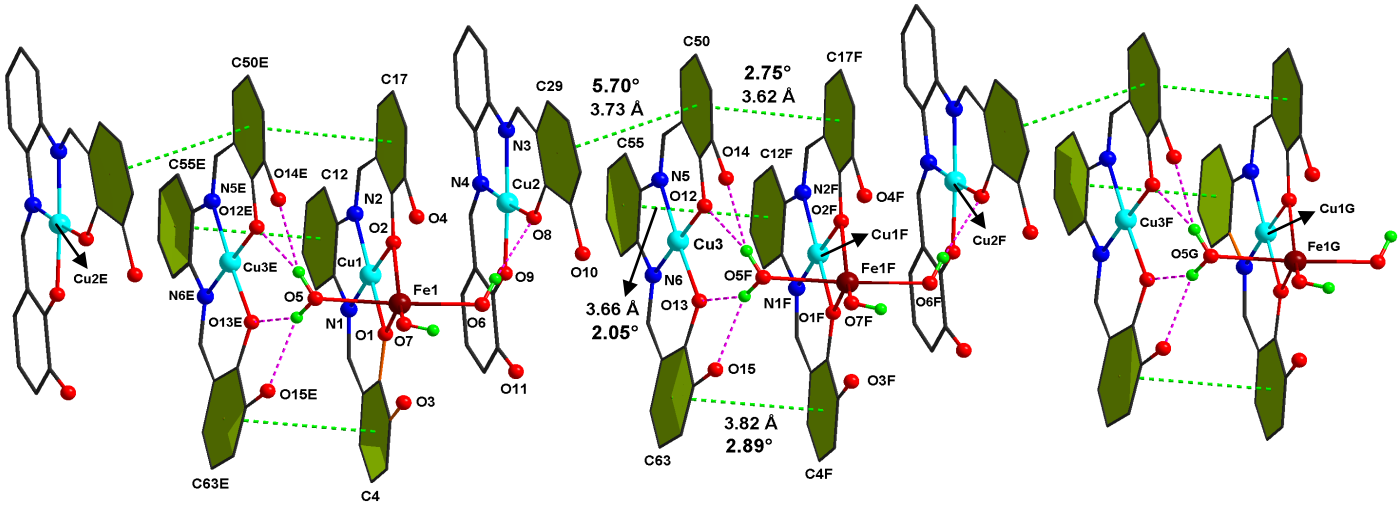

Fig. S1 Perspective view of $[\{Cu^{II}L^{2}Fe^{II}(H_2O)(MeOH)_2\}(Cu^{II}L^{2})_2](ClO_4)_2\cdot MeOH$ (**4**) showing hydrogen bonding and π···π stacking interactions and one-dimensional self-assembly. Methyl groups of methoxy moieties, perchlorate anions and methanol as solvent of crystallization have been omitted. Only those hydrogen atoms are shown which participate in hydrogen bonding. The values in Å and ° are the centroid-to-centroid distances and dihedral angles between the aromatic rings responsible for π···π stacking interactions. Symmetry codes: E, 1+x, y, z; F, −1+x, y, z; G, −2+x, y, z.

The equations used for simulation of magnetic data of 1–4 are mentioned below:

$Cu^{II}Mn^{II}$ (1):	$Cu^{II}Fe^{II}$ (2):
$\chi_M = \frac{\chi_D}{1 - 2zJ'\chi_D / N\beta^2 g^2}$ where $\chi_D = \frac{N\beta^2 g^2}{kT} \frac{10 + 28e^{6J/kT}}{5 + 7e^{6J/kT}} + TIP$	$\chi_M = \frac{\chi_D}{1 - 2zJ'\chi_D / N\beta^2 g^2}$ where $\chi_D = \frac{N\beta^2 g^2}{4kT} \frac{10 + 35e^{5J/kT}}{2 + 3e^{5J/kT}} + TIP$
$Cu^{II}Mn^{II}\cdots 2Cu^{II}$ (3):	$Cu^{II}Fe^{II}\cdots 2Cu^{II}$ (4):
$\chi_M = \frac{\chi_M^1}{1 - 2zJ'\chi_M^1 / N\beta^2 g^2}$ where $\chi_M^1 = \frac{7.997\chi_D T + 2\mu_{Cu}{}^2}{7.997T} + TIP$ with $\chi_D = \frac{N\beta^2 g^2}{kT} \frac{10 + 28e^{6J/kT}}{5 + 7e^{6J/kT}}$	$\chi_M = \frac{\chi_M^1}{1 - 2zJ'\chi_M^1 / N\beta^2 g^2}$ where $\chi_M^1 = \frac{7.997\chi_D T + 2\mu_{Cu}{}^2}{7.997T} + TIP$ with $\chi_D = \frac{N\beta^2 g^2}{4kT} \frac{10 + 35e^{5J/kT}}{2 + 3e^{5J/kT}}$