Electronic Supplementary Information

Homo- and heterodinuclear complexes of the tris(catecholamide) derivative of a tetraazamacrocycle with Fe^{3+}, Cu^{2+} and Zn^{2+} metal ions

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Table S1. Spectroscopic UV-vis data for the solutions of 1:1 and 2:1 Cu^{2+}ion to H_6L^1 ratios at different pH values. ($I = 0.1$ mol dm^{-3} KNO_3, $T = 298$ K).

pH, ratio, colour	UV-vis λ_{max}/nm (ε_{molar}/dm^3 mol^{-1} cm^{-1})
5.4, 1:1, greenish blue	250 (9.8×10^3), 316 (5.9×10^3), 326 (sh., 5.7×10^3), 340 (sh., 4.0×10^3), 430 (sh., 268), 550 (sh., 142), 626 (125), 740 (sh., 78)
7.1, (1:1) greenish yellow	250 (sh., 1.25×10^4), 316 (7.4×10^3), 326 (sh., 7.3×10^3), 340 (sh., 5.5×10^3), 430 (sh., 531), 550 (sh., 275), 626 (224), 740 (sh., 151)
10.0, 1:1, greenish yellow	250 sh., 316, 326 sh., 340 sh., 430 sh., 550 sh., 626, 740 sh.
9.1, 2:1, yellow	250 (sh., 1.77×10^4), 316 (12.1×10^3), 326 (sh., 11.5×10^3), 340 (sh., 8.3×10^3), 430 (sh., 479), 550 (sh., 255), 626 (234), 740 (sh., 160)

Table S2. Spectroscopic UV-Vis data for Fe^{3+}/H_6L^1 1:1 ratio solutions at different pH regions ($I = 0.10$ mol dm^{-3} KNO$_3$, $T = 298$ K).

pH, colour	UV-vis λ_{max}/nm(ε_{molar}/dm^3 mol^{-1} cm^{-1})
5.0, light purple	250 (sh., 1.6×10^4), 316 (sh., 8.6×10^3), 330 (sh., 7.3×10^3), 410 (sh., 3.1×10^3), 520 (2.3×10^3), 750 (sh., 846)
6.9, purple	250 (sh., 23.4×10^3), 316 (13.5×10^3), 330 (sh., 10.3×10^3), 410 (sh., 3.4×10^3), 520 (2.5×10^3), 750 (sh., 584)
11.4, red	250 (3.0×10^4), 316 (2.5×10^4), 326 (sh., 2.1×10^4), 330 (sh., 2.0×10^4), 410 (sh., 5.0×10^3), 474 (4.8×10^3), 750 (sh., 947)

Table S3. Spectroscopic UV-vis data of $Cu^{2+}/Fe^{3+}/H_6L^1$ 1:1:1 ratio solutions at different pH ($I = 0.1$ mol dm^{-3}, KNO_3, $T = 298$ K)

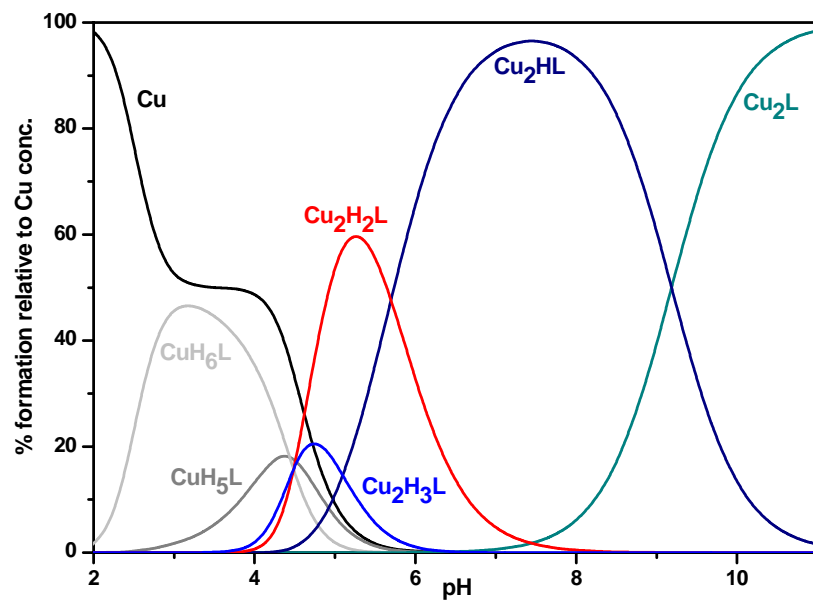| pH	colour	UV-vis λ_{max}/nm (ε_{molar}/dm^3 mol^{-1} cm^{-1})
7.0	red purple	250 (1.4×10^4), 294 (sh., 1.1×10^4), 316 (sh., 8.9×10^3), 326 (sh., 8.1×10^3), 340 (sh., 6.1×10^3), 406 (sh., 2.7×10^3), 622 (sh., 1.5×10^3), 740 (sh., 930)
10.0	dark red purple	250 (1.8×10^4), 316 (1.7×10^4), 326 (sh., 1.3×10^4), 340 (sh., 8.4×10^3), 370 (sh., 2.7×10^3), 454 (2.45×10^3), 740 (sh., 725)

Fig. S1. Species distribution curves calculated for the Cu^{2+}/H_6L^1 system in aqueous solution. $C_{Cu} = 2 \times C_L = 2.0 \times 10^{-3}$ mol dm^{-3}. L = L^1.

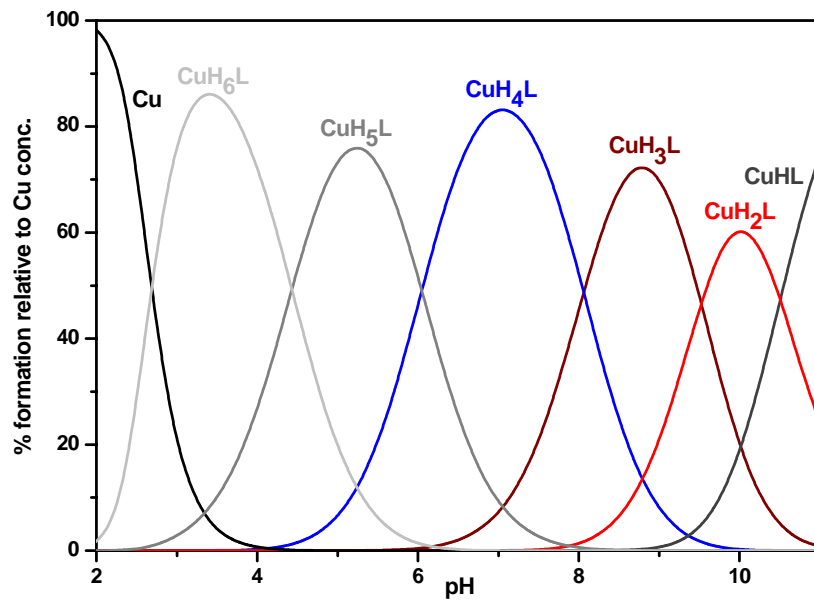**Fig. S2.** Species distribution curves calculated for the Cu^{2+}/H_6L^1 system in aqueous solution. $C_{Cu} = C_L = 1.0 \times 10^{-3}$ mol dm^{-3}. $L = L^1$.

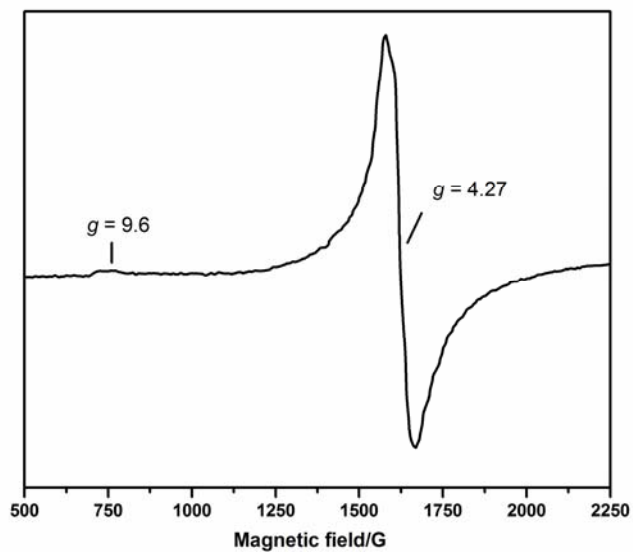**Fig. S3**. X-band EPR signal of the Fe^{3+}/H_6L^1 1:1 ratio solution at pH 10.2, recorded in water/DMSO (1:1 v/v), at 4.7 K. Microwave power of 2.35 mW, modulation amplitude of 1 mT and frequency of 9.64 GHz.