Supporting Information

Calix[4]pyrrole Schiff base macrocycles.
Novel binucleating ligands for Cu(I) and Cu(II).

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I. Magnetic Measurements for complexes 4 and 5.

Evans Method. Solution magnetic measurements were made using the Evans method. Solutions of the metal complex were prepared in $CDCl_3$ and placed in 5 mm NMR tubes, while pure $CDCl_3$ was placed in a concentric capillary tubes within the NMR tubes. Calculations of the magnetic moments (μ) were based on the difference in chemical shift observed (400.269 MHz) for the residual $CHCl_3$ signal in neat solvent and in the solution containing the paramagnetic species.

Complex 4, $[C_{38}H_{32}N_8)Cu^{II}_2]$.

1) Concentration of **4** = 0.0066 M, $\Delta\delta$ = 19.2129 Hz, μ_{eff} = 2.06 μ_B
2) Concentration of **4** = 0.0026 M, $\Delta\delta$ = 6.8046 Hz, μ_{eff} = 1.95 μ_B

Complex 5, $[(C_{42}H_{40}N_8O_4)Cu^{II}_2]$.

1) Concentration of **5** = 0.0027 M, $\Delta\delta$ = 6.8046 Hz, μ_{eff} = 1.92 μ_B
2) Concentration of **5** = 0.0032 M, $\Delta\delta$ = 8.8059 Hz, μ_{eff} = 1.99 μ_B

SQUID. Solid State magnetic susceptibilities were measured using a Quantum Design MPMS SQUID system in the temperature range of 4−300 K in a field of 1 kOE. The crystalline sample was placed inside a gelatin capsule. The susceptibility contribution from the capsule was measured separately and subtracted from the data.

Complex 3, $[C_{38}H_{32}N_8)Cu^{II}_2]$

The molar magnetic susceptibility data for **3** were fitted to a modified Bleaney-Bowers equation:

$$\chi_{molar} = (1-p)\frac{2Ng^2\beta^2}{kT}\left(\frac{1}{3+e^{\frac{-J}{kT}}}\right) + p\frac{2Ng^2\beta^2}{3kT}S(S+1) + \chi_0$$

Where,
p = molar fraction of paramagnetic impurity
N = Avogadro's Number
g = g-factor
β = Bohr magneton
k = Boltzmann constant
J = exchange coupling constant
S = spin quantum number
χ_0 = temperature independent susceptibility (sum of a negative contribution from Langevin diamagnetism and a positive contribution from Van Vleck paramagnetism).

A reasonable fit ($R = \Sigma_i[(\chi_{obs})_i-(\chi_{calc})_i]^2/\Sigma_i(\chi_{obs})^2 = 0.00037$) was obtained using the following parameters:

$p = 0.0118 \pm 0.0007$
$g = 1.9 \pm 0.1$
$J = -41.0 \pm 0.2\ cm^{-1}$
$S = ½$
$\chi_0 = 0.00065 \pm 0.00005$