Electronic Supplementary Information
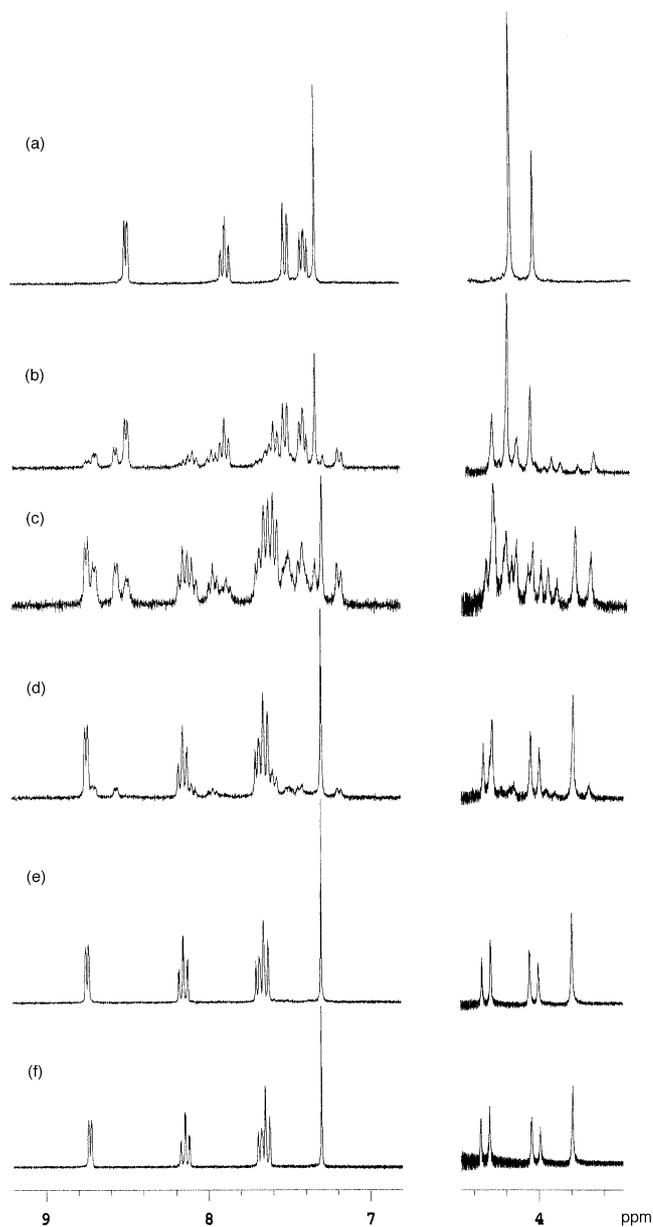

Fig. S1 ^{1}H NMR spectra of the $Zn(NO_3)_2$ + **3** system at rt (pD 7). The concentration of **3** was fixed at 5 mM, and that of $Zn(NO_3)_2$ was varied. (a) $[Zn(NO_3)_2]$ = 0 mM, (b) $[Zn(NO_3)_2]$ = 2.5 mM, (c) $[Zn(NO_3)_2]$ = 5 mM, (d) $[Zn(NO_3)_2]$ = 7.5 mM, (e) $[Zn(NO_3)_2]$ = 10 mM, (f) $[Zn(NO_3)_2]$ = 50 mM. The region of pyridyl and phenyl proton signals (left) and that of other proton signals (right) are shown separately.
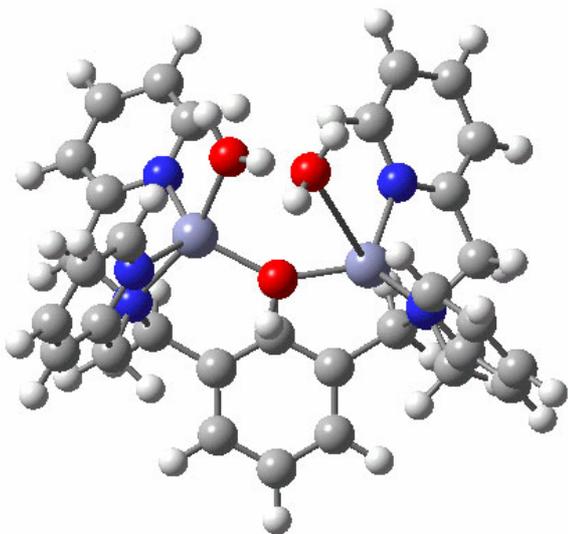
(a)

(b)

(c)
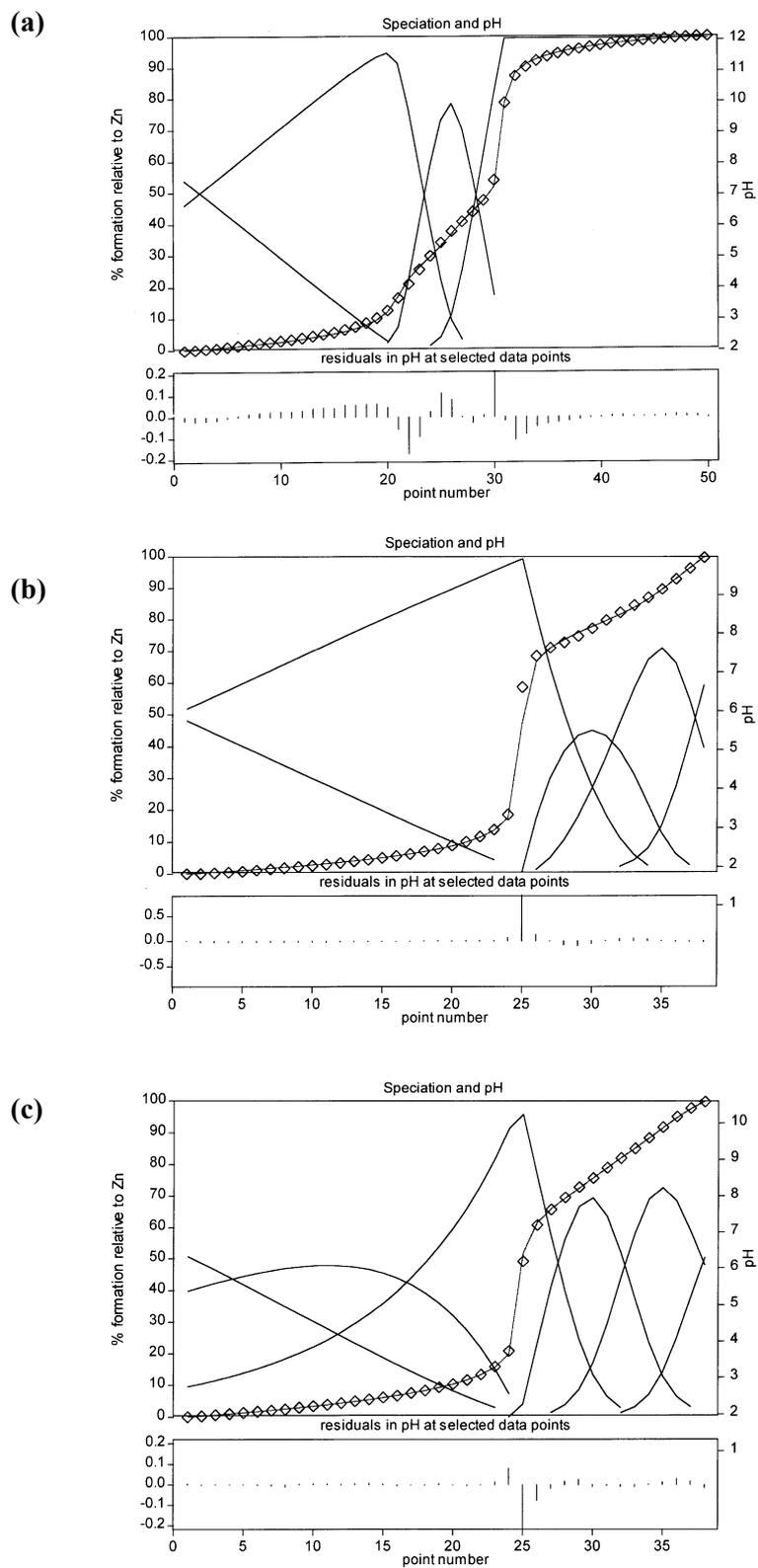
Fig. S2 Titration data and theoretical curves. (a) The 2:1 mixture of $Zn(NO_3)_2$ and **1**, (b) the 2:1 mixture of $Zn(NO_3)_2$ and **2** and (c) the 2:1 mixture of $Zn(NO_3)_2$ and **3**.

(a)
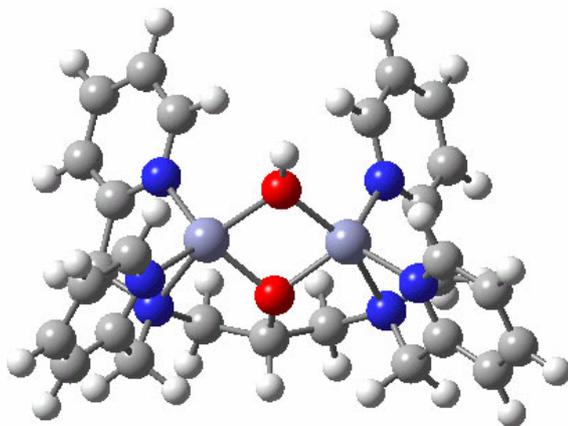
(b)

Fig. S3 Optimized structures of (a) $Zn_2\mathbf{1}H_{-2}$ and (b) $Zn_2\mathbf{2}H_{-1}$, obtained by *ab intio* molecular orbital calculations using the Hartree-Fock method with the 3-21G basis set. Program used was Gaussian 03W, and these figures were drawn using GaussView 3.0.