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Supplementary Information

Anion and ion-pair binding by a G-2 poly(ethylene imine) dendrimer

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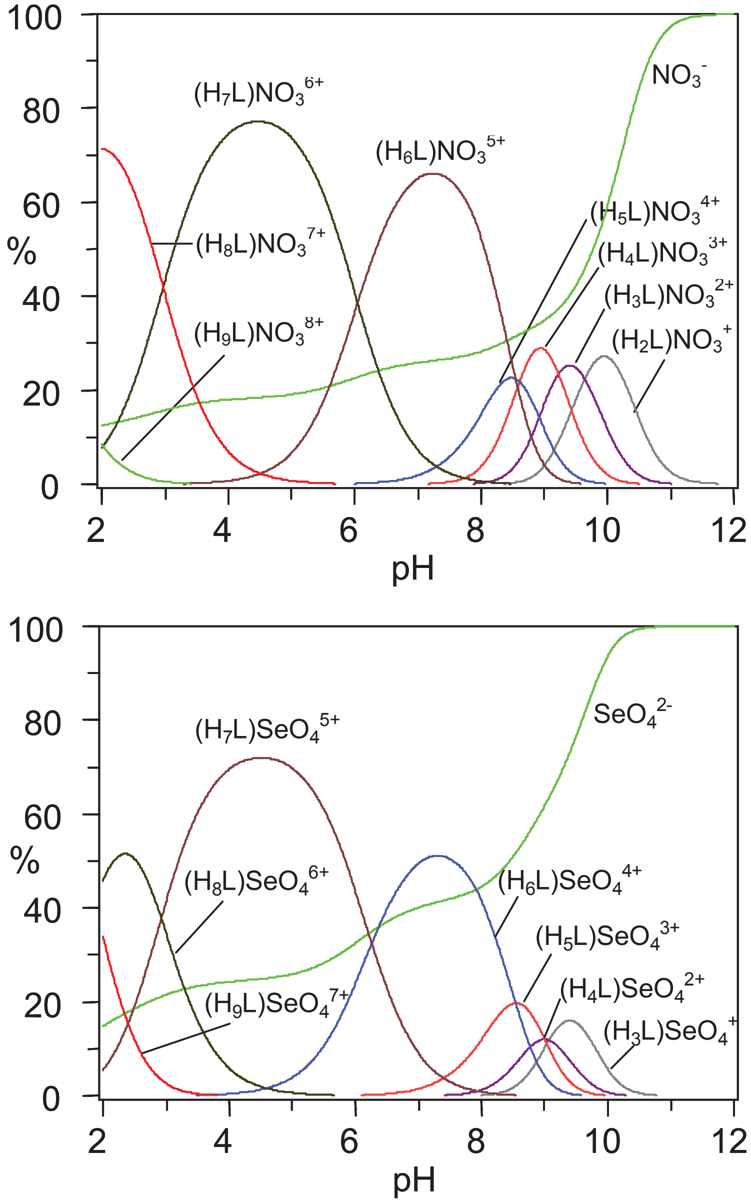

Figure S1. Distribution diagrams of the anion complexes formed in the system L/NO_3^- and L/SeO_4^{2-}. [L] = [anion] = 1×10^{-2} M.

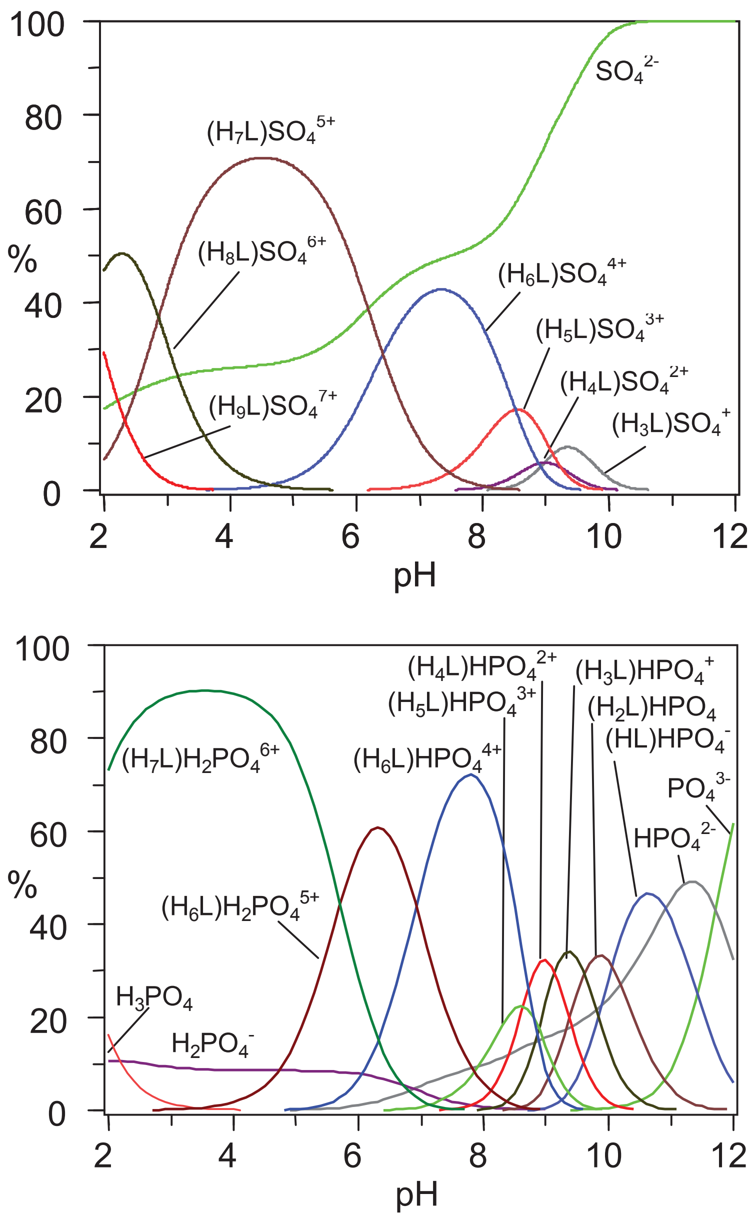

Figure S2. Distribution diagrams of the anion complexes formed in the system L/SO_4^{2-} and L/PO_4^{3-} . [L] = [anion] = 1×10^{-2} M.

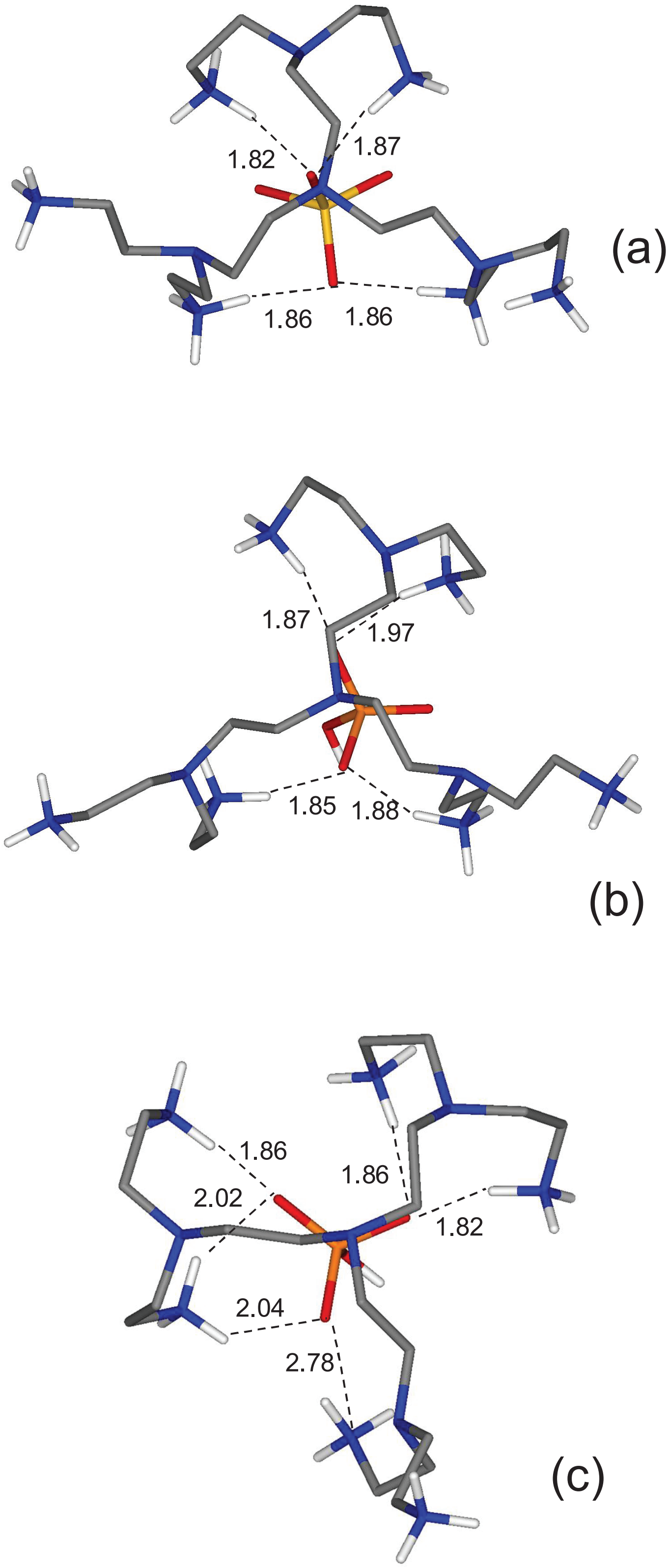

Figure S3. Less abundant conformers calculated for $(H_6L)SO_4^{4+}$ (a) and $(H_6L)HPO_4^{4+}$ (b) (c).

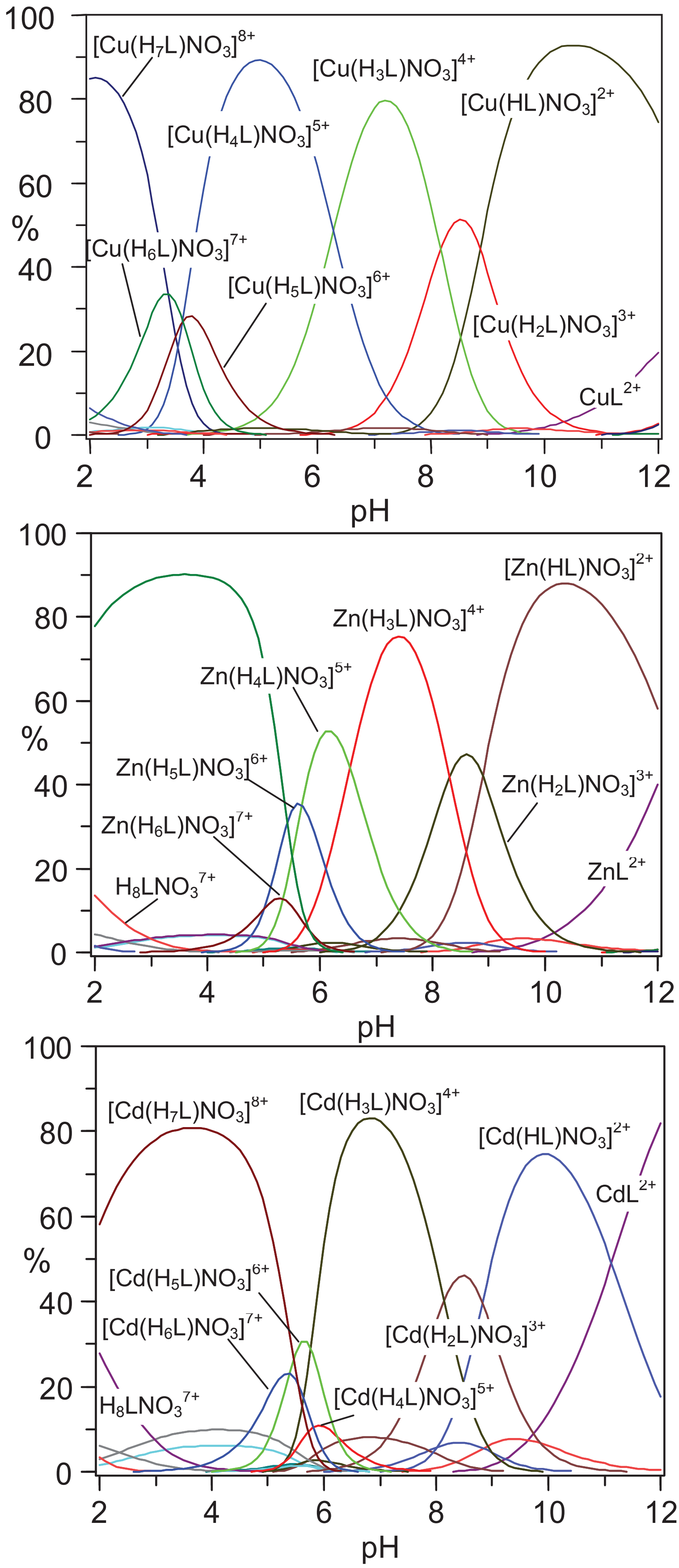

Figure S4. Distribution diagrams of the ion-pair complexes formed by L with M^{2+} (Cu^{2+}, Zn^{2+}, Cd^{2+}) and nitrate as a function of pH. [L] = $[M^{2+}]$ = [anion] = 1×10^{-2} M.

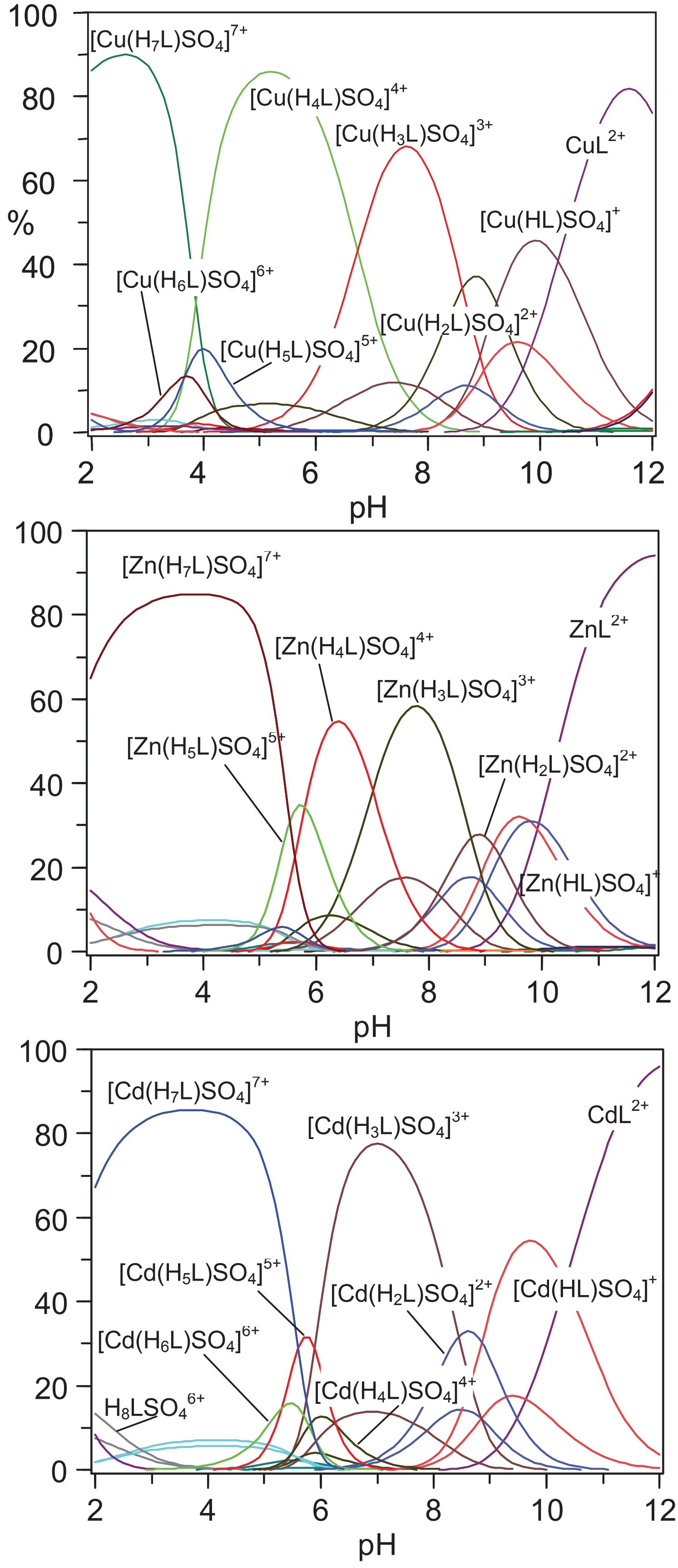

Figure S5. Distribution diagrams of the ion-pair complexes formed by L with M^{2+} (Cu^{2+}, Zn^{2+}, Cd^{2+}) and sulfate as a function of pH. [L] = [M^{2+}] = [anion] = 1×10^{-2} M.

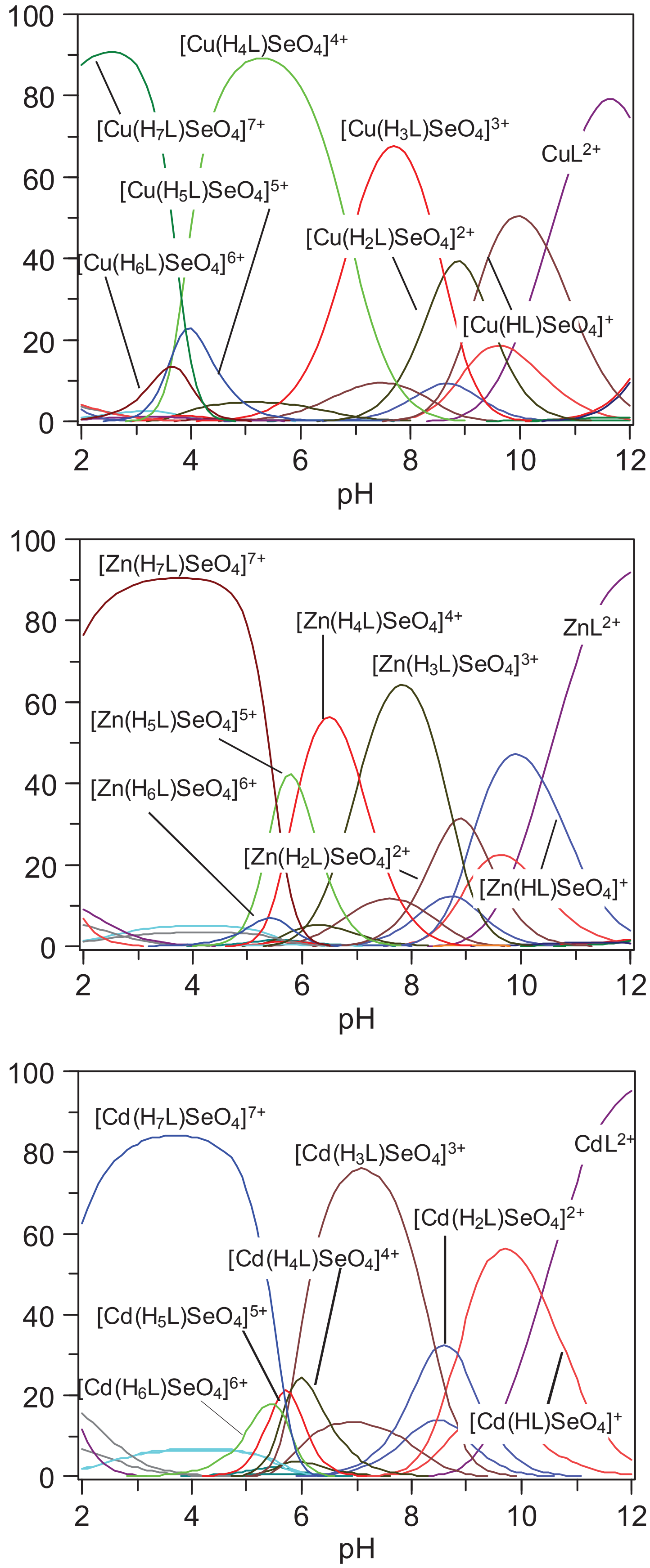

Figure S6. Distribution diagrams of the ion-pair complexes formed by L with M^{2+} (Cu^{2+}, Zn^{2+}, Cd^{2+}) and selenate as a function of pH. [L] = [M^{2+}] = [anion] = 1×10^{-2} M.

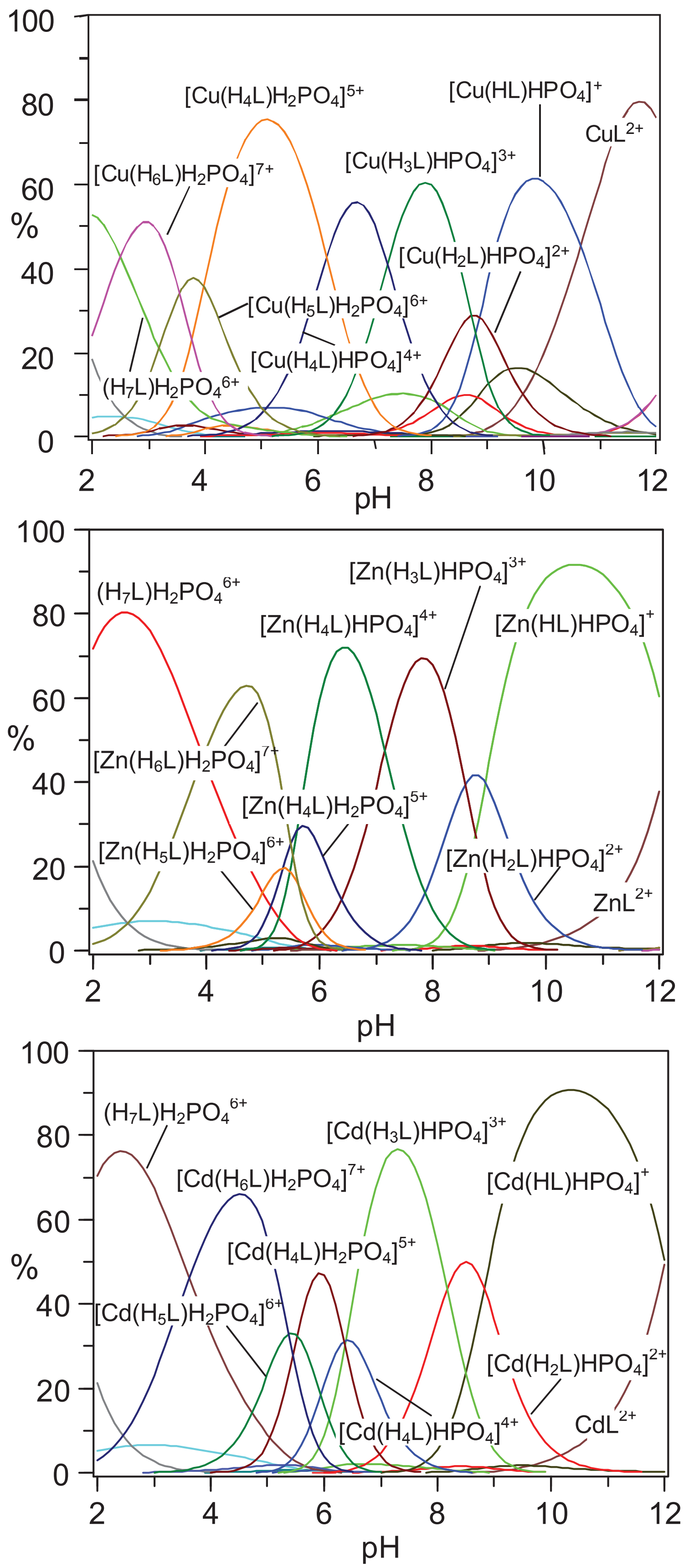

Figure S7. Distribution diagrams of the ion-pair complexes formed by L with M^{2+} (Cu^{2+}, Zn^{2+}, Cd^{2+}) and phosphate as a function of pH. [L] = [M^{2+}] = [anion] = 1×10^{-2} M.

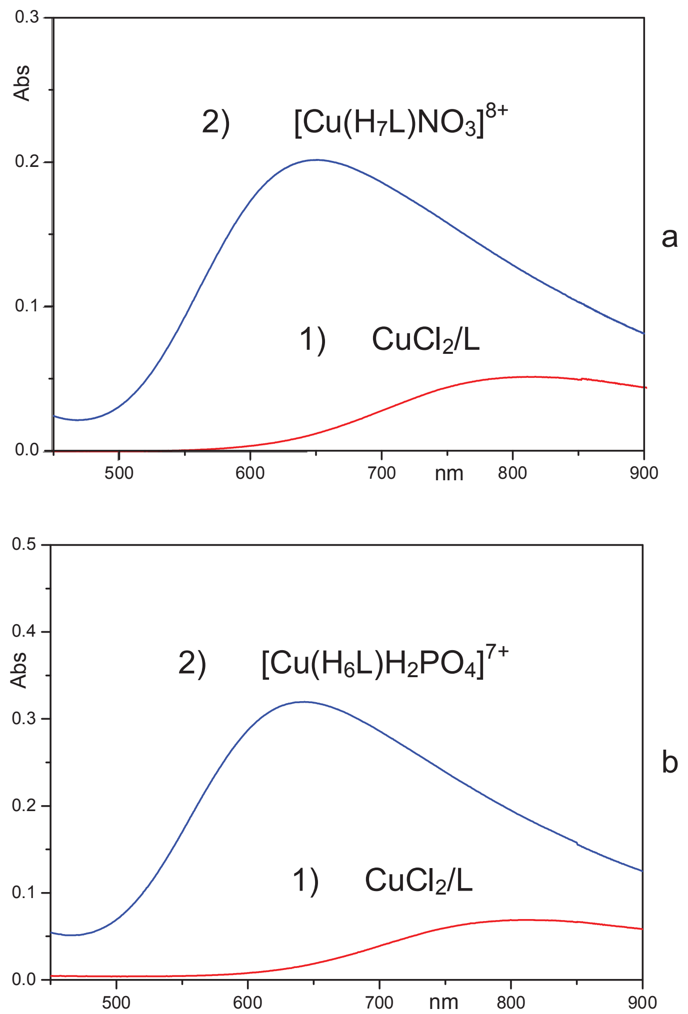

Figure S8. Adsorption spectra of solutions containing $CuCl_2$ and L before (1) and after (2) addition of (a) 1 eq. of NO_3^- and (b) 1 eq. of $H_2PO_4^-$. (a) $[Cu^{2+}] = [L] = [NO_3^-] = 4.39\times10^{-3}$ M, pH 2.5; $[Cu(H_7L)NO_3]^{8+}$: λ_{max} = 651nm, ε = 56 $M^{-1}cm^{-1}$). (b) $[Cu^{2+}] = [L] = [H_2PO_4^-] = 4.95\times10^{-3}$ M, pH 2.4; $[Cu(H_6L)H_2PO_4]^{7+}$: λ_{max} = 643 nm, ε = 65 $M^{-1}cm^{-1}$).

Table S1. Stability constants of ion-pair complexes formed by L with M^{2+}/SeO_4^{2-} (M = Cu, Zn, Cd). 0.10 M Me_4NCl, 298.1 ± 0.1 K.

M =	Cu^{2+}	Zn^{2+}	Cd^{2+}
	log*K*		
$M^{2+} + SeO_4^{2-} + HL^{+} = M(HL)SeO_4^{+}$	23.07(9)	16.64(8)	17.89(8)
$M^{2+} + SeO_4^{2-} + H_2L^{2+} = M(H_2L)SeO_4^{2+}$	22.34(9)	15.82(5)	16.74(8)
$M^{2+} + SeO_4^{2-} + H_3L^{3+} = M(H_3L)SeO_4^{3+}$	21.69(8)	15.32(5)	15.92(4)
$M^{2+} + SeO_4^{2-} + H_4L^{4+} = M(H_4L)SeO_4^{4+}$	19.37(8)	13.14(4)	12.51(7)
$M^{2+} + SeO_4^{2-} + H_5L^{5+} = M(H_5L)SeO_4^{5+}$	14.48(9)	10.52(5)	9.72(7)
$M^{2+} + SeO_4^{2-} + H_6L^{6+} = M(H_6L)SeO_4^{6+}$	9.74(9)	7.01(5)	6.92(5)
$M^{2+} + SeO_4^{2-} + H_7L^{7+} = M(H_7L)SeO_4^{7+}$	8.27(9)	7.57(5)	7.04(3)
$MHL^{3+} + SeO_4^{2-} = M(HL)SeO_4^{+}$	2.88(9)	2.71(8)	3.00(8)
$MH_2L^{4+} + SeO_4^{2-} = M(H_2L)SeO_4^{2+}$	3.31(9)	2.98(5)	2.98(8)
$MH_3L^{5+} + SeO_4^{2-} = M(H_3L)SeO_4^{3+}$	3.75(8)	3.52(5)	3.55(4)
$MH_4L^{6+} + SeO_4^{2-} = M(H_4L)SeO_4^{4+}$	4.49(8)	4.03(4)	3.68(7)
$MH_5L^{7+} + SeO_4^{2-} = M(H_5L)SeO_4^{5+}$	4.48(9)	4.66(5)	
$M^{2+} + (H_3L)SeO_4^{+} = M(H_3L)SeO_4^{3+}$	19.66(8)	13.29(8)	13.89(4)
$M^{2+} + (H_4L)SeO_4^{2+} = M(H_4L)SeO_4^{4+}$	17.49(8)	11.26(5)	10.63(7)
$M^{2+} + (H_5L)SeO_4^{3+} = M(H_5L)SeO_4^{5+}$	12.18(9)	8.21(5)	7.42(7)
$M^{2+} + (H_6L)SeO_4^{4+} = M(H_6L)SeO_4^{6+}$	7.21(9)		
$M^{2+} + (H_7L)SeO_4^{5+} = M(H_7L)SeO_4^{7+}$	5.17(9)	4.47(5)	3.94(3)

[a] Values in parentheses are standard deviations on the last significant figures.