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SUPPORTING INFORMATION

Title: Study of Thermodynamic and Kinetic Stability of Transition Metal and Lanthanide Complexes of DTPA Analogues with a Phosphorus Acid Pendant Arm
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Table S1

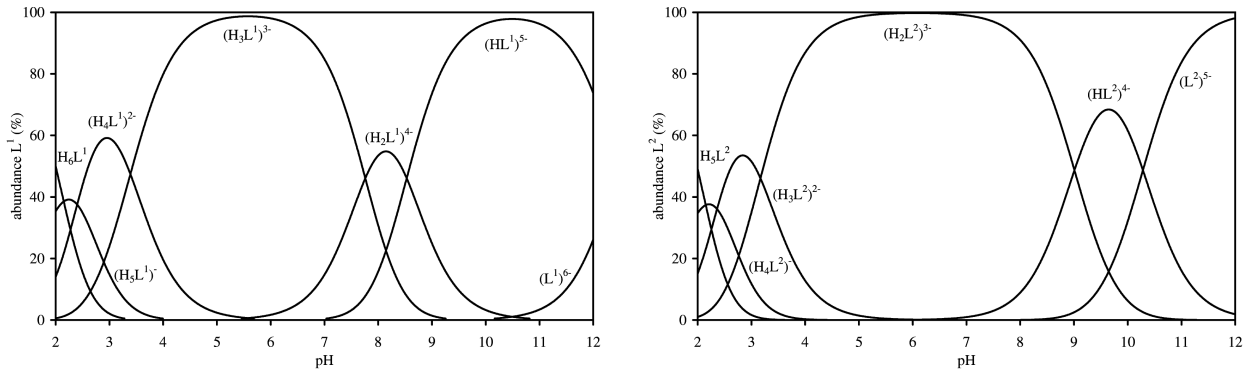
Parameters of the hydrogen bond network in the structure of $H_6L^1 \cdot HCl \cdot 1.5H_2O$[a].

D–H	*d*(D–H), Å	*d*(H···A), Å	<DHA, °	*d*(D···A), Å	A	symmetry
O1–H1	0.79(3)	1.86(3)	172(3)	2.649(2)	O112	[x+1, y, z]
N1–H11	0.87(2)	1.88(3)	167(2)	2.735(2)	O3	[–x+1, –y, -z+1]
N4–H41	0.93(3)	1.71(3)	172(2)	2.638(2)	O3	[–x+1, –y, –z+1]
N7–H71	0.86(2)	2.02(2)	146(2)	2.775(2)	O412	[–x+1, –y+1, –z+1]
N7–H71	0.86(2)	2.24(2)	114(2)	2.706(2)	O412	
O111–H111	1.01(3)	1.49(3)	171(3)	2.489(2)	O2	[x–1, y, z]
O211–H211	1.04(4)	1.45(4)	158(3)	2.445(2)	O411	[x, y–1, z]
O211–H211	1.04(4)	2.65(4)	132(3)	3.425(2)	O412	[x, y–1, z]
O311–H311	0.99(3)	1.56(3)	176(3)	2.543(2)	O1W	[x, y, z–1]
O1W–H1W1	0.87(4)	2.31(4)	176(3)	3.179(2)	Cl1	[x–1, y, z]
O1W–H1W2	0.86(3)	2.19(3)	172(2)	3.042(2)	Cl1	[–x+1, –y+1, –z+2]
O2W–H2W1	0.70(4)	2.30(4)	161(3)	2.964(4)	O212	[x+1, y+1, z]
O2W–H2W2	0.89(4)	2.34(4)	161(3)	3.204(3)	Cl1	

[a] D = donor; A = acceptor

Figure S1

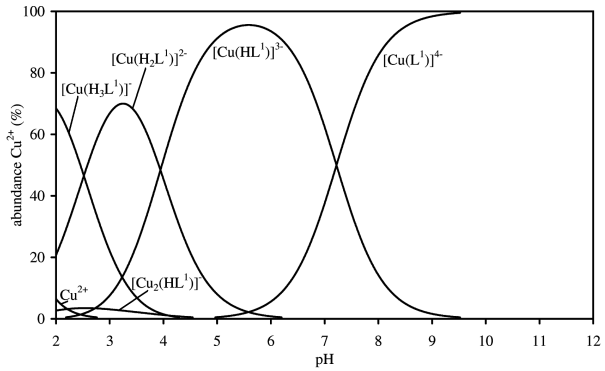
Distribution diagrams of H_6L^1 (A) and H_5L^2 (B).



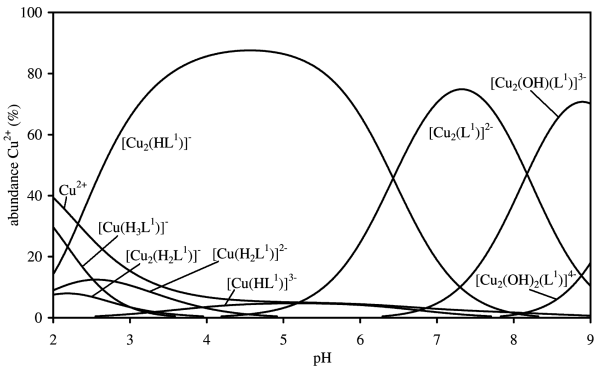
A B

Figure S2

Distribution diagrams of H_6L^1-Cu^{2+} systems in (A) 1:1 and (B) 1:2 ratios ($c(H_6L^1)$ = 0.004 M).



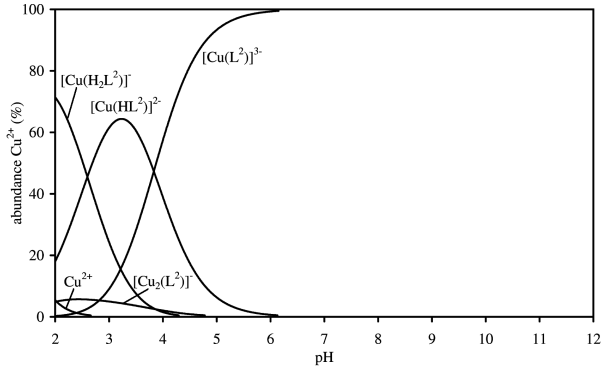
A



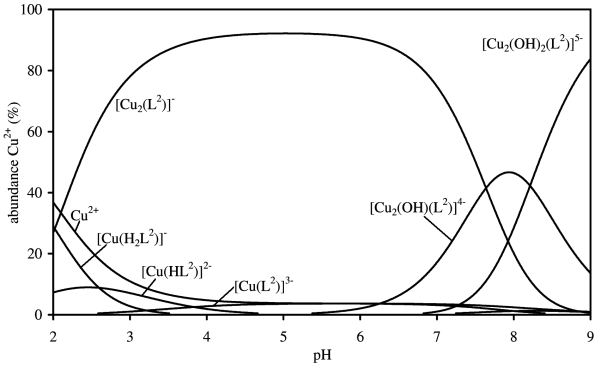
B

Figure S3

Distribution diagrams of H_5L^2-Cu^{2+} systems in (A) 1:1 and (B) 1:2 ratios ($c(H_5L^2)$ = 0.004 M).



A



B