Electronic Supplementary Information for Dalton Transactions

Electronic Suplementary Information

Properties of a new 4-imidazolyl derivative of a 14-membered tetraazamacrocyclic chelating agent

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Content

Table S1. Stability constants (log units) for the complexes of L^1 and related ligands* with selected metal ions. T = 298.2 K, I = 0.10 mol dm^{-3} in KNO_3.

Equilibrium reaction	L^{1} [a]	L^{3} [b]	L^{4} [c]	L^{8} [d]	L^{9} [d]
$K^+ + L \rightleftharpoons [KL]^+$	1.86(4)	–	–	–	–
$Mn^{2+} + L \rightleftharpoons [MnL]^{2+}$	7.95(1)	–	–	–	–
$[MnL]^{2+} + H^+ \rightleftharpoons [M(HL)]^{3+}$	6.09(4)	–	–		
$Fe^{2+} + L \rightleftharpoons [FeL]^{2+}$	9.73(2)	–	–	–	–
$[FeL]^{2+} + H^+ \rightleftharpoons [Fe(HL)]^{3+}$	6.06(4)	–		–	–
$Co^{2+} + L \rightleftharpoons [CoL]^{2+}$	12.77(5)	14.4	13.5	11.55	11.36
$[CoL]^{2+} + H^+ \rightleftharpoons [Co(HL)]^{3+}$	5.73(3)	4.1	–	–	3.99
$[CoHL]^{3+} + H^+ \rightleftharpoons [Co(H_2L)]^{4+}$	3.88(5)	–		–	–
$Ni^{2+} + L \rightleftharpoons [NiL]^{2+}$	16.97(2)	16.59	16.94	15.01	14.93
$[NiL]^{2+} + H^+ \rightleftharpoons [Ni(HL)]^{3+}$	3.79(2)	2.94	2.1	2.59	3.23
$[NiHL]^{3+} + H^+ \rightleftharpoons [Ni(H_2L)]^{4+}$	2.64(2)	–	–	–	–
$Cu^{2+} + L \rightleftharpoons [CuL]^{2+}$	20.70(4)	21.61	20.13	18.46	18.96
$[CuL]^{2+} + H^+ \rightleftharpoons [Cu(HL)]^{3+}$	4.99(5)	2.28	–	2.93	3.62
$[CuL]^{2+} \rightleftharpoons [ML(OH)]^+ + H^+$	-11.09(6)	–	–	–	–
$Zn^{2+} + L \rightleftharpoons [ZnL]^{2+}$	14.28(5)	14.01	14.65	11.90	11.83
$[ZnL]^{2+} + H^+ \rightleftharpoons [Zn(HL)]^{3+}$	5.84(2)	4.05	1.84	3.0	4.52
$[ZnHL]^{3+} + H^+ \rightleftharpoons [Zn(H_2L)]^{4+}$	3.44(3)	–	–	–	–
$[ZnL]^{2+} \rightleftharpoons [ZnL(OH)]^+ + H^+$	-10.64(8)	-7.66	-8.35	–	–
$Cd^{2+} + L \rightleftharpoons [CdL]^{2+}$	14.67(1)	14.56	14.85	–	–
$[CdL]^{2+} + H^+ \rightleftharpoons [Cd(HL)]^{3+}$	4.99(2)	3.84	1.91	–	–
$[CdHL]^{3+} + H^+ \rightleftharpoons [Cd(H_2L)]^{4+}$	3.55(5)	–	–	–	–
$[CdL]^{2+} \rightleftharpoons [CdL(OH)]^+ + H^+$	-10.13(6)	–	–	–	–
$Pb^{2+} + L \rightleftharpoons [PbL]^{2+}$	8.93(1)	10.89	10.69	–	–
$[PbL]^{2+} + H^+ \rightleftharpoons [Pb(HL)]^{3+}$	6.35(2)	4.96	3.95	–	–
$[PbL]^{2+} \rightleftharpoons [PbL(OH)]^+ + H^+$	-11.04(3)	-9.9	-10.59	–	–
$Fe^{3+} + L \rightleftharpoons [FeL]^{3+}$	20.18(4)	20.64	15.87	–	–
$[FeL]^{3+} + H^+ \rightleftharpoons [Fe(HL)]^{4+}$	3.44(5)	2.84	3.31	–	–

*The structure of ligands can be seen in Scheme 1. [a] Values in parentheses are standard deviations on the last significant figure. [b] I = 0.10 mol dm^{-3} in NMe_4NO_3, ref. 18. [c] I = 0.10 mol dm^{-3} in NMe_4NO_3, ref. 19. [d] I = 0.10 mol dm^{-3} in KNO_3, ref. 5.

Ref. 18 - J. Costa, R. Delgado, M. C. Figueira, R. T. Henriques and M. Teixeira, *J. Chem. Soc., Dalton Trans.,* 1997, 65.

Ref. 19 - J. Costa, R. Delgado, M. G. B. Drew and V. Félix, *J. Chem. Soc.,Dalton Trans.*, 1999, 4331.

Ref. 5 - J. H. Timmons, W. R. Harris, I. Murase and A. E. Martell, *Inorg. Chem.*, 1978, **17**, 2192.

Table S2. Spectroscopic UV-vis-near IR data and magnetic moments (μ) for the Co^{2+}, Ni^{2+} and Cu^{2+} complexes of L^1 (T = 298.0 K).

Complex (colour)	pH	UV-vis-near IR λ_{max} / nm (ε_{molar}/ $dm^3mol^{-1}cm^{-1}$)	μ (MB)
$[CoL^1]^{2+}$ (pink)	7.56	1067 (4.1), 930 (sh., 4.7), 581 (sh., 52.5), 506 (170.6), 260 (7.74×10^4).	4.9
$[NiL^1]^{2+}$ (green)	7.78	1115 (sh, 2.8), 1072 (3.7), 905 (sh., 6.2), 769 (10.8), 625 (sh., 16.4), 572 (25.5), 264 (2.66×10^4).	3.1
$[CuL^1]^{2+}$ (blue)	8.01	994 (sh, 45.2), 777 (sh, 92.8), 639 (234.6), 266 (4.06×10^4).	–