Supplementary Material

Table S1. Protonation constants (log $K_{H_hL_l}$) of ligands L^1, L^2, L^5 – L^7, L^{12}, L^{13} and stability constants (log $K_{M_mH_hL_l}$) of their metal complexes with divalent metal ions (T = 298.2 K and I = 0.10 mol dm^{-3} KNO_3).

Ion	Equilibrium quotient	L^1 [a]	L^2 [a]	L^5 (L^6) [b]	L^7 [c]	L^{12} [d]	L^{13} [e]
H^+	[HL]/[L]×[H]	10.570	10.74	9.74 (9.92)	11.1	10.83	10.511 (10.58)[f]
	[H_2L]/[HL]×[H]	9.836	10.08	8.67 (8.56)	10.1	10.15	9.824 (9.92)[f]
	[H_3L]/[H_2L]×[H]	8.92	9.49	4.67 (4.66)	9.4	9.30	9.129 (9.28)[f]
	[H_4L]/[H_3L]×[H]	5.80	7.76	–	8.5	8.45	5.615 (5.80)[f]
	[H_5L]/[H_4L]×[H]	4.03	5.57	–	3.4	7.30	–
	[H_6L]/[H_5L]×[H]	–	3.52	–	1.9	4.98	–
Ni^{2+}	[ML]/[M]×[L]	13.07	12.65	– (16.27)	–	12.23	8.702
	[MHL]/[ML]×[H]	9.23	9.16	–	–	9.7	5.27
	[MH_2L]/[MHL]×[H]	5.82	9.00	–	–	8.46	–
	[MH_3L]/[MH_2L]×[H]	–	5.34	–	–	6.2	–
	[M_2L]/[ML]×[M]	4.08	5.03	–	–	–	–
	[M_2L]/[M_2LOH]×[H]	8.50	7.64	–	–	7.83*	–
	[M_2LOH]/[M_2L(OH)$_2$]×[H]	–	10.00	–	–	10.5	–
Cu^{2+}	[ML]/[M]×[L]	20.12	18.08	20.23 (19.76)	19.8	19.35	13.117 (13.21)[f]
	[MHL]/[ML]×[H]	8.76	9.44	–	10.1	9.75	10.757 (10.92)[f]
	[MH_2L]/[MHL]×[H]	6.26	8.30	–	5.9	7.69	–
	[MH_3L]/[MH_2L]×[H]	1.88	6.527	–	3.7	4.06	–
	[MH_4L]/[MH_3L]×[H]	–	2.32	–	–	–	–
	[ML]/[MLOH]×[H]	11.73	11.61	–	10.53	–	9.789 (9.9)[f]
	[MLOH]/[ML(OH)$_2$]×[H]	–	–	–	14.13	–	–
	[M_2L]/[ML]×[M]	6.38	10.55	–	–	7.82	–
	[M_2L]/[M_2LOH]×[H]	5.94	9.14	–	–	7.81	–
	[M_2LOH]/[M_2L(OH)$_2$]×[H]	9.10	10.70	–	–	9.4	–
Zn^{2+}	[ML]/[M]×[L]	13.07	12.24	11.91 (12.816	18.91	10.53	10.702
	[MHL]/[ML]×[H]	8.98	9.28	–	5.97	9.56	–
	[MH_2L]/[MHL]×[H]	5.41	8.58	–	–	8.16	–
	[MH_3L]/[MH_2L]×[H]	–	5.54	–	–	–	–
	[ML]/[MLOH]×[H]	11.72	11.31	8.06 (8.48	10.28	–	–
	[M_2L]/[ML]×[M]	–	6.53	–	–	–	–
	[M_2L]/[M_2LOH]×[H]	9.71*	8.41	–	–	7.55*	–
	[M_2LOH]/[M_2L(OH)$_2$]×[H]	9.91	9.74	–	–	9.5	–
Cd^{2+}	[ML]/[M]×[L]	10.19	9.49	8.77 (9.759	–	9.46	–
	[MHL]/[ML]×[H]	8.61	9.36	–	–	9.89	–
	[MH_2L]/[MHL]×[H]	6.70	8.93	–	–	8.23	–
	[MH_3L]/[MH_2L]×[H]	–	6.33	–	–	–	–
	[ML]/[MLOH]×[H]	–	11.88	9.62 (10.30)	–	–	–
	[M_2L]/[ML]×[M]	4.00	4.69	–	–	–	–
	[M_2L]/[M_2LOH]×[H]	8.69	–	–	–	4.19*	–
	[M_2LOH]/[M_2L(OH)$_2$]×[H]	8.91	–	–	–	9.69	–

[a] Present work. [b] I = 0.1 mol dm^{-3} KNO_3, ref. 23. [c] I = 0.1 mol dm^{-3} NMe_4Cl, ref. 10. [d] I = 0.15 mol dm^{-3} $NaClO_4$, ref. 20. [e] I = 0.1 mol dm^{-3} KCl, ref. 21. [f] I = 0.15 mol dm^{-3} NaCl, ref. 22. * log $\beta_{M_mH_hL_1}$

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Table S2. pM values determined for the complexes of the indicated ligands and divalent metal ions.[a]

Ion	Ligand	pH = 7.5	pH = 11
Ni^{2+}	L^{1} [b]	5.44	9.91
	L^{2} [b]	5.21	10.93
	L^{7} [c]	–	–
	L^{12} [d]	4.63	9.61
	L^{13} [e]	2.81	7.39
Cu^{2+}	L^{1} [b]	10.61	16.66
	L^{2} [b]	10.19	15.38
	L^{7} [c]	8.15	14.50
	L^{12} [d]	9.18	15.88
	L^{13} [e]	6.21	11.61
Zn^{2+}	L^{1} [b]	5.37	10.83
	L^{2} [b]	5.31	11.25
	L^{7} [c]	6.35	14.35
	L^{12} [d]	3.70	10.08
	L^{13} [e]	3.41	10.03
Cd^{2+}	L^{1} [b]	3.87	9.26
	L^{2} [b]	3.74	7.36
	L^{7} [c]	–	–
	L^{12} [d]	3.31	8.13
	L^{13} [e]	–	–

[a] $C_L = 1.67\times10^{-3}$ mol dm^{-3}; $T = 298.2$ K, using the Hyss program, ref. 28. [b] $I = 0.10$ mol dm^{-3} in KNO_3. [c] $I = 0.10$ mol dm^{-3} in NMe_4Cl. [d] $I = 0.15$ mol dm^{-3} in $NaClO_4$.[e] $I = 0.1$ mol dm^{-3} KCl.

Table S3 Spectroscopic UV-vis-NIR data for the mono- and dinuclear complexes of Ni^{2+} and Cu^{2+} with L^1 and L^2 at 298.2 K

Complex (M:L ratio)	pH (color)	λ_{max} /nm (ε/dm^3 mol^{-1} cm^{-1})
Ni^{2+}/L^1 (1:1)	7.5 (purple)	> 1300, 1165 (sh., 1.9), 950 (sh., 1.5), 770 (5.6), 580 (13.4), 408 (sh., 16.9), 370 (45.0), 290 (1.5×10^3), 264 (5.2×10^3)
	11.12 (light blue)	1165 (sh.,19.3), 950 (sh.,23.2), 770 (sh., 26.9), 570 (66.6), 420 (sh., 101.8), 354 (193.4), 290 (1.5×10^3), 264 (4.9×10^3)
Ni^{2+}/L^1 (2:1)	9.4 (pale green)	1165 (sh., 10.6), 950 (sh.,14.6), 770 (sh., 18.4), 580 (50.0), 420 (sh., 70.3), 370 (sh., 181.6), 308 (sh.,1.5×10^3), 264 (6.0×10^3)
Ni^{2+}/L^2 (1:1)	7.8 (light blue)	1175 (sh., 1.8), 952 (sh., 1.2), 752 (3.0), 584 (9.2), 376 (32.9), 288 (sh., 1.9×10^3), 262 (4.7×10^3)
	10.8 (light blue)	1175 (sh., 9.8), 952 (sh., 11.2), 752 (sh.,12.3), 584 (23.3), 410 (sh., 31.0), 370 (64.5), 288 (1.8×10^3), 264 (4.3×10^3)
Ni^{2+}/L^2 (2:1)	8.9 (light blue)	1175 (sh., 29.9), 952 (sh., 34.1), 709 (sh., 45.6), 570 (67.5), 410 (sh., 90.5), 370 (136.3), 288 (2.4×10^3), 262 (5.8×10^3)
	11.4 (light blue)	1175 (sh., 44.3), 952 (sh., 50.6), 702 (sh., 72.9), 570 (93.6), 410 (sh., 129.6), 370 (sh.,184.5), 288 (2.2×10^3), 262 (4.9×10^3)
Cu^{2+}/L^1 (1:1)	4.3 (blue)	910 (sh., 15.6), 624 (271.7), 284 (sh., 5.3×10^3), 266 (9.9×10^3)
	7.15 (purple)	910 (sh., 21.2), 728 (sh., 87.2), 622 (211.7), 294 (sh., 4.2×10^3), 276 (4.7×10^3), 264 (6.2×10^3)
	10.57 (blue)	910 (sh., 31.5), 728 (sh., 81.2), 622 (203.3), 292 (sh., 3.7×10^3), 280 (3.7×10^3), 264 (7.2×10^3)
Cu^{2+}/L^1 (2:1)	8.2 (blue)	938 (sh., 49.0), 774 (sh., 72.9), 622 (294.7), 414 (sh., 183.5), 394 (sh., 226.5), 296 (4.8×10^3), 264 (1.1×10^4)
	11.4 (pale green)	938 (sh., 92.1), 774 (sh., 113.5), 588 (175.5), 412 (sh., 216.3), 304 (3.9×10^3), 266 (5.4×10^3)
Cu^{2+}/L^2 (1:1)	4.7 (light blue)	922 (sh., 12.3), 781 (sh., 41.9), 620 (214.3), 292 (3.2×10^3), 282 (sh., 2.8), 264 (6.2×10^3)
	7.2 (purple)	922 (sh., 23.0), 781 (sh., 45.1), 620 (192.5), 416 (sh., 69.0), 292 (3.2×10^3), 280 (sh., 3.1×10^3), 264 (6.4×10^3)
	11.2 (light blue)	922 (sh., 26.0), 781 (sh., 36.5), 630 (102.6), 420 (sh., 35.5), 294 (3.3×10^3), 264 (6.4×10^3)
Cu^{2+}/L^2 (2:1)	7.8 (blue)	953 (sh., 54.2), 790 (sh., 62.5), 626 (201.9), 416 (sh., 92.7), 302 (2.7×10^3), 280 (3.2×10^3), 264 (5.1×10^3)
	11.4 (light blue)	953 (sh., 71.2), 790 (sh., 96.9.), 614 (283.1), 426 (sh., 275.4), 298 (3.8×10^3), 264 (7.7×10^3)