

Supplementary Information

Table 1 Overall ($\log \beta_{\text{HhL}}$) and stepwise ($\log K_{\text{HhL}}$)^{a,b} protonation constants of L^1 and L^2 , and stability constants ($\log \beta_{\text{MmHhL}_1}$ and $\log K_{\text{MmHhL}_1}$) of their complexes with several divalent metal ions. Values for $[\text{17}](\text{DBF})\text{N}_2\text{O}_2$ and $[\text{22}](\text{DBF})\text{N}_2\text{O}_3$ are also presented for comparison. $T = 298.2 \text{ K}$; $I = 0.10 \text{ mol dm}^{-3}$ in aqueous KNO_3

Ion	Species	L^1		$[\text{17}](\text{DBF})\text{N}_2\text{O}_2^c$		L^2		$[\text{22}](\text{DBF})\text{N}_2\text{O}_3^c$
	mhl	$\log \beta_{\text{MmHhL}_1}$	$\log K_{\text{MmHhL}_1}$	$\log K_{\text{MmHhL}_1}$	$\log \beta_{\text{MmHhL}_1}$	$\log K_{\text{MmHhL}_1}$	$\log K_{\text{MmHhL}_1}$	
H^+	011	10.23(1)	10.23	8.01	10.00(1)	10.00	8.78	
	021	19.09(2)	8.86	7.13	19.02(1)	9.02	7.81	
	031	23.62(2)	4.53	-	23.97(1)	4.95	-	
	041	27.12(3)	3.50	-	27.55(1)	3.58	-	
	101	7.17(1)	7.17	2.92	5.96(4)	5.96	3.77	
	111	14.56(4)	7.39	7.79	-	-	7.91	
	1-11	-2.46(7)	-9.63	-	-3.46(5)	-9.42	-7.65	
	1-21	-	-	-	-	-	-8.75	
	201	-	-	-	8.94(7)	2.98	-	
Co^{2+}	2-21	-	-	-	-7.79(8)	-	-	
	101	8.34(3)	8.34	3.38	7.04(1)	7.04	4.18	
	111	15.28(7)	6.94	-	14.35(3)	7.31	-	
	1-11	-0.64(9)	8.98	-	-	-	-7.90	
	1-21	-	-	-	-	-	-8.59	
	201	-	-	-	10.17(4)	3.13	-	
	2-21	-	-	-	-5.96(4)	-	-	
	101	15.2(2) ^d	15.15	6.99	12.53(2)	12.53	8.91	
	111	[19.2] ^d	[4.0]	6.05	17.20(4)	4.67	-	
Cu^{2+}	1-11	[6.2] ^d	[9.0]	-7.64	-	-	-7.90	
	1-21	-	-	-8.88	-	-	-8.82	
	201	-	-	-	15.06(7)	2.53	-	
	2-11	-	-	-	10.03(4)	-5.03	-	
	2-21	-	-	-	4.19(2)	-5.84	-	
	2-31	-	-	-	-6.51(7)	-10.70	-	
	101	7.78(1)	7.78	3.46	6.37(2)	6.37	4.24	
	1-11	-2.36(9)	-10.14	-	-2.58(6)	-8.95	-7.36	
	1-21	-	-	-	-12.65(7)	-10.07	-8.77	
Zn^{2+}	201	-	-	-	9.77(3)	3.40	-	
	2-11	-	-	-	2.80(1)	-6.97	-	
	2-21	-	-	-	-4.47(2)	-7.27	-	
	101	9.96(2)	9.96	5.51	5.68(5)	5.68	3.15	
	111	15.81(7)	5.85	5.78	-	-	8.34	
	1-11	-0.62(3)	-10.58	-9.24	-3.39(7)	-9.07	-8.52	
	1-21	-	-	-	-	-	-8.61	
	201	-	-	-	8.45(5)	2.77	-	
	2-11	-	-	-	0.93(1)	-7.52	-	
Cd^{2+}	101	9.11(1)	9.12	-	8.20(4)	8.20	-	
	111	-	-	-	15.54(2)	7.34	-	
	1-11	-0.35(3)	-9.45	-	-1.15(4)	-9.35	-	

1-21	-11.32(3)	-10.97	-	-11.73(6)	-10.58	-
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^a See experimental, calculation of stability constants, for definitions. ^b Values in parentheses are standard deviations in the last significant figures. ^c Ref. 22. ^d Values obtained by batch titration.
