Supplementary Material

Table S1 Results for curve fitting of pH titration data with Eqs. (1),[a] (2),[b] and (3).[c]

	$Zn_{4.9}$-cicMT2	$Cd_{5.2}$-cicMT2	$Zn_{4.9}$-cicMT2 (10 mM NaCl)	$Cd_{5.2}$-cicMT2 (10 mM NaCl)	$Zn_{4.9}$-cicMT2 (100 mM NaCl)	$Cd_{5.2}$-cicMT2 (100 mM NaCl)
Eq. (1)						
A_{MT}	47955 ± 281	54606 ± 162	47315 ± 473	53906 ± 150	48432 ± 209	52803 ± 159
A_{MTHn}	-448 ± 362	-224 ± 246	-891 ± 529	86 ± 249	29 ± 237	815 ± 215
pK_1	4.68 ± 0.01	3.439 ± 0.006	4.78 ± 0.02	3.561 ± 0.007	4.707 ± 0.007	3.857 ± 0.006
n	1.45 ± 0.05	1.38 ± 0.03	1.33 ± 0.08	1.32 ± 0.02	1.58 ± 0.04	1.33 ± 0.02
Eq. (2)						
A_{MT}	49701 ± 283	55246 ± 144	50328 ± 600	54750 ± 125	55032 ± 9654	53361 ± 231
A_{MTHm}	24553 ± 10455	49072 ± 2564	27044 ± 7313	48663 ± 2179	44067 ± 3624	31169± 40551
A_{MTHm+n}	381 ± 106	288 ± 148	167 ± 136	696 ± 106	328 ± 106	1117 ± 180
pK_1	4.57 ± 0.03	3.38 ± 0.01	4.62 ± 0.01	3.513 ± 0.006	4.69 ± 0.03	3.9 ± 0.3
pK_2	4.9 ± 0.4	4.6 ± 0.3	5.3 ± 0.4	4.8 ± 0.3	7.0 ± 1.3	3.9 ± 1.5
n	2.06 ± 0.10	1.62 ± 0.03	2.32 ± 0.10	1.52 ± 0.03	1.73 ± 0.02	1.3 ± 0.6
m	0.8 ± 0.1	1.3 ± 0.4	0.72 ± 0.16	1.0 ± 0.3	0.4 ± 0.5	0.8 ± 0.3
Eq. (3)						
A'_{MT}[d]	49790 ± 13	55237 ± 139	49830 ± 320	54707 ± 109	54493 ± 1742	53821 ± 114
A'_{MTHm}[d]	26882 ± 1619	50036 ± 1426	29892 ± 3221	50292 ± 761	42076 ± 1121	17027 ± 3534
A'_{MTHm+n}[d]	381 ± 130	288 ± 149	167 ± 251	696 ± 108	328 ± 373	1117 ± 155
pK_1	4.537 ± 0.007	3.38 ± 0.01	4.60 ± 0.01	3.514± 0.008	4.676 ± 0.005	3.76 ± 0.02
pK_2	5.07 ± 0.05	4.7 ± 0.2	5.5 ± 0.1	5.0 ± 0.1	6.1 ± 0.5	3.94 ± 0.02
n	2.8 ± 0.1	1.62 ± 0.04	2.7 ± 0.2	1.53 ± 0.03	1.89 ± 0.05	2.7 ± 0.4

m	0.92 ± 0.03	1.3 ± 0.4	0.92 ± 0.10	1.2 ± 0.3	0.36 ± 0.07	1.00 ± 0.05

a $$A_{\text{total}} = \frac{A_{\text{MT}} + A_{\text{MTH}_n} 10^{n(\text{p}K_1 - \text{pH})}}{1 + 10^{n(\text{p}K_1 - \text{pH})}}$$

b $$\text{A}_{\text{total}} = \frac{\text{A}_{\text{MT}} + \text{A}_{\text{MTH}_m} 10^{\text{m}(\text{p}K_2 - \text{pH})} + \text{A}_{\text{MTH}_{n+m}} 10^{\text{n}\cdot\text{p}K_1 + \text{m}\cdot\text{p}K_2 - (\text{n}+\text{m})\text{pH}}}{1 + 10^{\text{m}(\text{p}K_2 - \text{pH})} + 10^{\text{n}\cdot\text{p}K_1 + \text{m}\cdot\text{p}K_2 - (\text{n}+\text{m})\text{pH}}}$$

c $$\text{A}_{\text{total}} = \frac{\text{A}_{\text{MTH}_m} + \text{A}_{\text{MTH}_{n+m}} 10^{\text{n}(\text{p}K_1 - \text{pH})}}{1 + 10^{\text{n}(\text{p}K_1 - \text{pH})}} + \frac{\text{A}_{\text{MT}} + \text{A}_{\text{MTH}_m} 10^{\text{m}(\text{p}K_2 - \text{pH})}}{1 + 10^{\text{m}(\text{p}K_2 - \text{pH})}}$$

d The absorption values obtained from the original curve-fitting with Eq. (3) were shifted by $\{ A_{\text{H}m+n\text{MT2}}$ (Eq. (2)) $+|A_{\text{H}m+n\text{MT2}}|$(Eq. (3))$\}$ to result into A' and allow direct comparison with values from Eq. (2).