TABLE 1S: Bond overlap populations, Q_{M-O}, between M^{z+} and O, effective charges, n, on M^{z+}, O and H obtained by the MO calculation of monohydrated ion clusters, $M^{z+}\cdot H_2O$ and hydration numbers obtained experimentally, N_{hyd}.

ion	Q_{M-O}	n_M	n_O	n_H [a]	N_{hyd} [b]
Li^+	0.385	+0.73	−0.30	+0.28	4.3
Na^+	0.273	+0.81	−0.37	+0.28	5.6
K^+	0.168	+0.89	−0.41	+0.26	5.5
Rb^+	0.147	+0.90	−0.43	+0.26	6.3 [c]
Cs^+	0.109	+0.92	−0.44	+0.26	7.0
Ag^+	0.311	+0.73	−0.31	+0.29	3.4
Be^{2+}	0.745	+1.15	−0.01	+0.43	4.0
Mg^{2+}	0.501	+1.48	−0.06	+0.29	6.0
Ca^{2+}	0.366	+1.66	−0.17	+0.25	6.3
Sr^{2+}	0.293	+1.73	−0.23	+0.25	8.1
Ba^{2+}	0.227	+1.79	−0.28	+0.24	8.1
V^{2+}	0.483	+1.39	+0.02	+0.30	6.0
Cr^{2+}	0.482	+1.30	+0.03	+0.33	6.0
Mn^{2+}	0.480	+1.43	−0.01	+0.29	6.0
Fe^{2+}	0.484	+1.36	+0.02	+0.31	6.0
Co^{2+}	0.497	+1.27	+0.03	+0.35	6.0
Ni^{2+}	0.486	+1.21	+0.05	+0.38	6.0
Cu^{2+}	0.450	+1.11	+0.08	+0.41	6.0
Zn^{2+}	0.488	+1.35	−0.03	+0.33	6.0

[a] Values for two H atoms in a H_2O were identical each other. [b] Mean of values reported in the reference 22 (at 25 °C). [c] The value assumed by the authors as a mean of values of K^+ and Cs^+.

TABLE 2S: Fundamental data used in the calculation of enthalpies due to the ligand field stabilization, $H°_{LF}$

d^n [a]	ion	N_t [b]	N_e [c]	CFSE [d]	10Dq [e]	$-H°_{LF}$ [f]
					/ kJ mol^{-1}	/ kJ mol^{-1}
			divalent 3d elements			
d^0	Ca^{2+}	0	0	0Dq	0	0
d^2	Ti^{2+}	2	0	−8Dq	–	–
d^3	V^{2+}	3	0	−12Dq	14	169
d^4	Cr^{2+}	3	1	−6Dq	17	100
d^5	Mn^{2+}	3	2	0Dq	9	0
d^6	Fe^{2+}	4	2	−4Dq	12	48
d^7	Co^{2+}	5	2	−8Dq	12	96
d^8	Ni^{2+}	6	2	−12Dq	10	123
d^9	Cu^{2+}	6	3	−6Dq	16	93
d^{10}	Zn^{2+}	6	4	0Dq	0	0
			trivalent 3d elements			
d^0	Sc^{3+}	0	0	0Dq	0	0
d^1	Ti^{3+}	1	0	−4Dq	24	97
d^2	V^{3+}	2	0	−8Dq	22	172
d^3	Cr^{3+}	3	0	−12Dq	21	253
d^4	Mn^{3+}	3	1	−6Dq	25	151
d^5	Fe^{3+}	3	2	0Dq	17	0
d^{10}	Ga^{3+}	6	4	0Dq	–	–

[a] d^n Electronic configuration of ion. [b] Number of electrons in t_{2g} orbital. [c] Number of electrons in e_g orbital. [d] Stabilization estimated by the crystal field theory. [e] 10Dq obtained experimentally.[37] [f] Ligand field stabilization enthalpy calculated by eq 5.