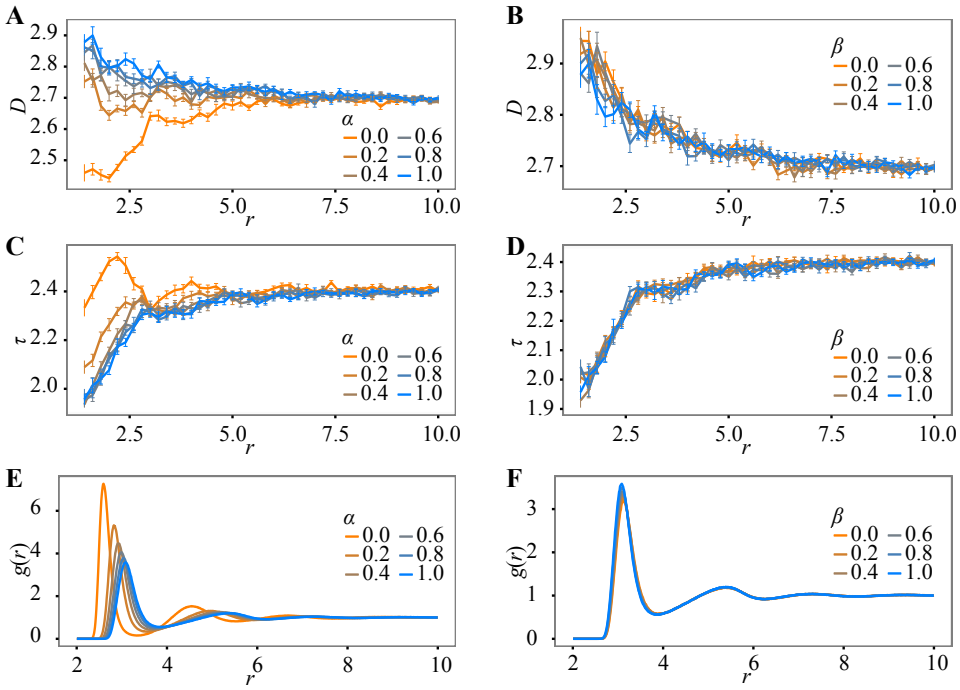

Figure S1. Distance profile of the hydration properties (A, B) D, (C, D) τ, and (E, F) $g(r)$ for fixed parameters (A, C, E) $\beta = 1.0$ and (B, D, F) $\alpha = 1.0$. See also the legend of Figure 1.

Table S1. Parameters used in this work

X	A_{XX}[*1]	B_{XX}[*2]	radius[*3]
H	1.47e+04	5.85e+01	
Li^+	4.32e+03	2.40e+01	1.14
Na^+	1.48e+04	4.64e+01	1.87
K^+	7.81e+04	1.11e+02	2.66
Rb^+	1.42e+05	1.54e+02	2.97
Cs^+	2.94e+05	2.29e+02	3.40
F^-	4.07e+04	8.74e+01	1.75
Cl^-	2.53e+05	3.18e+02	2.40
Br^-	4.04e+05	4.12e+02	2.22
I^-	7.86e+05	6.20e+02	2.95

[*1] (kcal/mol/Å^6), [*2] (kcal/mol/Å^{12}), [*3] The second term of the Eq (11) in the manuscript (Å).

Table S2. Cell dimensions (Å)

	X	*Y*	*Z*
Li^+	28.68	31.60	30.09
Na^+	28.64	31.56	30.05
K^+	31.81	31.55	27.06
Rb^+	28.68	31.60	30.09
Cs^+	28.68	31.60	30.09
F^-	28.65	31.57	30.06
Cl^-	28.76	31.69	30.18
Br^-	28.68	31.60	30.09
I^-	31.88	31.61	27.09

Table S3. Experimental values[*1]

	$N(D_{hyd})^{exp}$	$N(\tau_{hyd})^{exp}$	r_{MO}^{exp} (Å)
Li^+	0.89	0.41	1.3
Na^+	0.92	0.65	2.1
K^+	1.0	1.1	2.9
Rb^+	-	1.3	3.3
Cs^+	0.99	1.5	3.7
F^-	0.89	0.39	2.0
Cl^-	1.0	1.1	2.7
Br^-	1.1	1.4	2.6
I^-	1.1	2.4	3.3

[*1] The experimental values were obtained from Refs. [22], [23], and [24]

Table S4. PCCs between α and the hydration properties with fixed β.

	D_{hyd}		τ_{hyd}		r_{MO}	
β	0.0	1.0	0.0	1.0	0.0	1.0
Li^+	–0.578	–0.473	0.836	0.920	0.866	0.751
Na^+	0.945	0.926	–0.937	–0.928	0.939	0.914
K^+	0.938	0.897	–0.927	–0.871	0.948	0.936
Rb^+	0.929	0.898	–0.846	–0.873	0.953	0.944
Cs^+	0856	0.896	–0.735	–0.840	0.964	0.958
F^-	0.949	0.930	–0.907	–0.899	0.892	0.824
Cl^-	0.904	0.924	–0.889	–0.898	0.961	0.945
Br^-	0.859	0.862	–0.797	–0.839	0.937	0.893
I^-	0.820	0.800	–0.793	–0.786	0.949	0.824

Table S5. PCCs between β and the hydration properties with fixed α.

	D_{hyd}		τ_{hyd}		r_{MO}	
α	0.0	1.0	0.0	1.0	0.0	1.0
Li^+	–0.857	–0.211	0.921	0.118	–0.995	–0.729
Na^+	–0.779	–0.326	0.694	0.006	–0.976	–0.520
K^+	–0.875	–0.440	0.694	0.059	–0.962	–0.563
Rb^+	–0.833	–0.278	0.466	–0.480	–0.971	–0.736
Cs^+	–0.731	0.038	0.103	–0.619	–0.968	–0.687
F^-	–0.937	–0.627	0.675	–0.099	–0.991	–0.636
Cl^-	–0.862	–0.669	0.767	–0.636	–0.756	–0.814
Br^-	–0.955	–0.709	0.837	–0.575	–0.993	–0.814
I^-	–0.972	–0.557	0.877	–0.487	–0.994	–0.860

Table S6. PCC between the hydration properties

	$N(D_{hyd})$–$N(\tau_{hyd})$	$N(D_{hyd})$–r_{MO}	$N(\tau_{hyd})$–r_{MO}
Li^+	0.889	–0.809	–0.869
Na^+	0.987	0.995	0.989
K^+	0.979	0.988	0.980
Rb^+	0.956	0.984	0.939
Cs^+	0.882	0.969	0.827
F^-	0.986	0.976	0.975
Cl^-	0.947	0.986	0.945
Br^-	0.966	0.987	0.961
I^-	0.955	0.964	0.926

Table S7. Representative parameters.

	D_{hyd}*1		τ_{hyd}*2		r_{MO}*3	
	α	β	α	β	α	β
Li^+	0	0	1.0	1.0	0	1.0
Na^+	0	0	0	1.0	0	1.0
K^+	0.2	0.6	1.0	0.2	0.4	0.6
Rb^+	-	-	1.0	1.0	1.0	0.6
Cs^+	0	0.4	0.8	1.0	1.0	0
F^-	0	0.2	0	0.8	0	1.0
Cl^-	0	0	0.4	0.2	0	1.0
Br^-	0.2	0	1.0	1.0	0	1.0
I^-	0.8	0.2	0.8	1.0	0	0.2

*1 Parameters yielding the minimum error of D_{hyd}. *2 Those of τ_{hyd}. *3 Those of r_{MO}.