Revised ionic radii of lanthanoid(III) ions in aqueous solution

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Supporting online information

Table 1S. B_{ij} and C_{ij} parameters for the MD simulations using the new ionic radii. B_{ij} is in Å^{-1} and C_{ij} is in kJ $\text{mol}^{-1}\text{Å}^6$.

	B_{ij}	$C_{ij}/10^{+4}$
La-O	3.446	3.884
Ce-O	3.476	3.730
Pr-O	3.496	3.628
Nd-O	3.523	3.489
Sm-O	3.554	3.330
Eu-O	3.576	3.198
Gd-O	3.586	3.167
Tb-O	3.606	3.064
Dy-O	3.626	2.962
Ho-O	3.640	2.859
Er-O	3.656	2.808
Tm-O	3.671	2.731
Yb-O	3.688	2.644
Lu-O	3.701	2.577

Table 2S. Ln-O first shell structural parameters of Ln(III) ions in aqueous solution obtained from the MD simulations using the 8-fold Shannon ionic radii. N is the coordination number, R is the average distance of the Ln-O distribution, σ^2 is the Debye-Waller factor, and β is the asymmetry parameter.

	N	R(Å)	σ^2(Å^2)	β
Sm-O	8.9	2.450	0.009	0.54
Eu-O	8.8	2.440	0.008	0.57
Gd-O	8.6	2.425	0.007	0.60
Tb-O	8.5	2.410	0.007	0.62
Dy-O	8.3	2.390	0.006	0.62
Ho-O	8.2	2.370	0.006	0.62
Er-O	8.1	2.360	0.006	0.62
Tm-O	8.1	2.350	0.005	0.50
Yb-O	8.1	2.340	0.005	0.46
Lu-O	8.0	2.340	0.005	0.44

Table 3S. Ln-O first shell structural parameters of Ln(III) ions in aqueous solution obtained from the MD simulations using the 9-fold Shannon ionic radii. N is the coordination number, R is the average distance of the Ln-O distribution, σ^2 is the Debye-Waller factor, and β is the asymmetry parameter.

	N	R(Å)	σ^2(Å^2)	β
La-O	9.1	2.540	0.008	0.47
Ce-O	9.0	2.530	0.008	0.48
Pr-O	9.0	2.520	0.008	0.50
Nd-O	9.0	2.510	0.008	0.51
Sm-O	9.0	2.480	0.008	0.51
Eu-O	9.0	2.475	0.008	0.55
Gd-O	9.0	2.470	0.008	0.58
Tb-O	8.9	2.460	0.008	0.60
Dy-O	8.8	2.450	0.008	0.64
Ho-O	8.7	2.435	0.008	0.64
Er-O	8.6	2.420	0.008	0.65
Tm-O	8.5	2.410	0.007	0.54
Yb-O	8.2	2.390	0.006	0.49
Lu-O	8.2	2.370	0.006	0.46

Table 4S. Ln-O first shell structural parameters of Ln(III) ions in aqueous solution obtained from the MD simulations using the new ionic radii. N is the coordination number, R is the average distance of the Ln-O distribution, σ^2 is the Debye-Waller factor, and β is the asymmetry parameter.

	N	R(Å)	σ^2(Å^2)	β
La-O	9.1	2.585	0.008	0.47
Ce-O	9.0	2.565	0.008	0.48
Pr-O	9.0	2.540	0.008	0.49
Nd-O	9.0	2.520	0.008	0.50
Sm-O	9.0	2.490	0.008	0.52
Eu-O	9.0	2.475	0.008	0.55
Gd-O	9.0	2.460	0.008	0.59
Tb-O	8.9	2.445	0.008	0.61
Dy-O	8.7	2.430	0.008	0.64
Ho-O	8.6	2.415	0.008	0.65
Er-O	8.5	2.395	0.008	0.65
Tm-O	8.2	2.380	0.007	0.52
Yb-O	8.1	2.365	0.006	0.47
Lu-O	8.1	2.355	0.006	0.44