Supporting Information for

Parametrization of Trivalent and Tetravalent Metal Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models

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Methods for simulating the archaea superoxide reductase.

First, the H++ server[1] was used to determine the protonation states of the amino acids, after which the charged groups and binding site residues were carefully examined, with protonation states were correctly if necessary. Afterwards, the protein, which was described by AMBER ff14SB force field[2], was solvated in a water box with a distance of at least 12 Å between the edge of the box and the solute atoms. Different parameter sets for the Fe^{3+} ion, *i.e.* the 12-6 HFE, 12-6 IOD, and 12-6-4 parameter sets, were investigated in conjunction with three different water models, namely the OPC, OPC3, and TIP3P water models, resulting in a total of 9 sets of topologies and simulations. No counter-ions were needed to neutralize the systems. Finally, MD simulations were performed for each set of topology to assess the performance of different combinations of ion parameter set and water model. AMBER 18[3] was used to run the simulations. For each simulation, five steps of minimization were first performed to remove close contacts: the first step minimizes the water molecules and counter-ions, with the protein restrained; the second, third, and fourth steps restrain the heavy atoms, backbone heavy atoms, and backbone carbon and oxygen atoms of the protein, respectively; while the last step minimizes the entire system. Each minimization step consisted of 10000 cycles of steepest descent minimization. After the minimization steps, the system was heated from 0 to 300 K gradually by 1 ns NVT simulation, with the solute restrained by a 5 kcal/mol·$Å^2$ restraining potential. Then the system was equilibrated at 300 K and 1 atm by 6 ns NPT simulation, with the restraining potential gradually released. Finally, 100 ns NPT production simulation at 300 K and 1 atm was performed. Snapshots were saved every 20 ps for analyses. The Langevin thermostat with a collision frequency of 2 ps^{-1} was used to control the temperature in the MD simulations, and the Berendsen barostat with a pressure relaxation time of 5 ps was used for the pressure control in the NPT simulations. SHAKE[4] was used to constrain bonds involving hydrogen atoms and the three-point SHAKE[5] was used to constrain the water molecules. Time step was set as 2 fs for all the MD simulations. The nonbonded cutoff was set as 10 Å in the minimization and MD simulations.

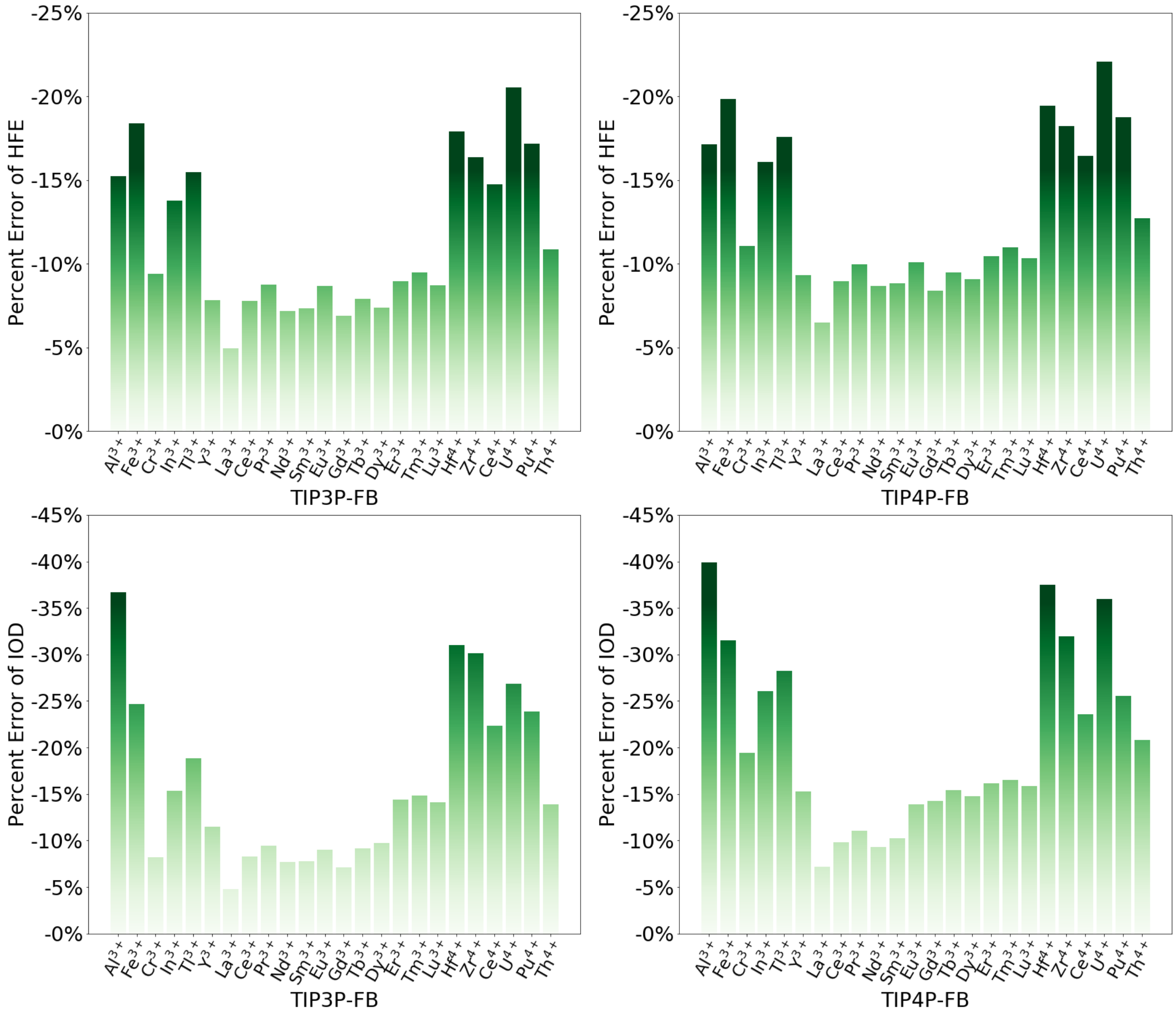

Figure S1. HFE and IOD percent errors for the 12-6 nonbonded model of highly charged metal ions in conjunction with TIP3P-FB and TIP4P-FB water models. The HFE percent errors were for the 12-6 IOD parameter set which can reproduce the experimental IOD values (Tables 3 and S5). The IOD percent errors were for the 12-6 HFE parameter set which can reproduce the experimental HFE values (Tables 2 and S4).

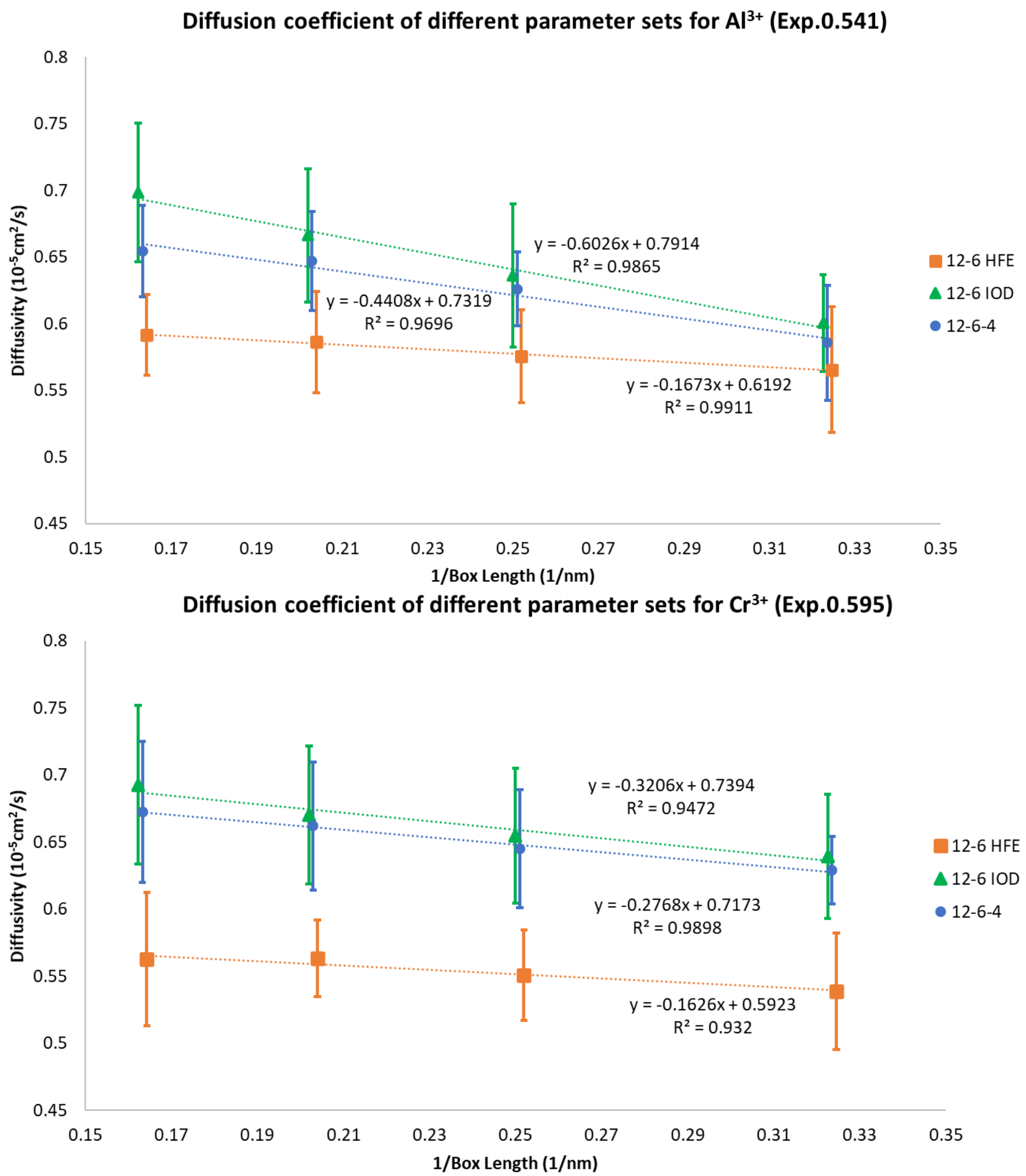

Figure S2. Diffusion coefficients of Al^{3+} and Cr^{3+} under different ion concentrations. Error bar is the standard deviation over multiple simulations, while the dashed lines are linear extrapolations for each parameter set, with their Y-intercepts are the final diffusion coefficients.

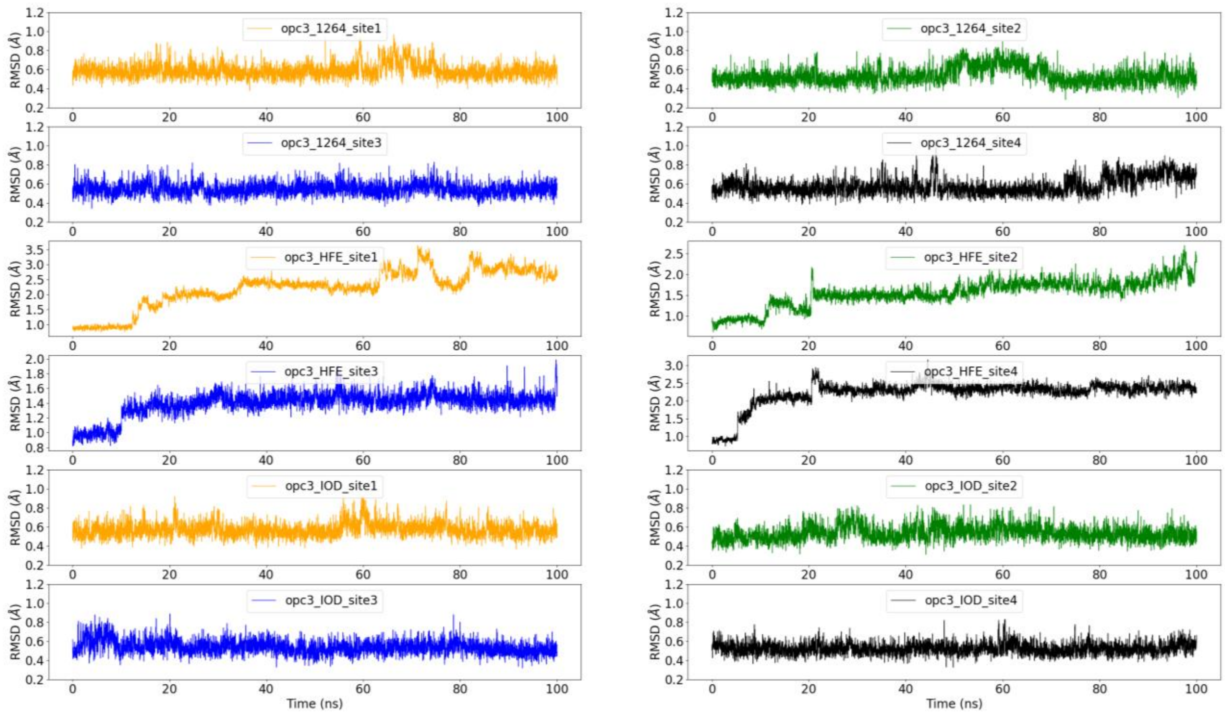

Figure S3. RMSDs of the binding site residues from the simulations using the 12-6-4, 12-6 HFE, and 12-6 IOD parameter sets for Fe^{3+} in conjunction with the OPC3 water model. The RMSDs were calculated against the initial coordinates generated based on the crystal structure.

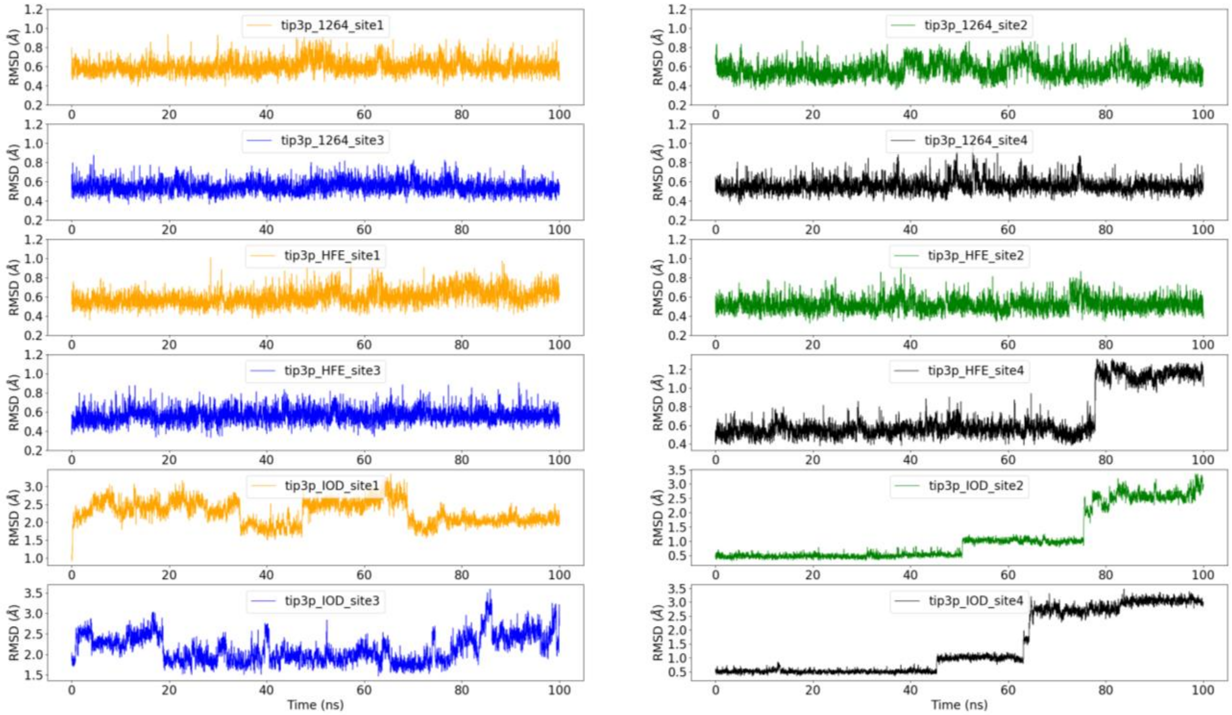

Figure S4. RMSDs of the binding site residues from the simulations using the 12-6-4, 12-6 HFE, and 12-6 IOD parameter sets for Fe^{3+} in conjunction with the TIP3P water model. The RMSDs were calculated against the initial coordinates generated based on the crystal structure. Metal site 4 has its RMSD increased from 0.6 to 1.2 Å at ~80 ns when using the HFE/TIP3P parameter combination, which is due to the rotation of a coordinated HIS residue. This HIS residue is still bound to the metal ion after the rotation.

Table S1. Parameters for the Eight Different Water Models[a]

Water model	Q(O) or Q(M) (e)	Q(H) (e)	r(O-H) (Å)	H-O-H (º)	r(O-M) (Å)	R_{min}/2 for O (Å)	ε for O (kcal/mol)
TIP3P	-0.834	+0.417	0.9572	104.52	N/A	1.7683	0.1520
SPC/E	-0.8476	+0.4238	1.0	109.47	N/A	1.7767	0.1553
TIP4P	-1.04	+0.52	0.9572	104.52	0.15	1.7699	0.1550
$TIP4P_{Ew}$	-1.04844	+0.52422	0.9572	104.52	0.125	1.775931	0.16275
OPC3	-0.8952	+0.4476	0.9789	109.47	N/A	1.7814990	0.163406
OPC	-1.3582	+0.6791	0.8724	103.6	0.1594	1.777167268	0.2128008130
TIP3P-FB	-0.84844	+0.42422	1.0118	108.15	N/A	1.7835723	0.155866
TIP4P-FB	-1.05174	+0.52587	0.9572	104.52	0.10527	1.77660486	0.179082

[a]Here M represents a dummy atom. For the 4-point water models, the oxygen atom has a charge of zero, while the dummy atom has a negative charge.

Table S2A. Calculated HFE Values (in kcal/mol) from the Parameter Space Scan for Trivalent and Tetravalent Metal Ions in Conjunction with the OPC3 Water Model[ab]

		Trivalent Metal Ion					Tetravalent Metal Ion				
$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C_4 (kcal/mol*Å^4)					C_4 (kcal/mol*Å^4)				
		0	125	250	375	500	0	250	500	750	1000
0.9	0.00000062	-1163.4	-1356.2	-1514.3	-1656.3	N/A	-1874.1	N/A	N/A	N/A	N/A
1.0	0.00001422	-1084.6	-1228.1	-1365.8	N/A	-1636.5	-1765.6	-2075.6	-2372.7	N/A	N/A
1.1	0.00016377	-1033.5	-1150.6	-1273.1	-1396.6	-1521.3	-1695.7	-1959.1	-2230.1	-2499.6	-2781.4
1.2	0.00110429	-968.6	-1052.9	-1147.9	-1253.9	-1365.0	-1605.3	-1800.2	-2037.8	-2284.5	-2538.5
1.3	0.00490301	-921.0	-992.2	-1070.3	-1153.8	-1239.8	-1525.0	-1701.0	-1885.6	-2086.6	-2295.6
1.4	0.01570749	-855.5	-916.7	-980.9	-1047.7	-1116.7	-1435.7	-1575.3	-1725.6	-1892.4	-2066.9
1.5	0.03899838	-808.5	-856.9	-912.6	-965.7	-1023.1	-1374.6	-1492.7	-1619.2	-1746.2	-1880.1
1.6	0.07934493	-768.7	-812.9	-857.7	-904.6	-953.7	-1317.4	-1419.1	-1526.1	-1638.9	-1755.5
1.7	0.13818331	-731.4	-770.4	-811.0	-852.8	-895.2	-1260.2	-1349.6	-1443.9	-1542.6	-1647.8
1.8	0.21312875	-697.8	-731.7	-767.4	-803.9	-841.3	-1211.8	-1291.5	-1374.7	-1460.6	-1548.8
1.9	0.29896986	-667.0	-698.2	-729.4	-762.1	-797.6	-1173.2	-1243.8	-1323.0	-1404.8	-1481.7
2.0	0.38943250	-640.8	-668.1	-698.9	-728.8	-759.0	-1133.0	-1205.0	-1275.5	-1345.0	-1419.6
2.1	0.47874242	-614.5	-641.6	-670.2	-697.2	-725.9	-1097.4	-1158.0	-1220.7	-1284.3	-1353.3
2.2	0.56252208	-591.9	-615.9	-640.8	-665.7	-692.8	-1055.2	-1111.1	-1168.2	-1228.5	-1289.7
2.3	0.63803333	-567.1	-590.6	-614.1	-637.4	-660.1	-1017.5	-1068.1	-1121.0	-1175.4	-1229.5

[a]Here "N/A" means the simulation job failed. This point was not used in the curve fitting.
[b]At low $R_{min,M}/2$ and high C_4 region, HFE value (if not failed) will be more negative while using 12 window TI. It does not affect our final parameters, but we hope the readers are aware of this issue in case anyone needs to try uncommon $R_{min,M}/2$ and C_4 combinations.

Table S2B. Calculated HFE Values (in kcal/mol) from the Parameter Space Scan for Trivalent and Tetravalent Metal Ions in Conjunction with the OPC Water Model[ab]

		Trivalent Metal Ion					Tetravalent Metal Ion				
$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C_4 (kcal/mol*Å^4)					C_4 (kcal/mol*Å^4)				
		0	125	250	375	500	0	250	500	750	1000
0.9	0.00000062	-1098.2	-1279.0	N/A	N/A	N/A	-1771.3	-2144.3	N/A	N/A	N/A
1.0	0.00001422	-1029.2	-1165.8	-1298.3	-1426.3	N/A	-1677.1	N/A	N/A	N/A	N/A
1.1	0.00016377	-985.8	-1093.4	-1205.9	-1323.2	-1439.6	-1616.0	-1860.6	-2111.2	-2369.3	N/A
1.2	0.00110429	-925.4	-1002.8	-1095.3	-1196.1	-1300.1	-1534.3	-1722.6	-1943.8	-2176.9	-2415.5
1.3	0.00490301	-880.9	-949.4	-1022.7	-1099.5	-1181.6	-1468.1	-1628.2	-1799.1	-1984.5	-2182.4
1.4	0.01570749	-824.0	-882.6	-942.1	-1004.5	-1070.4	-1384.3	-1515.1	-1656.9	-1811.7	-1977.1
1.5	0.03899838	-778.8	-827.5	-877.8	-927.5	-981.5	-1325.9	-1433.7	-1548.0	-1665.0	-1799.5
1.6	0.07934493	-743.8	-785.6	-828.5	-872.0	-919.3	-1273.0	-1367.9	-1467.0	-1580.7	-1685.6
1.7	0.13818331	-708.7	-747.1	-785.9	-824.0	-864.4	-1220.2	-1304.8	-1393.8	-1488.8	-1587.2
1.8	0.21312875	-678.4	-711.0	-745.1	-778.8	-814.1	-1174.2	-1250.2	-1327.1	-1410.5	-1493.6
1.9	0.29896986	-647.6	-679.9	-709.3	-740.9	-772.1	-1141.8	-1209.3	-1285.9	-1358.2	-1434.7
2.0	0.38943250	-623.2	-650.7	-681.6	-710.5	-740.7	-1104.0	-1171.2	-1234.9	-1299.8	-1374.9
2.1	0.47874242	-600.1	-627.1	-651.6	-679.6	-708.6	-1068.0	-1126.2	-1186.6	-1249.1	-1310.7
2.2	0.56252208	-576.4	-602.1	-627.5	-650.0	-676.2	-1028.5	-1081.6	-1137.3	-1195.1	-1255.8
2.3	0.63803333	-554.9	-576.9	-600.1	-621.5	-646.0	-991.6	-1041.0	-1091.3	-1141.1	-1196.7

[a]Here "N/A" means the simulation job failed. These points were not used in the curve fittings.
[b]At low $R_{min,M}/2$ and high C_4 region, HFE value (if not failed) will be more negative while using 12 window TI. It does not affect our final parameters, but we hope the readers are aware of this issue in case anyone needs to try uncommon $R_{min,M}/2$ and C_4 combinations.

Table S2C. Calculated HFE Values (in kcal/mol) from the Parameter Space Scan for Trivalent and Tetravalent Metal Ions in Conjunction with the TIP3P-FB Water Model[ab]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	Trivalent Metal Ion C_4 (kcal/mol*Å^4) 0	125	250	375	500	Tetravalent Metal Ion C_4 (kcal/mol*Å^4) 0	250	500	750	1000
0.9	0.00000062	N/A	-1335.5	-1492.6	N/A	N/A	-1844.5	N/A	N/A	N/A	N/A
1.0	0.00001422	-1069.4	-1210.8	-1350.0	-1484.2	N/A	-1740.5	-2049.4	N/A	N/A	-2948.5
1.1	0.00016377	-1019.6	-1135.2	-1257.9	-1382.8	-1509.0	-1672.4	-1937.4	-2207.2	-2480.1	-2757.6
1.2	0.00110429	-956.4	-1042.6	-1134.4	-1242.4	-1353.6	-1586.1	-1780.2	-2018.7	-2265.0	-2518.4
1.3	0.00490301	-908.7	-980.6	-1058.7	-1141.9	-1228.6	-1508.4	-1682.4	-1867.6	-2068.8	-2277.7
1.4	0.01570749	-845.9	-906.9	-970.8	-1037.2	-1107.8	-1420.9	-1559.9	-1708.3	-1875.1	-2052.3
1.5	0.03899838	-799.5	-850.8	-904.0	-957.6	-1014.6	-1363.1	-1476.6	-1600.2	-1730.9	-1867.1
1.6	0.07934493	-760.4	-805.5	-849.0	-896.8	-946.3	-1304.5	-1406.5	-1513.8	-1625.7	-1742.5
1.7	0.13818331	-724.8	-763.6	-803.0	-846.3	-889.0	-1249.8	-1336.7	-1432.9	-1531.5	-1635.4
1.8	0.21312875	-690.4	-726.4	-760.5	-797.3	-834.7	-1200.4	-1280.1	-1364.1	-1451.2	-1541.7
1.9	0.29896986	-660.9	-692.7	-724.4	-756.5	-790.0	-1168.4	-1237.7	-1317.3	-1390.6	-1472.3
2.0	0.38943250	-632.3	-662.4	-692.6	-722.6	-756.1	-1122.9	-1191.9	-1261.2	-1335.7	-1411.4
2.1	0.47874242	-610.2	-637.7	-664.7	-692.5	-719.4	-1088.5	-1148.5	-1211.1	-1276.8	-1343.5
2.2	0.56252208	-586.3	-611.6	-635.8	-661.7	-687.1	-1048.5	-1103.3	-1160.1	-1220.7	-1280.1
2.3	0.63803333	-563.8	-587.4	-609.4	-633.1	-656.9	-1010.0	-1061.0	-1113.9	-1168.5	-1222.1

[a]Here "N/A" means the simulation job failed. This point was not used in the curve fitting.
[b]At low $R_{min,M}/2$ and high C_4 region, HFE value (if not failed) will be more negative while using 12 window TI. It does not affect our final parameters, but we hope the readers are aware of this issue in case anyone needs to try uncommon $R_{min,M}/2$ and C_4 combinations.

Table S2D. Calculated HFE Values (in kcal/mol) from the Parameter Space Scan for Trivalent and Tetravalent Metal Ions in Conjunction with the TIP4P-FB Water Model[ab]

		Trivalent Metal Ion					Tetravalent Metal Ion				
		C_4 (kcal/mol*Å^4)					C_4 (kcal/mol*Å^4)				
$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	0	125	250	375	500	0	250	500	750	1000
0.9	0.00000062	-1092.1	N/A	-1429.2	N/A	N/A	-1762.9	N/A	-2451.3	N/A	N/A
1.0	0.00001422	-1025.4	-1163.3	-1297.8	N/A	-1559.5	-1673.1	-1971.6	-2256.9	-2548.1	N/A
1.1	0.00016377	-983.1	-1093.3	-1211.8	-1331.8	-1452.6	-1611.2	-1865.4	-2125.3	-2391.9	-2666.5
1.2	0.00110429	-922.0	-1008.2	-1098.2	-1201.8	-1309.6	-1529.8	-1720.5	-1951.2	-2190.9	-2439.7
1.3	0.00490301	-878.0	-949.1	-1025.1	-1105.8	-1190.1	-1463.3	-1627.2	-1807.4	-2001.6	-2204.1
1.4	0.01570749	-819.2	-880.0	-941.9	-1006.5	-1075.0	-1380.1	-1512.3	-1661.0	-1820.0	-1992.4
1.5	0.03899838	-777.6	-827.5	-879.1	-931.4	-987.8	-1324.7	-1437.2	-1557.4	-1681.0	-1816.8
1.6	0.07934493	-742.8	-784.9	-828.1	-874.9	-922.8	-1270.8	-1369.5	-1473.7	-1584.9	-1697.7
1.7	0.13818331	-708.0	-745.6	-785.3	-826.5	-868.1	-1218.8	-1305.0	-1397.6	-1494.3	-1595.0
1.8	0.21312875	-676.9	-710.3	-744.0	-779.9	-816.4	-1174.0	-1250.5	-1331.5	-1417.2	-1506.1
1.9	0.29896986	-648.2	-678.0	-709.9	-742.9	-774.6	-1140.4	-1209.9	-1288.5	-1363.9	-1443.9
2.0	0.38943250	-623.0	-651.2	-681.2	-708.6	-741.3	-1103.9	-1171.1	-1237.4	-1306.2	-1381.2
2.1	0.47874242	-599.1	-626.3	-653.0	-680.0	-708.6	-1065.8	-1124.5	-1187.0	-1249.3	-1315.9
2.2	0.56252208	-576.7	-601.1	-625.5	-651.5	-676.5	-1026.3	-1081.6	-1135.7	-1197.2	-1256.5
2.3	0.63803333	-555.7	-577.0	-600.5	-623.4	-645.9	-990.6	-1040.9	-1092.0	-1147.2	-1201.1

[a]Here "N/A" means the simulation job failed. These points were not used in the curve fittings.
[b]At low $R_{min,M}/2$ and high C_4 region, HFE value (if not failed) will be more negative while using 12 window TI. It does not affect our final parameters, but we hope the readers are aware of this issue in case anyone needs to try uncommon $R_{min,M}/2$ and C_4 combinations.

Table S3A. Calculated IOD and CN Values from the Parameter Space Scan for the Trivalent (top) and Tetravalent (bottom) Metal Ions in Conjunction with the OPC3 Water Model[a]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=125 kcal/mol*Å^4		C4=250 kcal/mol*Å^4		C4=375 kcal/mol*Å^4		C4=500 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.09	2.0	1.03	2.0	0.99	2.0	0.96	2.0	N/A	N/A
1.0	0.00001422	1.35	3.0	1.23	2.3	1.14	2.0	N/A	N/A	1.08	2.0
1.1	0.00016377	1.53	4.0	1.49	4.0	1.46	4.0	1.43	4.0	1.41	4.0
1.2	0.00110429	1.81	6.0	1.77	6.0	1.74	6.0	1.55	4.0	1.53	4.0
1.3	0.00490301	1.89	6.0	1.86	6.0	1.83	6.0	1.81	6.0	1.79	6.0
1.4	0.01570749	2.00	6.0	1.97	6.0	1.95	6.0	1.92	6.0	1.90	6.0
1.5	0.03899838	2.24	8.0	2.22	8.0	2.19	8.0	2.17	8.0	2.16	8.0
1.6	0.07934493	2.36	8.7	2.33	8.5	2.30	8.3	2.28	8.2	2.26	8.1
1.7	0.13818331	2.48	9.0	2.46	9.0	2.44	9.0	2.42	5.0	2.40	9.0
1.8	0.21312875	2.60	9.6	2.59	9.7	2.57	9.7	2.55	9.7	2.54	9.7
1.9	0.29896986	2.72	10.0	2.70	10.0	2.68	10.0	2.66	10.0	2.65	10.0
2.0	0.38943250	2.88	12.0	2.86	12.0	2.84	12.0	2.82	12.0	2.81	12.0
2.1	0.47874242	2.96	12.0	2.95	12.0	2.93	12.0	2.91	12.0	2.89	12.0
2.2	0.56252208	3.05	12.0	3.03	12.0	3.02	12.0	3.00	12.0	2.98	12.0
2.3	0.63803333	3.14	12.0	3.12	12.0	3.11	12.0	3.09	12.0	3.08	12.0

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=250 kcal/mol*Å^4		C4=500 kcal/mol*Å^4		C4=750 kcal/mol*Å^4		C4=1000 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.06	2.0	N/A	N/A	N/A	N.A	N/A	N/A	N/A	N/A
1.0	0.00001422	1.32	3.0	1.13	1.8	1.07	2.0	N/A	N/A	N/A	N/A
1.1	0.00016377	1.48	4.0	1.43	4.0	1.38	4.0	1.35	4.0	1.32	4.0
1.2	0.00110429	1.75	6.0	1.71	6.0	1.50	4.0	1.47	4.0	1.44	4.0
1.3	0.00490301	1.83	6.0	1.79	6.0	1.75	6.0	1.72	6.0	1.69	6.0
1.4	0.01570749	1.99	6.1	1.90	6.0	1.86	6.0	1.82	6.1	1.81	6.0
1.5	0.03899838	2.18	8.0	2.14	8.0	2.11	8.0	2.08	8.0	2.06	8.0
1.6	0.07934493	2.30	8.9	2.25	7.1	2.21	8.2	2.18	8.0	2.16	8.0
1.7	0.13818331	2.41	9.1	2.37	9.0	2.34	9.0	2.32	9.0	2.29	9.0
1.8	0.21312875	2.54	10.0	2.51	10.0	2.48	10.0	2.46	10.0	2.44	10.0
1.9	0.29896986	2.71	12.0	2.68	12.0	2.65	12.0	2.63	12.0	2.60	12.0
2.0	0.38943250	2.78	12.0	2.75	12.0	2.73	12.0	2.70	12.0	2.68	12.0
2.1	0.47874242	2.86	12.0	2.84	12.0	2.81	12.0	2.79	12.0	2.77	12.0
2.2	0.56252208	2.95	12.0	2.92	12.0	2.90	12.0	2.87	12.0	2.85	12.0
2.3	0.63803333	3.04	12.1	3.02	12.4	2.99	12.0	2.96	12.0	2.97	12.8

[a]Here "N/A" means the simulation job failed. These points were not used in the curve fittings.

Table S3B. Calculated IOD and CN Values from the Parameter Space Scan for the Trivalent (top) and Tetravalent (bottom) Metal Ions in Conjunction with the OPC Water Model[a]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=125 kcal/mol*Å^4		C4=250 kcal/mol*Å^4		C4=375 kcal/mol*Å^4		C4=500 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.12	2.0	1.06	2.0	N/A	N/A	N/A	N/A	N/A	N/A
1.0	0.00001422	1.38	3.0	1.21	1.9	1.16	2.0	1.12	2.0	N/A	N/A
1.1	0.00016377	1.56	4.0	1.52	4.0	1.49	4.0	1.46	4.0	1.44	4.0
1.2	0.00110429	1.84	6.0	1.81	6.0	1.61	4.0	1.58	4.0	1.55	4.0
1.3	0.00490301	1.92	6.0	1.89	6.0	1.87	6.0	1.85	6.0	1.82	6.0
1.4	0.01570749	2.03	6.0	2.00	6.0	1.98	6.0	1.96	6.0	1.94	6.0
1.5	0.03899838	2.27	8.0	2.25	8.0	2.22	7.9	2.20	7.9	2.18	7.8
1.6	0.07934493	2.39	8.6	2.36	8.4	2.34	8.1	2.32	8.1	2.30	8.0
1.7	0.13818331	2.52	9.0	2.49	9.0	2.47	9.0	2.46	9.0	2.44	5.4
1.8	0.21312875	2.64	9.7	2.62	9.7	2.61	9.8	2.59	9.8	2.57	9.8
1.9	0.29896986	2.75	10.0	2.73	10.1	2.72	10.1	2.72	10.7	2.74	11.4
2.0	0.38943250	2.91	12.0	2.89	12.0	2.88	12.0	2.86	12.0	2.84	12.0
2.1	0.47874242	3.00	12.0	2.98	12.0	2.96	12.0	2.95	12.0	2.93	12.0
2.2	0.56252208	3.08	12.0	3.07	12.0	3.05	12.0	3.03	12.0	3.02	12.0
2.3	0.63803333	3.17	12.0	3.15	12.0	3.14	12.0	3.12	12.0	3.11	12.0

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=250 kcal/mol*Å^4		C4=500 kcal/mol*Å^4		C4=750 kcal/mol*Å^4		C4=1000 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.09	2.0	1.01	2.0	N/A	N/A	N/A	N/A	N/A	N/A
1.0	0.00001422	1.35	3.0	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
1.1	0.00016377	1.52	4.0	1.46	4.0	1.42	4.0	1.38	4.0	N/A	N/A
1.2	0.00110429	1.79	6.0	1.74	6.0	1.53	4.0	1.49	4.0	1.47	4.0
1.3	0.00490301	1.87	6.0	1.82	6.0	1.79	6.0	1.76	6.0	1.73	6.0
1.4	0.01570749	1.97	6.0	1.93	6.0	1.90	6.0	1.86	6.0	1.84	6.0
1.5	0.03899838	2.22	8.0	2.18	8.0	2.15	8.0	2.12	8.0	2.10	8.0
1.6	0.07934493	2.32	8.5	2.28	8.1	2.25	8.0	2.22	8.0	2.19	8.0
1.7	0.13818331	2.44	9.0	2.41	9.0	2.38	9.0	2.35	9.0	2.33	9.0
1.8	0.21312875	2.67	12.0	2.55	10.0	2.52	10.0	2.50	10.0	2.47	10.0
1.9	0.29896986	2.74	12.0	2.72	12.0	2.69	12.0	2.67	12.0	2.64	12.0
2.0	0.38943250	2.82	12.0	2.79	12.0	2.77	12.0	2.74	12.0	2.72	12.0
2.1	0.47874242	2.90	12.0	2.87	12.0	2.85	12.0	2.82	12.0	2.80	12.0
2.2	0.56252208	2.98	12.0	2.96	12.0	2.93	12.0	2.91	12.0	2.89	12.0
2.3	0.63803333	3.07	12.3	3.05	12.3	3.03	12.2	3.01	12.3	3.02	13.1

[a]Here "N/A" means the simulation job failed. These points were not used in the curve fittings.

Table S3C. Calculated IOD and CN Values from the Parameter Space Scan for the Trivalent (top) and Tetravalent (bottom) Metal Ions in Conjunction with the TIP3P-FB Water Model[a]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=125 kcal/mol*Å^4		C4=250 kcal/mol*Å^4		C4=375 kcal/mol*Å^4		C4=500 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	N/A	N/A	1.03	2.0	0.99	2.0	N/A	N/A	N/A	N/A
1.0	0.00001422	1.36	3.0	1.24	0.9	1.14	2.0	1.10	2.0	N/A	N/A
1.1	0.00016377	1.53	4.0	1.49	4.0	1.46	4.0	1.43	4.0	1.40	4.0
1.2	0.00110429	1.81	6.0	1.77	6.0	1.74	6.0	1.55	4.0	1.53	4.0
1.3	0.00490301	1.89	6.0	1.86	6.0	1.83	6.0	1.81	6.0	1.79	6.0
1.4	0.01570749	2.00	6.0	1.97	6.0	1.95	6.0	1.92	6.0	1.90	6.0
1.5	0.03899838	2.24	8.0	2.22	8.0	2.19	8.0	2.17	8.0	2.15	8.0
1.6	0.07934493	2.36	8.8	2.33	8.7	2.31	8.5	2.28	8.3	2.26	8.2
1.7	0.13818331	2.48	9.0	2.46	9.0	2.44	9.0	2.42	9.0	2.40	9.0
1.8	0.21312875	2.61	9.7	2.59	9.8	2.57	9.8	2.56	9.8	2.54	9.9
1.9	0.29896986	2.72	10.0	2.70	10.0	2.68	10.0	2.66	10.0	2.65	10.0
2.0	0.38943250	2.88	11.9	2.86	12.0	2.84	12.0	2.82	12.0	2.80	12.0
2.1	0.47874242	2.96	12.0	2.94	12.0	2.93	12.0	2.91	12.0	2.89	12.0
2.2	0.56252208	3.05	12.0	3.03	12.0	3.02	12.0	3.00	12.0	2.98	12.0
2.3	0.63803333	3.14	12.0	3.12	12.0	3.11	12.0	3.09	12.0	3.07	12.0

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=250 kcal/mol*Å^4		C4=500 kcal/mol*Å^4		C4=750 kcal/mol*Å^4		C4=1000 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.06	2.0	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
1.0	0.00001422	1.32	3.0	1.13	2.0	N/A	N/A	N/A	N/A	1.00	2.0
1.1	0.00016377	1.48	4.0	1.43	4.0	1.38	4.0	1.35	4.0	1.32	4.0
1.2	0.00110429	1.75	6.0	1.71	6.0	1.66	6.0	1.47	4.0	1.44	4.0
1.3	0.00490301	1.83	6.0	1.79	6.0	1.75	6.0	1.72	6.0	1.69	6.0
1.4	0.01570749	2.00	6.1	1.90	6.0	1.86	6.0	1.83	6.0	1.80	6.0
1.5	0.03899838	2.18	8.0	2.14	8.0	2.11	8.0	2.08	8.0	2.06	8.0
1.6	0.07934493	2.30	8.9	2.25	8.6	2.21	8.2	2.18	8.1	2.15	8.0
1.7	0.13818331	2.41	9.1	2.37	9.0	2.34	9.0	2.32	9.0	2.29	9.0
1.8	0.21312875	2.63	12.0	2.51	10.0	2.48	10.0	2.46	10.0	2.43	10.0
1.9	0.29896986	2.70	12.0	2.68	12.0	2.65	12.0	2.62	12.0	2.60	12.0
2.0	0.38943250	2.78	12.0	2.75	12.0	2.73	12.0	2.70	12.3	2.68	12.0
2.1	0.47874242	2.86	12.0	2.84	12.0	2.81	12.0	2.79	12.0	2.76	12.0
2.2	0.56252208	2.95	12.0	2.92	12.0	2.90	12.0	2.87	12.0	2.85	12.0
2.3	0.63803333	3.04	12.1	3.01	12.1	3.00	12.5	2.97	12.3	2.98	13.1

[a]Here "N/A" means the simulation job failed. These points were not used in the curve fittings.

Table S3D. Calculated IOD and CN Values from the Parameter Space Scan for the Trivalent (top) and Tetravalent (bottom) Metal Ions in Conjunction with the TIP4P-FB Water Model[a]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=125 kcal/mol*Å^4		C4=250 kcal/mol*Å^4		C4=375 kcal/mol*Å^4		C4=500 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.11	2.0	N/A	N/A	1.00	2.0	N/A	N/A	N/A	N/A
1.0	0.00001422	1.37	3.0	1.22	1.5	1.15	2.0	N/A	N/A	1.09	2.0
1.1	0.00016377	1.54	4.0	1.50	4.0	1.47	4.0	1.44	4.0	1.42	4.0
1.2	0.00110429	1.82	6.0	1.79	6.0	1.76	6.0	1.56	4.0	1.54	4.0
1.3	0.00490301	1.91	6.0	1.88	6.0	1.85	6.0	1.82	6.0	1.80	6.0
1.4	0.01570749	2.02	6.0	1.99	6.0	1.96	6.0	1.94	6.0	1.92	6.0
1.5	0.03899838	2.26	8.0	2.23	8.0	2.21	8.0	2.19	8.0	2.17	8.0
1.6	0.07934493	2.38	8.9	2.35	8.9	2.33	8.6	2.30	8.5	2.28	8.2
1.7	0.13818331	2.50	9.0	2.48	9.0	2.46	9.0	2.44	9.0	2.42	9.0
1.8	0.21312875	2.63	9.8	2.61	9.9	2.59	9.9	2.58	9.9	2.56	9.9
1.9	0.29896986	2.76	10.8	2.74	10.9	2.72	10.9	2.69	10.3	2.66	10.1
2.0	0.38943250	2.89	12.0	2.88	12.0	2.86	12.0	2.84	12.0	2.82	12.0
2.1	0.47874242	2.98	12.0	2.96	12.0	2.94	12.0	2.93	12.0	2.91	12.0
2.2	0.56252208	3.07	12.0	3.05	12.0	3.03	12.0	3.01	12.0	3.00	12.0
2.3	0.63803333	3.15	12.0	3.14	12.0	3.12	12.0	3.11	12.0	3.09	12.0

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=250 kcal/mol*Å^4		C4=500 kcal/mol*Å^4		C4=750 kcal/mol*Å^4		C4=1000 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.08	2.0	N/A	N/A	0.94	2.0	N/A	N/A	N/A	N/A
1.0	0.00001422	1.34	3.0	1.14	2.0	1.08	2.0	1.04	2.0	N/A	N/A
1.1	0.00016377	1.50	4.0	1.44	4.0	1.40	4.0	1.36	4.0	1.33	4.0
1.2	0.00110429	1.77	6.0	1.72	6.0	1.51	4.0	1.48	4.0	1.45	4.0
1.3	0.00490301	1.85	6.0	1.80	6.0	1.77	6.0	1.73	6.0	1.71	6.0
1.4	0.01570749	2.01	6.0	1.91	6.0	1.88	6.0	1.85	6.0	1.82	6.0
1.5	0.03899838	2.20	8.0	2.16	8.0	2.13	6.9	2.10	8.0	2.07	8.0
1.6	0.07934493	2.31	8.8	2.27	8.4	2.23	8.1	2.20	8.0	2.17	8.0
1.7	0.13818331	2.43	9.2	2.39	9.0	2.36	9.0	2.33	9.0	2.31	9.0
1.8	0.21312875	2.65	12.0	2.61	11.6	2.58	11.5	2.48	10.0	2.45	10.0
1.9	0.29896986	2.72	12.0	2.69	12.0	2.67	12.0	2.64	12.0	2.62	12.0
2.0	0.38943250	2.80	12.0	2.77	12.0	2.74	12.0	2.72	12.0	2.70	12.0
2.1	0.47874242	2.88	12.0	2.85	12.0	2.83	12.0	2.80	12.0	2.78	12.0
2.2	0.56252208	2.96	12.0	2.94	12.0	2.91	12.0	2.89	12.0	2.87	12.0
2.3	0.63803333	3.07	12.6	3.05	9.2	3.02	12.6	3.00	12.7	2.98	12.9

[a]Here "N/A" means the simulation job failed. These points were not used in the curve fittings.

Table S4. Calculated HFE, IOD, and CN Values for the 12-6 HFE Parameter Set for the Four New Water Models (Parameters in Table 2).

	OPC3			OPC			TIP3P-FB			TIP4P-FB		
	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN
Al^{3+}	-1082.8	1.36	3.0	-1082.8	1.14	2.0	-1083.4	1.19	2.0	-1082.2	1.13	2.0
Fe^{3+}	-1019.6	1.55	4.0	-1019.2	1.41	3.0	-1019.9	1.53	4.0	-1020.1	1.39	3.0
Cr^{3+}	-958.6	1.82	6.0	-958.3	1.60	4.0	-958.4	1.80	6.0	-956.9	1.58	4.0
In^{3+}	-952.5	1.84	6.0	-949.8	1.62	4.0	-949.7	1.82	6.0	-951.8	1.59	4.0
Tl^{3+}	-949.0	1.85	6.0	-949.8	1.62	4.0	-949.7	1.81	6.0	-948.4	1.60	4.0
Y^{3+}	-821.6	2.16	7.7	-824.3	2.03	6.0	-825.1	2.09	6.9	-825.3	2.00	6.0
La^{3+}	-752.1	2.43	9.0	-751.6	2.35	8.1	-752.8	2.40	9.0	-751.9	2.34	8.2
Ce^{3+}	-764.2	2.37	8.8	-766.7	2.32	8.0	-764.8	2.34	8.7	-763.7	2.30	8.0
Pr^{3+}	-773.8	2.33	8.2	-777.4	2.28	8.0	-774.7	2.30	8.0	-775.3	2.26	8.0
Nd^{3+}	-783.8	2.30	8.0	-782.3	2.25	7.9	-784.3	2.28	8.0	-782.6	2.24	8.0
Sm^{3+}	-794.0	2.27	8.0	-794.4	2.18	8.3	-795.4	2.25	8.0	-793.4	2.19	8.2
Eu^{3+}	-802.0	2.26	8.0	-803.0	2.14	8.1	-801.4	2.23	8.0	-803.7	2.11	7.0
Gd^{3+}	-805.4	2.25	8.0	-805.5	2.09	6.2	-805.3	2.22	8.0	-807.5	2.05	6.2
Tb^{3+}	-814.5	2.21	8.0	-811.6	2.06	6.0	-814.3	2.18	8.0	-814.4	2.03	6.0
Dy^{3+}	-820.0	2.19	8.0	-819.0	2.04	6.0	-818.8	2.14	7.4	-820.0	2.02	6.0
Er^{3+}	-835.0	2.06	6.5	-835.1	2.01	6.0	-834.8	2.02	6.0	-835.8	1.98	6.0
Tm^{3+}	-839.8	2.03	6.0	-839.9	2.00	6.0	-838.4	2.01	6.0	-841.7	1.97	6.0
Lu^{3+}	-839.8	2.03	6.0	-840.5	2.00	6.0	-838.4	2.01	6.0	-841.7	1.97	6.0
Hf^{4+}	-1662.1	1.51	4.0	-1664.0	1.37	3.0	-1664.9	1.49	4.0	-1665.1	1.35	3.0
Zr^{4+}	-1623.0	1.55	4.0	-1623.1	1.51	4.0	-1622.6	1.53	4.0	-1621.0	1.49	4.0
Ce^{4+}	-1463.2	1.90	6.0	-1463.7	1.87	6.0	-1463.8	1.88	6.0	-1462.6	1.85	6.0
U^{4+}	-1567.1	1.79	6.0	-1568.9	1.57	4.0	-1567.3	1.77	6.0	-1568.9	1.55	4.0
Pu^{4+}	-1520.2	1.84	6.0	-1520.5	1.81	6.0	-1520.4	1.82	6.0	-1520.0	1.78	6.0
Th^{4+}	-1389.2	2.15	8.0	-1390.0	1.96	6.0	-1389.6	2.11	8.3	-1388.2	1.94	6.0

Table S5. Calculated HFE, IOD, and CN Values for the 12-6 IOD Parameter Set for the Four New Water Models (Parameters in Table 3).

	OPC3			OPC			TIP3P-FB			TIP4P-FB		
	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN
Al^{3+}	-929.6	1.88	6.0	-907.9	1.88	6.0	-917.3	1.88	6.0	-896.5	1.88	6.0
Fe^{3+}	-842.8	2.02	6.0	-823.5	2.03	6.0	-832.5	2.02	6.0	-817.3	2.02	6.0
Cr^{3+}	-879.0	1.96	6.0	-861.2	1.96	6.0	-868.5	1.96	6.0	-852.6	1.95	6.0
In^{3+}	-825.0	2.15	8.1	-801.3	2.14	6.9	-820.4	2.14	8.0	-798.6	2.15	8.3
Tl^{3+}	-810.4	2.24	8.0	-785.1	2.24	8.0	-802.5	2.24	8.0	-782.5	2.24	8.0
Y^{3+}	-767.3	2.36	8.7	-752.7	2.35	8.2	-760.4	2.36	8.8	-747.9	2.35	8.7
La^{3+}	-719.9	2.52	9.0	-710.0	2.52	9.0	-714.6	2.51	9.0	-703.1	2.51	9.0
Ce^{3+}	-710.3	2.54	9.0	-702.2	2.54	9.0	-705.5	2.54	9.0	-696.7	2.54	9.0
Pr^{3+}	-714.3	2.53	9.0	-704.7	2.53	9.0	-707.8	2.53	9.0	-698.5	2.53	9.0
Nd^{3+}	-735.1	2.48	9.0	-722.9	2.48	9.0	-727.9	2.48	9.0	-716.3	2.47	9.0
Sm^{3+}	-744.5	2.45	9.0	-730.6	2.45	9.0	-736.6	2.45	9.0	-724.8	2.45	9.0
Eu^{3+}	-741.6	2.46	9.0	-727.9	2.46	9.0	-733.7	2.46	9.0	-722.4	2.46	9.0
Gd^{3+}	-759.3	2.40	9.0	-744.1	2.39	8.6	-751.4	2.40	9.0	-739.3	2.39	9.0
Tb^{3+}	-756.6	2.41	9.0	-741.8	2.40	9.0	-748.5	2.41	9.0	-735.7	2.41	9.0
Dy^{3+}	-765.4	2.37	8.9	-750.4	2.36	8.2	-758.6	2.38	8.9	-744.4	2.37	8.8
Er^{3+}	-768.5	2.36	8.7	-752.5	2.35	8.1	-760.8	2.36	8.8	-748.1	2.35	8.5
Tm^{3+}	-768.3	2.36	8.7	-752.9	2.35	8.1	-760.7	2.36	8.7	-748.0	2.35	8.6
Lu^{3+}	-775.2	2.33	8.2	-758.7	2.33	8.0	-767.1	2.33	8.4	-753.5	2.33	8.1
Hf^{4+}	-1380.3	2.17	8.0	-1349.9	2.16	7.9	-1367.0	2.17	8.0	-1341.4	2.16	7.9
Zr^{4+}	-1367.8	2.19	8.0	-1331.3	2.20	8.0	-1357.6	2.19	8.0	-1327.9	2.19	8.0
Ce^{4+}	-1255.7	2.42	9.2	-1229.8	2.42	9.0	-1247.6	2.41	9.2	-1222.4	2.42	9.0
U^{4+}	-1256.0	2.42	9.2	-1229.7	2.42	9.0	-1246.8	2.42	9.2	-1222.4	2.42	9.1
Pu^{4+}	-1272.8	2.39	9.0	-1244.2	2.40	9.0	-1259.7	2.39	9.0	-1235.8	2.39	9.0
Th^{4+}	-1249.3	2.44	9.7	-1219.2	2.44	9.1	-1239.5	2.44	9.7	-1213.3	2.44	9.6

Table S6. Calculated HFE, IOD, and CN Values for the 12-6-4 Parameter Set for the Four New Water Models (Parameters in Table 4).

	OPC3			OPC			TIP3P-FB			TIP4P-FB		
	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN
Al^{3+}	-1081.3	1.88	6.0	-1081.0	1.88	6.0	-1081.1	1.88	6.0	-1080.4	1.88	6.0
Fe^{3+}	-1019.0	2.03	6.7	-1018.8	2.03	6.4	-1020.1	2.03	6.7	-1020.2	2.02	6.5
Cr^{3+}	-958.7	1.96	6.0	-956.4	1.95	6.0	-957.6	1.95	6.0	-958.1	1.96	6.0
In^{3+}	-951.4	2.16	8.0	-952.9	2.15	7.4	-950.2	2.16	8.0	-951.9	2.15	7.8
Tl^{3+}	-950.1	2.23	8.0	-949.1	2.23	8.0	-949.7	2.24	8.0	-950.3	2.24	8.0
Y^{3+}	-822.9	2.37	9.0	-823.9	2.37	8.9	-825.0	2.37	9.0	-825.7	2.36	9.0
La^{3+}	-753.0	2.51	9.0	-752.6	2.51	9.0	-750.8	2.51	9.1	-752.4	2.52	9.1
Ce^{3+}	-765.4	2.54	9.3	-765.3	2.55	9.2	-764.6	2.55	9.6	-764.2	2.55	9.5
Pr^{3+}	-775.6	2.54	9.4	-775.5	2.53	9.1	-776.0	2.55	9.7	-755.5	2.54	9.5
Nd^{3+}	-784.0	2.46	9.0	-782.2	2.47	9.0	-784.2	2.46	9.0	-785.7	2.46	9.0
Sm^{3+}	-794.8	2.44	9.0	-794.9	2.44	9.0	-795.0	2.44	9.0	-794.5	2.44	9.0
Eu^{3+}	-803.9	2.45	9.0	-802.4	2.45	9.0	-804.2	2.45	9.0	-803.3	2.45	9.0
Gd^{3+}	-807.4	2.40	9.0	-807.1	2.39	8.9	-807.4	2.39	9.0	-808.0	2.39	9.0
Tb^{3+}	-812.5	2.40	9.0	-814.2	2.4	9.0	-813.6	2.40	9.0	-813.8	2.40	9.0
Dy^{3+}	-818.1	2.38	9.0	-817.9	2.37	8.9	-818.8	2.38	9.0	-817.8	2.37	9.0
Er^{3+}	-835.0	2.37	9.0	-835.6	2.36	8.9	-835.5	2.37	9.0	-836.3	2.36	9.0
Tm^{3+}	-839.2	2.37	9.0	-841.2	2.36	9.0	-841.9	2.35	9.0	-842.0	2.36	9.0
Lu^{3+}	-839.8	2.34	8.8	-840.3	2.34	8.2	-841.5	2.35	9.0	-841.2	2.34	9.0
Hf^{4+}	-1663.2	2.15	8.0	-1664.0	2.16	8.0	-1663.7	2.15	8.0	-1664.1	2.15	8.0
Zr^{4+}	-1621.6	2.18	8.1	-1622.0	2.19	8.0	-1624.0	2.20	8.3	-1622.0	2.19	8.2
Ce^{4+}	-1462.5	2.42	10.0	-1462.8	2.41	9.9	-1463.3	2.42	10.0	-1461.2	2.42	10.0
U^{4+}	-1568.7	2.41	10.0	-1569.8	2.42	9.9	-1567.9	2.42	10.0	-1566.4	2.43	10.0
Pu^{4+}	-1521.9	2.40	9.9	-1521.3	2.38	9.0	-1519.8	2.39	9.9	-1521.4	2.39	10.0
Th^{4+}	-1388.2	2.44	10.0	-1389.8	2.45	10.0	-1390.1	2.45	10.0	-1391.2	2.45	10.0

Table S7. Performance of the Parameters Sets Developed in the Present Study in Simulating the Diffusivity Coefficients of Al^{3+} and Cr^{3+} When Used in Conjunction with the OPC Water Model

Al^{3+}		Cr^{3+}	
Parameter Set	Diffusion coefficient (10^{-5} cm^2/s)	Parameter Set	Diffusion coefficient (10^{-5} cm^2/s)
12-6 HFE	0.619±0.110	12-6 HFE	0.592±0.099
12-6 IOD	0.791±0.078	12-6 IOD	0.739±0.076
12-6-4	0.732±0.061	12-6-4	0.717±0.103
Experiment[6]	0.541	Experiment[6]	0.595

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