Supporting Information of

ADVANCES IN METAL ION MODELING

By

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Table SI.1a. The simulated HFE values of the LJ grids for the divalent cations in the TIP3P water model. The X axis is ε (kcal/mol) while the Y axis is $R_{min}/2$ (Å).[a]

	1	0.1	0.01	10^{-3}	10^{-4}	10^{-5}	10^{-6}
0.3	-502.8	-518.6	-536.1	-561.9	-585.1	-605.2	-641.3
0.4	-482.7	-508.3	-528.8	-546.6	-574.7	-593.9	-621.9
0.5	-470.1	-497.1	-517.4	-535.7	-562.8	-585.6	-606.8
0.6	-455.0	-478.8	-507.0	-528.3	-548.7	-576.5	-594.2
0.7	-448.0	-463.0	-497.7	-518.6	-537.2	-565.6	-587.0
0.8	-428.8	-452.8	-482.3	-508.9	-531.0	-553.6	-579.8
0.9	-413.2	-447.1	-465.9	-501.1	-523.0	-540.9	-570.7
1.0	-394.8	-428.9	-457.6	-488.7	-512.8	-533.7	-559.7
1.1	-379.0	-414.6	-448.1	-473.1	-504.1	-528.3	-548.4
1.2	-365.8	-397.3	-437.8	-460.0	-497.2	-518.8	-538.1
1.3	-352.7	-381.0	-421.7	-452.2	-484.6	-510.1	-532.4
1.4	-339.3	-367.0	-407.7	-445.4	-469.8	-504.1	-526.8
1.5	-325.6	-354.9	-392.4	-434.5	-458.2	-497.0	-518.8
1.6	-313.3	-342.6	-376.6	-420.7	-452.2	-484.7	-510.2
1.7	-301.5	-330.4	-364.1	-406.8	-443.9	-472.2	-504.1
1.8	-289.7	-318.1	-352.9	-393.1	-437.0	-461.7	-499.2
1.9	-278.1	-306.2	-341.0	-379.3	-423.7	-455.4	-488.6
2.0	-267.2	-294.4	-330.2	-366.4	-411.5	-444.3	-477.4
2.1	-257.9	-283.2	-318.6	-355.7	-399.1	-442.7	-464.4
2.2	-248.0	-272.8	-307.6	-345.6	-386.4	-431.0	-457.0
2.3	-239.7	-262.8	-296.7	-335.1	-374.4	-419.4	-452.4
2.4	-231.6	-252.9	-286.3	-324.1	-362.9	-408.0	-441.7
2.5	-223.8	-244.0	-275.9	-314.3	-353.3	-396.7	-440.4

a. Units of the HFE values are kcal/mol.

Table SI.1b. The simulated HFE values of the LJ grids for the divalent cations in the SPC/E water model. The X axis is ε (kcal/mol) while the Y axis is $R_{min}/2$ (Å).[a]

	1	0.1	0.01	10^{-3}	10^{-4}	10^{-5}	10^{-6}
0.3	-505.2	-521.4	-538.9	-565.5	-588.5	-608.9	-645.4
0.4	-484.7	-509.1	-531.3	-550.0	-578.3	-596.0	-625.6
0.5	-468.7	-499.9	-519.7	-538.5	-565.1	-588.6	-610.2
0.6	-456.8	-480.5	-508.5	-531.9	-551.4	-579.1	-598.1
0.7	-449.0	-464.4	-499.7	-521.9	-540.2	-568.3	-590.3
0.8	-430.3	-454.9	-484.1	-509.7	-533.3	-556.1	-582.6
0.9	-413.5	-446.7	-466.2	-503.0	-525.9	-544.0	-573.3
1.0	-394.7	-431.1	-459.9	-490.8	-515.4	-535.7	-562.9
1.1	-377.0	-414.2	-443.6	-476.0	-505.7	-530.3	-551.2
1.2	-363.7	-397.6	-439.4	-461.3	-498.8	-522.2	-541.0
1.3	-349.3	-381.0	-422.8	-454.6	-487.3	-513.7	-535.8
1.4	-336.9	-365.1	-406.8	-440.6	-472.2	-504.8	-529.5
1.5	-323.2	-352.7	-392.7	-436.3	-460.6	-498.1	-522.3
1.6	-310.0	-339.9	-377.0	-421.9	-455.1	-487.6	-513.4
1.7	-298.2	-328.5	-362.2	-408.3	-441.9	-473.6	-506.3
1.8	-285.5	-315.1	-350.5	-393.7	-436.9	-462.8	-500.5
1.9	-274.8	-302.7	-338.3	-379.9	-426.0	-458.2	-491.9
2.0	-263.2	-291.0	-327.5	-365.9	-411.6	-446.8	-480.3
2.1	-254.0	-279.9	-315.6	-353.0	-400.1	-439.1	-468.0
2.2	-244.3	-268.9	-304.0	-343.8	-387.0	-434.0	-458.8
2.3	-235.7	-258.6	-293.9	-332.2	-374.5	-420.8	-455.2
2.4	-227.7	-248.8	-282.6	-322.6	-362.3	-408.4	-445.0
2.5	-220.0	-239.8	-272.5	-311.7	-351.9	-397.2	-437.7

a. Units of the HFE values are kcal/mol.

Table SI.1c. The simulated HFE values of the LJ grids for the divalent cations in the TIP4P water model. The X axis is ε (kcal/mol) while the Y axis is $R_{min}/2$ (Å).[a]

	1	0.1	0.01	10^{-3}	10^{-4}	10^{-5}	10^{-6}
0.3	-460.8	-476.2	-490.1	-509.8	-527.9	-546.0	-588.6
0.4	-443.7	-467.7	-482.6	-497.0	-519.3	-534.9	-564.6
0.5	-435.2	-455.5	-473.1	-489.1	-509.6	-528.2	-546.9
0.6	-428.4	-439.5	-466.6	-482.8	-498.9	-520.7	-536.3
0.7	-414.0	-432.6	-455.4	-474.8	-490.7	-512.0	-529.3
0.8	-400.1	-420.3	-442.0	-467.6	-485.0	-502.1	-523.0
0.9	-384.3	-412.8	-429.9	-459.0	-477.2	-492.8	-515.9
1.0	-368.7	-398.8	-422.1	-447.4	-469.9	-487.0	-507.9
1.1	-354.9	-384.7	-416.8	-434.4	-463.6	-481.6	-498.4
1.2	-343.4	-370.6	-404.0	-426.6	-455.3	-474.6	-491.1
1.3	-331.1	-355.4	-392.3	-418.2	-444.1	-468.5	-485.7
1.4	-319.3	-343.8	-378.3	-413.7	-432.5	-462.9	-480.7
1.5	-307.7	-332.7	-365.2	-401.6	-426.4	-454.3	-474.7
1.6	-296.7	-322.7	-352.1	-389.7	-418.0	-443.8	-469.6
1.7	-285.3	-310.6	-340.4	-378.4	-413.7	-433.5	-464.0
1.8	-274.5	-299.2	-330.5	-366.0	-404.0	-425.8	-456.9
1.9	-264.6	-289.1	-320.2	-353.6	-392.5	-420.5	-448.5
2.0	-255.3	-279.0	-310.6	-342.4	-382.3	-414.7	-437.9
2.1	-246.3	-268.7	-300.3	-333.4	-371.0	-408.9	-429.3
2.2	-237.8	-259.3	-289.9	-324.4	-360.2	-399.0	-424.7
2.3	-229.8	-249.7	-279.3	-314.5	-348.9	-388.8	-418.2
2.4	-222.1	-240.7	-270.3	-304.8	-339.7	-380.1	-413.9
2.5	-215.1	-232.2	-261.3	-295.5	-330.8	-370.1	-407.3

a. Units of the HFE values are kcal/mol.

Table SI.1d. The simulated HFE values of the LJ grids for the divalent cations in the $TIP4P_{EW}$ water model. The X axis is ε (kcal/mol) while the Y axis is $R_{min}/2$ (Å).[a]

	1	0.1	0.01	10^{-3}	10^{-4}	10^{-5}	10^{-6}
0.3	-476.1	-490.9	-506.5	-527.3	-546.6	-563.7	-600.3
0.4	-458.0	-482.1	-498.8	-514.5	-538.2	-554.0	-579.7
0.5	-447.8	-470.6	-488.7	-505.3	-527.6	-547.1	-566.4
0.6	-437.0	-454.3	-481.2	-499.1	-516.3	-539.8	-555.1
0.7	-426.4	-440.7	-471.1	-490.6	-506.8	-530.5	-548.8
0.8	-410.2	-432.4	-456.5	-481.7	-500.0	-519.4	-542.3
0.9	-394.5	-425.4	-442.3	-474.6	-493.9	-510.5	-534.1
1.0	-377.3	-410.3	-435.8	-462.3	-485.1	-503.1	-525.4
1.1	-363.0	-395.7	-424.0	-448.7	-479.3	-498.0	-516.0
1.2	-349.5	-381.2	-417.4	-437.4	-470.6	-490.3	-506.9
1.3	-337.8	-364.6	-402.6	-431.4	-459.5	-483.2	-502.5
1.4	-325.6	-352.3	-389.5	-422.8	-445.3	-477.6	-498.2
1.5	-313.5	-339.8	-375.5	-413.5	-436.8	-470.1	-490.6
1.6	-300.8	-328.4	-361.4	-400.6	-430.9	-459.7	-484.3
1.7	-289.4	-316.8	-347.2	-388.9	-423.7	-447.9	-478.0
1.8	-278.1	-304.9	-338.9	-377.0	-415.9	-438.9	-471.9
1.9	-267.8	-294.0	-326.2	-363.4	-403.6	-433.6	-463.3
2.0	-258.2	-282.9	-316.3	-350.6	-394.2	-424.2	-452.6
2.1	-248.7	-272.1	-305.0	-340.6	-381.6	-421.6	-442.8
2.2	-239.6	-261.7	-294.8	-330.5	-370.4	-411.1	-435.6
2.3	-231.5	-252.3	-284.2	-320.3	-358.0	-400.8	-431.4
2.4	-223.7	-243.1	-274.3	-311.2	-346.3	-390.5	-422.5
2.5	-216.9	-234.5	-264.9	-300.9	-338.1	-380.5	-420.2

a. Units of the HFE values are kcal/mol.

Table SI.2a. The simulated IOD and CN values of the LJ grids for the divalent cations in the TIP3P water model. The X axis is ε (kcal/mol) while Y axis is $R_{min}/2$ (Å). The number before the slash is the IOD value while the one after is the CN value.[a]

	1	0.1	0.01	10^{-3}	10^{-4}	10^{-5}	10^{-6}
0.3	1.59/4.0	1.51/3.9	1.37/2.9	1.16/2.0	1.11/2.0	0.91/1.0	0.80/1.0
0.4	1.65/4.0	1.56/4.0	1.42/3.0	1.21/2.0	1.13/2.0	1.00/2.0	0.85/1.0
0.5	1.86/6.0	1.60/4.0	1.51/3.9	1.36/3.0	1.16/2.0	1.11/2.0	0.90/1.0
0.6	1.90/6.0	1.65/4.0	1.56/4.0	1.41/3.0	1.20/2.0	1.13/2.0	0.98/1.0
0.7	1.95/6.0	1.85/6.0	1.59/4.0	1.48/3.9	1.32/3.0	1.15/2.0	1.10/2.0
0.8	2.00/6.0	1.90/6.0	1.63/4.0	1.55/4.0	1.40/3.0	1.18/2.0	1.12/2.0
0.9	2.06/6.0	1.94/6.0	1.83/5.6	1.58/4.0	1.44/3.1	1.24/2.0	1.14/2.0
1.0	2.13/6.0	1.99/6.0	1.88/6.0	1.61/4.0	1.53/4.0	1.38/3.0	1.16/2.0
1.1	2.26/7.0	2.04/6.0	1.92/6.0	1.65/4.0	1.56/4.0	1.41/3.0	1.20/2.0
1.2	2.37/7.8	2.10/6.0	1.96/6.0	1.86/6.0	1.59/4.0	1.46/3.9	1.28/2.8
1.3	2.44/7.9	2.17/6.1	2.00/6.0	1.89/6.0	1.62/4.0	1.54/4.0	1.39/3.0
1.4	2.52/8.1	2.30/7.1	2.05/6.0	1.92/6.0	1.66/4.0	1.57/4.0	1.42/3.0
1.5	2.60/8.5	2.39/7.8	2.11/6.0	1.96/6.0	1.86/6.0	1.59/4.0	1.46/4.4
1.6	2.69/8.9	2.46/8.0	2.17/6.0	2.00/6.0	1.89/6.0	1.62/4.0	1.53/4.0
1.7	2.77/9.0	2.53/8.1	2.29/7.0	2.05/6.0	1.92/6.0	1.65/4.0	1.56/4.0
1.8	2.86/9.3	2.60/8.5	2.37/7.7	2.10/6.0	1.96/6.0	1.85/5.9	1.58/4.0
1.9	2.95/9.7	2.68/8.8	2.45/7.9	2.15/6.0	1.99/6.0	1.88/6.0	1.61/4.0
2.0	3.03/9.9	2.76/9.0	2.50/7.9	2.27/6.9	2.03/6.0	1.91/6.0	1.64/4.0
2.1	3.12/10.5	2.84/9.2	2.57/8.2	2.34/7.4	2.07/6.0	1.94/6.0	1.68/4.1
2.2	3.22/10.6	2.92/9.4	2.65/8.6	2.41/7.8	2.12/6.0	1.97/6.0	1.86/6.0
2.3	3.31/11.4	2.99/9.5	2.72/8.8	2.47/7.9	2.17/6.1	2.00/6.0	1.89/6.0
2.4	3.40/11.4	3.08/9.9	2.79/8.9	2.52/8.0	2.28/7.0	2.04/6.0	1.92/6.0
2.5	3.50/12.6	3.17/10.3	2.86/9.0	2.59/8.2	2.35/7.5	2.08/6.0	1.94/6.0

a. Units of the IOD values are Å.

Table SI.2b. The simulated IOD and CN values of the LJ grids for the divalent cations in the SPC/E water model. The X axis is ε (kcal/mol) while Y axis is $R_{min}/2$ (Å). The number before the slash is the IOD value while the one after is the CN value.[a]

	1	0.1	0.01	10^{-3}	10^{-4}	10^{-5}	10^{-6}
0.3	1.60/4.0	1.52/3.9	1.37/3.0	1.17/2.0	1.11/2.0	0.91/1.0	0.80/1.0
0.4	1.65/4.0	1.57/4.0	1.42/3.0	1.21/2.0	1.14/2.0	1.00/2.0	0.85/1.0
0.5	1.87/6.0	1.60/4.0	1.52/3.9	1.37/3.0	1.16/2.0	1.11/2.0	0.90/1.0
0.6	1.91/6.0	1.65/4.0	1.56/4.0	1.42/3.0	1.20/2.0	1.13/2.0	0.97/1.0
0.7	1.95/6.0	1.86/5.9	1.60/4.0	1.48/3.6	1.32/3.0	1.16/2.0	1.11/2.0
0.8	2.01/6.0	1.91/6.0	1.64/4.0	1.55/4.0	1.41/3.0	1.19/2.0	1.13/2.0
0.9	2.07/6.0	1.95/6.0	1.71/4.8	1.58/4.0	1.44/3.1	1.24/2.0	1.15/2.0
1.0	2.14/6.0	1.99/6.0	1.89/6.0	1.62/4.0	1.53/3.9	1.39/3.0	1.17/2.0
1.1	2.23/6.5	2.04/6.0	1.93/6.0	1.66/4.0	1.57/4.0	1.42/3.0	1.20/2.0
1.2	2.36/7.5	2.10/6.0	1.96/6.0	1.86/6.0	1.59/4.0	1.46/4.7	1.28/2.6
1.3	2.45/7.9	2.17/6.0	2.01/6.0	1.90/6.0	1.62/4.0	1.54/4.0	1.40/3.0
1.4	2.52/8.0	2.29/6.8	2.06/6.0	1.93/6.0	1.66/4.0	1.57/4.0	1.42/3.0
1.5	2.60/8.3	2.38/7.6	2.11/6.0	1.97/6.0	1.87/6.0	1.59/4.0	1.47/3.4
1.6	2.69/8.8	2.46/7.9	2.17/6.0	2.01/6.0	1.91/6.0	1.62/4.0	1.54/4.0
1.7	2.77/8.9	2.53/8.0	2.27/6.7	2.05/6.0	1.93/6.0	1.66/4.0	1.56/4.0
1.8	2.86/9.2	2.60/8.1	2.36/7.2	2.10/6.0	1.96/6.0	1.85/5.9	1.59/4.0
1.9	2.95/9.5	2.69/8.5	2.45/7.9	2.15/6.0	2.00/6.0	1.89/6.0	1.61/4.0
2.0	3.03/9.9	2.76/8.9	2.51/8.0	2.22/6.1	2.03/6.0	1.92/6.0	1.64/4.0
2.1	3.12/10.1	2.85/9.0	2.57/8.0	2.33/7.1	2.08/6.0	1.94/6.0	1.67/4.0
2.2	3.21/10.9	2.92/9.2	2.64/8.3	2.41/7.6	2.12/6.0	1.97/6.0	1.87/6.0
2.3	3.32/11.0	3.00/9.4	2.71/8.5	2.47/7.9	2.17/6.0	2.01/6.0	1.90/6.0
2.4	3.41/11.7	3.08/9.9	2.79/8.8	2.52/8.0	2.25/6.6	2.04/6.0	1.92/6.0
2.5	3.50/12.1	3.17/10.1	2.86/8.9	2.58/8.0	2.34/7.1	2.08/6.0	1.95/6.0

a. Units of the IOD values are Å.

Table SI.2c. The simulated IOD and CN values of the LJ grids for the divalent cations in the TIP4P water model. The X axis is ε (kcal/mol) while Y axis is $R_{min}/2$ (Å). The number before the slash is the IOD value while the one after is the CN value.[a]

	1	0.1	0.01	10^{-3}	10^{-4}	10^{-5}	10^{-6}
0.3	1.61/4.0	1.53/3.9	1.39/2.9	1.18/2.0	1.13/2.0	0.91/1.0	0.78/1.0
0.4	1.67/4.0	1.58/4.0	1.44/3.1	1.23/2.0	1.15/2.0	1.00/2.0	0.84/1.0
0.5	1.88/6.0	1.62/4.0	1.53/3.9	1.39/3.0	1.18/2.0	1.13/2.0	0.90/1.0
0.6	1.92/6.0	1.66/4.0	1.58/4.0	1.44/3.0	1.22/2.0	1.15/2.0	0.98/1.0
0.7	1.97/6.0	1.88/6.0	1.61/4.0	1.51/3.9	1.36/2.9	1.17/2.0	1.12/2.0
0.8	2.02/6.0	1.92/6.0	1.65/4.0	1.57/4.0	1.43/3.0	1.21/2.0	1.14/2.0
0.9	2.08/6.0	1.96/6.0	1.85/6.0	1.60/4.0	1.47/4.8	1.27/2.1	1.16/2.0
1.0	2.15/6.0	2.01/6.0	1.90/6.0	1.64/4.0	1.55/3.9	1.40/3.0	1.19/2.0
1.1	2.29/7.2	2.06/6.0	1.94/6.0	1.68/4.2	1.58/4.0	1.44/3.0	1.23/2.0
1.2	2.39/7.9	2.12/6.0	1.98/6.0	1.87/6.0	1.61/4.0	1.49/4.0	1.32/2.7
1.3	2.46/8.0	2.20/6.4	2.02/6.0	1.91/6.0	1.64/4.0	1.56/4.0	1.41/3.0
1.4	2.55/8.4	2.33/7.5	2.07/6.0	1.95/6.0	1.69/4.2	1.59/4.0	1.44/3.0
1.5	2.63/8.8	2.41/7.8	2.13/6.0	1.98/6.0	1.87/6.0	1.61/4.0	1.50/3.8
1.6	2.71/9.0	2.47/8.0	2.20/6.5	2.02/6.0	1.91/6.0	1.64/4.0	1.55/4.0
1.7	2.79/9.2	2.55/8.2	2.32/7.3	2.07/6.0	1.94/6.0	1.68/4.3	1.58/4.0
1.8	2.88/9.6	2.63/8.8	2.40/7.8	2.12/6.0	1.98/6.0	1.87/5.9	1.60/4.0
1.9	2.97/9.9	2.71/8.9	2.46/7.9	2.17/6.1	2.01/6.0	1.90/6.0	1.63/4.0
2.0	3.06/10.5	2.78/9.1	2.53/8.1	2.29/7.1	2.05/6.0	1.93/6.0	1.66/4.0
2.1	3.15/10.6	2.87/9.3	2.60/8.5	2.37/7.8	2.09/6.0	1.96/6.0	1.81/5.4
2.2	3.25/11.3	2.94/9.8	2.68/8.9	2.44/7.9	2.14/6.0	1.99/6.0	1.88/6.0
2.3	3.34/11.4	3.02/9.9	2.74/8.9	2.49/8.0	2.20/6.3	2.02/6.0	1.91/6.0
2.4	3.44/12.2	3.11/10.3	2.81/9.1	2.55/8.1	2.31/7.3	2.06/6.0	1.93/6.0
2.5	3.52/12.8	3.20/10.9	2.89/9.5	2.61/8.5	2.38/7.7	2.10/6.0	1.96/6.0

a. Units of the IOD values are Å.

Table SI.2d. The simulated IOD and CN values of the LJ grids for the divalent cations in the $TIP4P_{EW}$ water model. The X axis is ε (kcal/mol) while Y axis is $R_{min}/2$ (Å). The number before the slash is the IOD value while the one after is the CN value.[a]

	1	0.1	0.01	10^{-3}	10^{-4}	10^{-5}	10^{-6}
0.3	1.62/4.0	1.53/3.8	1.39/3.0	1.19/2.0	1.13/2.0	0.92/1.0	0.80/1.0
0.4	1.67/4.0	1.58/4.0	1.44/3.0	1.23/2.0	1.15/2.0	1.01/2.0	0.85/1.0
0.5	1.88/5.9	1.62/4.0	1.53/3.9	1.39/3.0	1.18/2.0	1.13/2.0	0.91/1.0
0.6	1.93/6.0	1.67/4.0	1.58/4.0	1.44/3.0	1.22/2.0	1.15/2.0	0.99/2.0
0.7	1.97/6.0	1.88/6.0	1.61/4.0	1.50/4.3	1.35/2.9	1.17/2.0	1.12/2.0
0.8	2.03/6.0	1.92/6.0	1.65/4.0	1.57/4.0	1.42/3.0	1.21/2.0	1.14/2.0
0.9	2.08/6.0	1.96/6.0	1.85/5.6	1.60/4.0	1.46/4.8	1.27/2.0	1.16/2.0
1.0	2.15/6.0	2.01/6.0	1.90/6.0	1.63/4.0	1.54/3.9	1.40/3.0	1.19/2.0
1.1	2.28/7.0	2.06/6.0	1.94/6.0	1.67/4.0	1.58/4.0	1.44/3.0	1.22/2.0
1.2	2.39/7.7	2.12/6.0	1.98/6.0	1.88/6.0	1.61/4.0	1.48/3.5	1.30/2.4
1.3	2.46/7.9	2.18/6.0	2.02/6.0	1.91/6.0	1.64/4.0	1.55/3.9	1.41/3.0
1.4	2.54/8.1	2.31/7.1	2.07/6.0	1.95/6.0	1.68/4.0	1.59/4.0	1.44/3.0
1.5	2.62/8.5	2.41/7.7	2.13/6.0	1.98/6.0	1.88/6.0	1.61/4.0	1.49/4.8
1.6	2.71/9.0	2.47/8.0	2.20/6.1	2.03/6.0	1.91/6.0	1.64/4.0	1.55/3.9
1.7	2.79/9.0	2.54/8.1	2.31/7.0	2.07/6.0	1.94/6.0	1.68/4.0	1.58/4.0
1.8	2.88/9.4	2.62/8.4	2.39/7.7	2.12/6.0	1.98/6.0	1.87/6.0	1.61/4.0
1.9	2.97/9.7	2.71/8.7	2.46/7.9	2.17/6.0	2.01/6.0	1.91/6.0	1.63/4.0
2.0	3.06/10.0	2.79/8.9	2.52/8.0	2.25/6.6	2.05/6.0	1.93/6.0	1.66/4.0
2.1	3.14/10.6	2.87/9.2	2.59/8.1	2.35/7.3	2.10/6.0	1.96/6.0	1.70/4.2
2.2	3.25/11.2	2.95/9.4	2.67/8.6	2.42/7.8	2.14/6.0	1.99/6.0	1.89/6.0
2.3	3.34/11.4	3.03/9.7	2.75/8.8	2.49/7.9	2.19/6.1	2.02/6.0	1.91/6.0
2.4	3.42/11.7	3.11/10.0	2.82/8.8	2.54/8.0	2.28/6.8	2.06/6.0	1.94/6.0
2.5	3.51/12.2	3.19/10.4	2.88/9.2	2.61/8.3	2.36/7.4	2.10/6.0	1.96/6.0

a. Units of the IOD values are Å.

Table SI.3a. The parameters and simulated HFE values from parameter space scans for monovalent cations and anions in the TIP3P water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	Positive M(I) ion without C_4 term	Positive M(I) ion with C_4 = 100 kcal/mol•Å^4	Negative M(I) ion without C_4 term	Negative M(I) ion with C_4 = -100 kcal/mol•Å^4
0.8	0.0000000113	-202.2	-489.2	-----	-----
0.9	0.00000062	-178.2	-309.9	-----	-----
1.0	0.00001423	-156.4	-237.8	-----	-----
1.1	0.00016377	-142.7	-204.0	-----	-----
1.2	0.00110429	-125.0	-172.6	-----	-----
1.3	0.00490301	-108.1	-144.2	-----	-----
1.4	0.01570749	-96.0	-126.2	-----	-----
1.5	0.03899838	-85.5	-110.7	-----	-----
1.6	0.07934493	-77.9	-99.1	-----	-----
1.7	0.13818331	-72.0	-90.9	-127.6	-107.7
1.8	0.21312875	-67.5	-84.4	-117.0	-99.4
1.9	0.29896986	-63.7	-79.0	-108.5	-92.8
2.0	0.38943250	-59.6	-74.4	-102.1	-87.5
2.1	0.47874242	-57.8	-71.0	-96.5	-83.3
2.2	0.56252208	-55.4	-67.8	-91.5	-79.4
2.3	0.63803333	-53.4	-64.7	-87.5	-76.3
2.4	0.70399643	-----	-----	-84.0	-73.1
2.5	0.76022647	-----	-----	-81.0	-70.7
2.6	0.80725180	-----	-----	-77.9	-68.3
2.7	0.84599584	-----	-----	-75.4	-66.5
2.8	0.87754630	-----	-----	-73.0	-64.3
2.9	0.90300541	-----	-----	-70.8	-62.7
3.0	0.92340323	-----	-----	-68.9	-61.5
3.1	0.93965518	-----	-----	-67.0	-59.7
3.2	0.95254766	-----	-----	-65.7	-58.4

a. Units of the HFE values are kcal/mol.

Table SI.3b. The parameters and simulated HFE values from parameter space scans for monovalent cations and anions in the SPC/E water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	Positive M(I) ion without C_4 term	Positive M(I) with C_4 = 100 kcal/mol•Å^4	Negative M(I) ion without C_4 term	Negative M(I) with C_4 = -100 kcal/mol•Å^4
0.8	0.0000000113	-203.8	-485.3	-----	-----
0.9	0.00000062	-179.0	-308.4	-----	-----
1.0	0.00001423	-156.9	-236.5	-----	-----
1.1	0.00016377	-141.6	-202.2	-----	-----
1.2	0.00110429	-124.7	-171.2	-----	-----
1.3	0.00490301	-106.9	-142.4	-----	-----
1.4	0.01570749	-93.9	-124.1	-----	-----
1.5	0.03899838	-83.5	-108.8	-----	-----
1.6	0.07934493	-76.2	-97.2	-----	-----
1.7	0.13818331	-70.5	-88.7	-133.0	-113.0
1.8	0.21312875	-65.7	-82.7	-121.4	-103.9
1.9	0.29896986	-61.9	-77.1	-112.8	-96.3
2.0	0.38943250	-58.6	-72.4	-105.0	-90.6
2.1	0.47874242	-56.0	-69.5	-99.2	-85.2
2.2	0.56252208	-53.8	-66.4	-93.7	-81.3
2.3	0.63803333	-51.9	-63.4	-89.2	-78.1
2.4	0.70399643	-----	-----	-85.4	-75.1
2.5	0.76022647	-----	-----	-81.8	-72.0
2.6	0.80725180	-----	-----	-78.8	-69.3
2.7	0.84599584	-----	-----	-75.9	-67.2
2.8	0.87754630	-----	-----	-73.7	-64.8
2.9	0.90300541	-----	-----	-71.5	-63.6
3.0	0.92340323	-----	-----	-69.2	-61.9
3.1	0.93965518	-----	-----	-67.8	-60.0
3.2	0.95254766	-----	-----	-65.5	-58.8

a. Units of the HFE values are kcal/mol.

Table SI.3c. The parameters and simulated HFE values from parameter space scans for monovalent cations and anions in the $TIP4P_{EW}$ water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	Positive M(I) ion without C_4 term	Positive M(I) ion with C_4 = 100 kcal/mol•Å^4	Negative M(I) ion without C_4 term	Negative M(I) ion with C_4 = -100 kcal/mol•Å^4
0.8	0.0000000113	-187.8	-471.1	-----	-----
0.9	0.00000062	-165.7	-290.7	-----	-----
1.0	0.00001423	-146.8	-224.8	-----	-----
1.1	0.00016377	-134.3	-193.4	-----	-----
1.2	0.00110429	-118.5	-163.9	-----	-----
1.3	0.00490301	-102.8	-137.8	-----	-----
1.4	0.01570749	-91.3	-121.2	-----	-----
1.5	0.03899838	-81.5	-106.8	-----	-----
1.6	0.07934493	-74.2	-95.7	-----	-----
1.7	0.13818331	-69.0	-88.0	-136.3	-115.8
1.8	0.21312875	-64.3	-81.2	-124.4	-106.2
1.9	0.29896986	-60.8	-76.5	-114.7	-98.5
2.0	0.38943250	-57.8	-72.2	-107.0	-92.8
2.1	0.47874242	-55.0	-68.2	-100.4	-87.3
2.2	0.56252208	-53.1	-65.7	-95.5	-83.3
2.3	0.63803333	-50.5	-62.4	-91.2	-78.8
2.4	0.70399643	-----	-----	-87.0	-76.0
2.5	0.76022647	-----	-----	-82.4	-73.0
2.6	0.80725180	-----	-----	-79.8	-70.7
2.7	0.84599584	-----	-----	-77.7	-67.8
2.8	0.87754630	-----	-----	-74.5	-66.1
2.9	0.90300541	-----	-----	-72.9	-63.8
3.0	0.92340323	-----	-----	-69.9	-63.1
3.1	0.93965518	-----	-----	-68.2	-60.8
3.2	0.95254766	-----	-----	-66.1	-59.2

a. Units of the HFE values are kcal/mol.

Table SI.4a. The parameters and simulated IOD and CN values from parameter space scans for monovalent cations and anions in the TIP3P water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	Positive M(I) ion without C_4 term	Positive M(I) ion with C_4 = 100 kcal/mol•Å^4	Negative M(I) ion without C_4 term	Negative M(I) ion with C_4 = -100 kcal/mol•Å^4
0.8	0.0000000113	0.88/1.0	0.74/1.0	-----	-----
0.9	0.00000062	1.20/2.0	1.09/2.0	-----	-----
1.0	0.00001423	1.47/3.0	1.27/2.0	-----	-----
1.1	0.00016377	1.69/4.0	1.61/4.0	-----	-----
1.2	0.00110429	1.84/4.0	1.76/4.0	-----	-----
1.3	0.00490301	2.04/4.7	2.01/5.5	-----	-----
1.4	0.01570749	2.24/5.5	2.19/6.0	-----	-----
1.5	0.03899838	2.40/5.9	2.35/6.0	-----	-----
1.6	0.07934493	2.55/6.2	2.51/6.6	-----	-----
1.7	0.13818331	2.71/6.9	2.66/7.2	2.58/6.3	2.62/6.2
1.8	0.21312875	2.85/7.9	2.82/8.2	2.73/6.7	2.77/6.6
1.9	0.29896986	2.99/8.4	2.95/9.4	2.87/7.1	2.90/6.8
2.0	0.38943250	3.11/9.4	3.09/10.3	3.00/7.2	3.03/7.1
2.1	0.47874242	3.24/10.6	3.22/11.1	3.12/8.0	3.15/7.5
2.2	0.56252208	3.37/11.9	3.34/12.1	3.24/7.7	3.26/7.7
2.3	0.63803333	3.49/16.6	3.47/15.6	3.34/8.1	3.38/7.6
2.4	0.70399643	-----	-----	3.46/8.5	3.48/8.5
2.5	0.76022647	-----	-----	3.56/9.4	3.60/7.9
2.6	0.80725180	-----	-----	3.67/10.1	3.70/8.5
2.7	0.84599584	-----	-----	3.78/10.8	3.79/8.5
2.8	0.87754630	-----	-----	3.89/10.1	3.89/10.2
2.9	0.90300541	-----	-----	3.99/13.3	4.01/11.0
3.0	0.92340323	-----	-----	4.09/12.5	4.09/10.4
3.1	0.93965518	-----	-----	4.18/15.3	4.22/12.0
3.2	0.95254766	-----	-----	4.29/15.2	4.34/13.9

a. In each data cell the value before the slash is the IOD value (unit is Å) while the value after the slash is the CN value. The cells filled with dashes means the data is unavailable from the present work.

Table SI.4b. The parameters and simulated IOD and CN values from parameter space scans for monovalent cations and anions in the SPC/E water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	Positive M(I) ion without C_4 term	Positive M(I) ion with C_4 = 100 kcal/mol•Å^4	Negative M(I) ion without C_4 term	Negative M(I) ion with C_4 = -100 kcal/mol•Å^4
0.8	0.0000000113	0.88/1.0	0.74/1.0	-----	-----
0.9	0.00000062	1.21/2.0	1.10/2.0	-----	-----
1.0	0.00001423	1.47/3.0	1.27/2.0	-----	-----
1.1	0.00016377	1.69/4.0	1.62/4.0	-----	-----
1.2	0.00110429	1.84/4.0	1.76/4.0	-----	-----
1.3	0.00490301	2.02/4.4	1.99/5.0	-----	-----
1.4	0.01570749	2.24/5.4	2.19/5.9	-----	-----
1.5	0.03899838	2.40/5.8	2.35/6.0	-----	-----
1.6	0.07934493	2.56/6.2	2.51/6.3	-----	-----
1.7	0.13818331	2.71/6.6	2.67/7.1	2.57/6.2	2.61/6.0
1.8	0.21312875	2.86/8.2	2.83/8.2	2.72/6.6	2.75/6.4
1.9	0.29896986	3.00/8.4	2.96/8.7	2.86/6.8	2.89/6.6
2.0	0.38943250	3.13/9.7	3.10/11.7	2.98/7.0	3.01/7.0
2.1	0.47874242	3.27/12.2	3.24/12.7	3.10/7.1	3.13/7.1
2.2	0.56252208	3.38/11.8	3.36/15.3	3.22/7.4	3.25/7.4
2.3	0.63803333	3.51/15.2	3.48/17.4	3.33/7.4	3.36/7.2
2.4	0.70399643	-----	-----	3.43/7.6	3.47/7.9
2.5	0.76022647	-----	-----	3.55/7.5	3.57/7.7
2.6	0.80725180	-----	-----	3.65/8.8	3.67/7.7
2.7	0.84599584	-----	-----	3.75/8.0	3.79/7.8
2.8	0.87754630	-----	-----	3.85/8.8	3.89/8.9
2.9	0.90300541	-----	-----	3.96/9.4	3.97/8.4
3.0	0.92340323	-----	-----	4.07/10.0	4.09/8.2
3.1	0.93965518	-----	-----	4.17/9.6	4.19/7.8
3.2	0.95254766	-----	-----	4.26/9.9	4.29/9.3

a. In each data cell the value before the slash is the IOD value (unit is Å) while the value after the slash is the CN value. The cells filled with dashes means the data is unavailable from the present work.

Table SI.4c. The parameters and simulated IOD and CN values from parameter space scans for monovalent cations and anions in the $TIP4P_{EW}$ water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	Positive M(I) ion without C_4 term	Positive M(I) ion with C_4 = 100 kcal/mol•Å^4	Negative M(I) ion without C_4 term	Negative M(I) ion with C_4 = -100 kcal/mol•Å^4
0.8	0.0000000113	0.89/1.0	0.74/1.0	-----	-----
0.9	0.00000062	1.22/2.0	1.11/2.0	-----	-----
1.0	0.00001423	1.49/3.1	1.29/2.0	-----	-----
1.1	0.00016377	1.71/4.0	1.63/4.0	-----	-----
1.2	0.00110429	1.86/4.0	1.78/4.0	-----	-----
1.3	0.00490301	2.07/5.0	2.04/5.6	-----	-----
1.4	0.01570749	2.26/5.7	2.21/6.0	-----	-----
1.5	0.03899838	2.42/5.9	2.37/6.0	-----	-----
1.6	0.07934493	2.58/6.3	2.53/6.6	-----	-----
1.7	0.13818331	2.73/6.7	2.69/7.1	2.57/6.1	2.60/6.0
1.8	0.21312875	2.87/7.5	2.83/8.5	2.71/6.3	2.74/6.1
1.9	0.29896986	3.01/8.3	2.97/8.6	2.85/6.6	2.88/6.3
2.0	0.38943250	3.14/9.2	3.10/9.0	2.98/6.7	3.01/6.5
2.1	0.47874242	3.27/10.3	3.24/10.9	3.10/6.9	3.13/6.7
2.2	0.56252208	3.38/9.9	3.35/11.9	3.21/6.9	3.24/7.0
2.3	0.63803333	3.50/12.0	3.48/14.2	3.32/7.4	3.35/7.1
2.4	0.70399643	-----	-----	3.44/8.0	3.46/7.3
2.5	0.76022647	-----	-----	3.53/7.7	3.57/7.5
2.6	0.80725180	-----	-----	3.65/7.7	3.67/7.2
2.7	0.84599584	-----	-----	3.75/9.5	3.77/8.4
2.8	0.87754630	-----	-----	3.84/8.8	3.87/7.8
2.9	0.90300541	-----	-----	3.94/9.9	3.97/8.1
3.0	0.92340323	-----	-----	4.06/11.7	4.08/9.9
3.1	0.93965518	-----	-----	4.15/9.6	4.18/8.2
3.2	0.95254766	-----	-----	4.26/12.1	4.27/8.4

a. In each data cell the value before the slash is the IOD value (unit is Å) while the value after the slash is the CN value. The cells filled with dashes means the data is unavailable from the present work.

Table SI.5a. The parameters and simulated HFE values from parameter space scans for trivalent and tetravalent cations in the TIP3P water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	M(III) ion without C_4 term	M(III) ion with C_4 = 500 kcal/mol•Å^4	M(IV) ion without C_4 term	M(IV) ion with C_4 = 500 kcal/mol•Å^4
0.9	0.00000062	-1138.1	-2334.2	-1833.3	-3106.5
1.0	0.00001423	-1064.4	-1805.0	-1731.3	-2526.1
1.1	0.00016377	-1015.0	-1553.2	-1663.5	-2249.9
1.2	0.00110429	-949.4	-1350.1	-1575.5	-2012.2
1.3	0.00490301	-903.2	-1228.3	-1503.6	-1868.8
1.4	0.01570749	-840.2	-1106.2	-1416.3	-1707.5
1.5	0.03899838	-798.9	-1014.8	-1359.8	-1603.5
1.6	0.07934493	-761.8	-948.4	-1303.2	-1513.4
1.7	0.13818331	-725.8	-891.9	-1246.3	-1434.3
1.8	0.21312875	-693.5	-840.2	-1205.6	-1366.4
1.9	0.29896986	-663.4	-798.7	-1166.8	-1318.9
2.0	0.38943250	-638.9	-761.1	-1130.9	-1267.5
2.1	0.47874242	-616.3	-726.5	-1089.1	-1212.2
2.2	0.56252208	-592.4	-693.4	-1049.7	-1162.3
2.3	0.63803333	-569.6	-661.6	-1013.9	-1117.9

a. Units of the HFE values are kcal/mol.

Table SI.5b. The parameters and simulated HFE values from parameter space scans for trivalent and tetravalent cations in the SPC/E water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	M(III) ion without C_4 term	M(III) ion with C_4 = 500 kcal/mol•Å^4	M(IV) ion without C_4 term	M(IV) ion with C_4 = 500 kcal/mol•Å^4
0.9	0.00000062	-1144.6	-2312.2	-1844.5	-3089.8
1.0	0.00001423	-1069.0	-1799.4	-1739.8	-2522.0
1.1	0.00016377	-1019.4	-1547.0	-1671.7	-2248.7
1.2	0.00110429	-955.9	-1346.8	-1585.1	-2012.7
1.3	0.00490301	-908.6	-1227.5	-1508.3	-1870.9
1.4	0.01570749	-844.7	-1106.6	-1424.0	-1710.9
1.5	0.03899838	-800.0	-1012.6	-1362.0	-1600.8
1.6	0.07934493	-761.0	-945.6	-1305.8	-1513.5
1.7	0.13818331	-724.8	-889.5	-1249.7	-1432.6
1.8	0.21312875	-692.1	-835.9	-1200.7	-1366.6
1.9	0.29896986	-661.3	-792.0	-1167.0	-1317.8
2.0	0.38943250	-635.9	-759.2	-1122.4	-1266.5
2.1	0.47874242	-612.3	-721.8	-1090.2	-1212.9
2.2	0.56252208	-587.0	-689.0	-1049.1	-1160.9
2.3	0.63803333	-565.8	-657.1	-1011.9	-1115.0

a. Units of the HFE values are kcal/mol.

Table SI.5c. The parameters and simulated HFE values from parameter space scans for trivalent and tetravalent cations in the $TIP4P_{EW}$ water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	M(III) ion without C_4 term	M(III) ion with C_4 = 500 kcal/mol•Å^4	M(IV) ion without C_4 term	M(IV) ion with C_4 = 500 kcal/mol•Å^4
0.9	0.00000062	-1068.5	-2196.5	-1726.6	-2921.2
1.0	0.00001423	-1004.8	-1710.8	-1641.4	-2393.8
1.1	0.00016377	-964.0	-1472.4	-1581.2	-2137.2
1.2	0.00110429	-905.0	-1287.2	-1504.4	-1920.8
1.3	0.00490301	-863.6	-1175.8	-1438.8	-1786.4
1.4	0.01570749	-806.4	-1061.8	-1360.3	-1637.7
1.5	0.03899838	-767.5	-975.2	-1305.3	-1540.5
1.6	0.07934493	-732.5	-913.6	-1254.5	-1457.3
1.7	0.13818331	-699.7	-859.1	-1202.2	-1380.7
1.8	0.21312875	-668.9	-810.3	-1164.9	-1318.9
1.9	0.29896986	-641.0	-770.3	-1128.8	-1274.5
2.0	0.38943250	-615.6	-736.3	-1087.0	-1226.2
2.1	0.47874242	-595.1	-703.4	-1054.0	-1174.5
2.2	0.56252208	-573.0	-671.3	-1015.7	-1127.2
2.3	0.63803333	-550.6	-641.6	-981.2	-1083.2

a. Units of the HFE values are kcal/mol.

Table SI.6a. The parameters and simulated IOD and CN values from parameter space scans for trivalent and tetravalent cations and anions in the TIP3P water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	M(III) ion without C_4 term	M(III) ion with C_4 = 500 kcal/mol•Å^4	M(IV) ion without C_4 term	M(IV) ion with C_4 = 500 kcal/mol•Å^4
0.9	0.00000062	1.09/2.0	0.92/2.0	1.06/2.0	0.92/2.0
1.0	0.00001423	1.34/3.0	1.07/2.0	1.31/3.0	1.06/2.0
1.1	0.00016377	1.52/4.0	1.39/4.0	1.47/4.0	1.37/4.0
1.2	0.00110429	1.79/6.0	1.51/4.0	1.74/6.0	1.49/4.0
1.3	0.00490301	1.88/6.0	1.77/6.0	1.82/6.0	1.74/6.0
1.4	0.01570749	1.99/6.0	1.89/6.0	1.99/9.0	1.85/6.0
1.5	0.03899838	2.23/8.0	2.14/8.0	2.17/8.0	2.10/8.0
1.6	0.07934493	2.36/9.0	2.25/8.4	2.29/8.9	2.21/9.9
1.7	0.13818331	2.47/9.0	2.39/9.0	2.41/9.9	2.33/9.0
1.8	0.21312875	2.61/10.0	2.53/10.0	2.62/12.0	2.56/12.0
1.9	0.29896986	2.77/11.8	2.70/12.0	2.69/12.0	2.63/12.0
2.0	0.38943250	2.86/12.0	2.79/12.0	2.77/12.0	2.71/12.0
2.1	0.47874242	2.95/12.0	2.88/12.0	2.85/12.0	2.80/12.0
2.2	0.56252208	3.04/12.0	2.97/12.0	2.93/12.0	2.88/12.0
2.3	0.63803333	3.13/12.0	3.06/12.0	3.08/13.7	3.03/13.8

a. In each data cell the value before the slash is the IOD value (unit is Å) while the value after the slash is the CN value.

Table SI.6b. The parameters and simulated IOD and CN values from parameter space scans for trivalent and tetravalent cations and anions in the SPC/E water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	M(III) ion without C_4 term	M(III) ion with C_4 = 500 kcal/mol•Å^4	M(IV) ion without C_4 term	M(IV) ion with C_4 = 500 kcal/mol•Å^4
0.9	0.00000062	1.09/2.0	0.93/2.0	1.06/2.0	0.93/2.0
1.0	0.00001423	1.35/3.0	1.07/2.0	1.32/3.0	1.06/2.0
1.1	0.00016377	1.52/4.0	1.40/4.0	1.48/4.0	1.38/4.0
1.2	0.00110429	1.80/6.0	1.52/4.0	1.75/6.0	1.50/4.0
1.3	0.00490301	1.88/6.0	1.78/6.0	1.83/6.0	1.74/6.0
1.4	0.01570749	1.99/6.0	1.90/6.0	1.99/8.8	1.86/6.0
1.5	0.03899838	2.23/8.0	2.15/8.0	2.17/8.0	2.10/8.0
1.6	0.07934493	2.36/8.9	2.26/9.2	2.29/9.0	2.21/9.9
1.7	0.13818331	2.48/9.0	2.40/9.0	2.41/9.3	2.34/9.0
1.8	0.21312875	2.61/9.8	2.54/10.0	2.53/10.0	2.48/10.0
1.9	0.29896986	2.74/10.7	2.67/10.9	2.70/12.0	2.64/12.0
2.0	0.38943250	2.87/12.0	2.80/12.0	2.78/12.0	2.72/12.0
2.1	0.47874242	2.96/12.0	2.89/12.0	2.86/12.0	2.80/12.0
2.2	0.56252208	3.04/12.0	2.98/12.0	2.94/12.0	2.89/12.0
2.3	0.63803333	3.13/12.0	3.07/12.0	3.04/12.3	2.98/12.2

a. In each data cell the value before the slash is the IOD value (unit is Å) while the value after the slash is the CN value.

Table SI.6c. The parameters and simulated IOD and CN values from parameter space scans for trivalent and tetravalent cations and anions in the $TIP4P_{EW}$ water model.[a]

$R_{min}/2$ (Å)	ε (kcal/mol)	M(III) ion without C_4 term	M(III) ion with C_4 = 500 kcal/mol•Å^4	M(IV) ion without C_4 term	M(IV) ion with C_4 = 500 kcal/mol•Å^4
0.9	0.00000062	1.11/2.0	0.94/2.0	1.08/2.0	0.93/2.0
1.0	0.00001423	1.37/3.0	1.08/2.0	1.33/3.0	1.07/2.0
1.1	0.00016377	1.54/4.0	1.41/4.0	1.50/4.0	1.39/4.0
1.2	0.00110429	1.82/6.0	1.53/4.0	1.77/6.0	1.51/4.0
1.3	0.00490301	1.90/6.0	1.79/6.0	1.84/6.0	1.76/6.0
1.4	0.01570749	2.01/6.0	1.91/6.0	2.02/9.0	1.87/6.0
1.5	0.03899838	2.25/8.0	2.16/8.0	2.19/8.0	2.12/8.0
1.6	0.07934493	2.38/9.0	2.28/8.4	2.31/9.0	2.23/9.9
1.7	0.13818331	2.49/9.0	2.41/9.0	2.43/9.8	2.35/9.0
1.8	0.21312875	2.63/10.0	2.55/10.0	2.64/12.0	2.58/12.0
1.9	0.29896986	2.74/10.6	2.73/12.0	2.71/12.0	2.66/12.0
2.0	0.38943250	2.89/12.0	2.81/12.0	2.79/12.0	2.73/12.0
2.1	0.47874242	2.97/12.0	2.90/12.0	2.87/12.0	2.82/12.0
2.2	0.56252208	3.06/12.0	2.99/12.0	2.96/12.0	2.91/12.0
2.3	0.63803333	3.15/12.0	3.08/12.0	3.09/13.3	3.05/13.7

a. In each data cell the value before the slash is the IOD value (unit is Å) while the value after the slash is the CN value.

Table SI.7. VDW Radii ($R_{min}/2$ values, in Å) of different parameter sets and their statistical analysis against the QMSP calculated values by Stokes[1] (see Table 23 in the main text). All the parameter sets were adopted using the Lorentz-Berthelot combining rules. Related water parameters are shown in Table 4 in the main text.

Year	1990	1992-2002	2006	2006	2008			2009		
Parameter set	Former AMBER FF (adapted from Åqvist[a])	Dang	JJ[i]	LR[j]	JC-TIP3P[k]	JC-SPC/E[k]	JC-TIP4P$_{EW}$[k]	HMN-5[l]	HMN-5a[l]	HMN-5b[l]
Na^+	1.868	1.319[b]/ 1.450[c]/ 1.275[d]	2.251	1.450	1.369	1.212	1.226	2.141	1.198	1.254
K^+	2.658	1.870[c]/ 1.770[e]	2.762	1.645	1.705	1.593	1.590	2.545	1.557	1.624
Rb^+	2.956	1.980[c]	2.947	1.750	1.813	1.737	1.709	---	---	---
Cs^+	3.395	2.180[c,f]	3.193	1.980	1.976	2.021	1.888	2.904	1.871	1.927
F^-	---	1.778[g]	1.711	2.260	2.303	2.257	2.538	1.927	1.927	1.927
Cl^-	---	2.497[b]/ 2.470[c,f]/ 2.435[d]	2.227	2.460	2.513	2.711	2.760	2.466	2.466	2.466
Br^-	---	2.550[d]	2.354	2.570	2.608	2.751	2.768	2.713	2.713	2.713
I^-	---	2.900[h]/ 2.876[d]	2.602	2.760	2.860	2.919	2.952	2.994	2.994	2.994
Average Error	1.014	0.150	0.527	0.131	0.165	0.172	0.200	0.523	0.100	0.125
Standard Deviation	0.372	0.144	0.605	0.152	0.170	0.259	0.329	0.344	0.258	0.232
UAE	1.014	0.184	0.583	0.154	0.170	0.242	0.302	0.523	0.212	0.187

a. From Åqvist.[2] b. From Smith and Dang.[3] c. From Dang.[4] d. From Dang.[5] e. From Chang and Dang.[6] f. From Dang.[7] g. From Dang.[8] h. From Dang and Garrett.[9] i. From Jesen and Jorgensen.[10] j From Lamoureux and Roux.[11] k .From Joung and Cheatham.[12] l. From Horinek *et al.*[13]

Table SI.7 (cont'd)

Year	2010	2012 /2014	2012	Present Work						
Parameter set	YWHL VAMR[m]	DVH[n]/ RDVH[o]	PCSN D[p]	HFE-TIP3P	HFE-SPC/E	HFE-TIP4P$_{EW}$	IOD	12-6-4-TIP3P	12-6-4-SPC/E	12-6-4-TIP4P$_{EW}$
Na^+	1.462	1.061	1.285	1.475	1.454	1.432	1.465	1.473	1.472	1.459
K^+	1.687	1.555	1.650	1.719	1.683	1.669	1.745	1.758	1.760	1.751
Rb^+	1.786	1.830	1.820	1.834	1.792	1.767	1.820	1.831	1.826	1.817
Cs^+	2.024	2.009	1.928	1.988	1.953	1.936	2.000	2.008	2.004	1.997
F^-	2.462	2.054	2.050	1.783	1.819	1.842	1.739	1.725	1.726	1.728
Cl^-	2.481	2.475	2.590	2.252	2.308	2.321	2.162	2.150	2.153	2.154
Br^-	2.626	2.548	2.720	2.428	2.470	2.520	2.331	2.314	2.324	2.326
I^-	2.758	2.683	2.950	2.724	2.770	2.819	2.590	2.567	2.579	2.585
Average Error	0.182	0.048	0.146	0.047	0.053	0.060	0.003	0.000	0.002	-0.001
Standard Deviation	0.192	0.182	0.212	0.096	0.107	0.128	0.091	0.099	0.098	0.095
UAE	0.186	0.150	0.185	0.081	0.088	0.101	0.068	0.071	0.073	0.068

m. From Yu *et al.*[14] n. From Deublein *et al.*[15] o. From Reiser *et al.*[16] p. From Peng *et al.*[17]

Table SI.8. VDW parameters of the H2 parameter set (adopted from set 5b of Horinek *et al.*[13] using the Lorentz-Berthelot combining rules).

Ions	$R_{min}/2$ (Å)	ε (kcal/mol)
Li^+	0.771	1.53899379
Na^+	1.198	1.53899379
K^+	1.557	1.53899379
Cs^+	1.871	1.53899379
F^-	1.927	0.46554562
Cl^-	2.466	0.41614392
Br^-	2.713	0.21068825
I^-	2.994	0.15759296

Table SI.9a. Percentage errors for the three parameter sets of monovalent ions against the target HFEs.[a]

	TIP3P	SPC/E	$TIP4P_{EW}$
Li^+	-0.4%(-6.6%)[-0.1%]	0.0%(-8.0%)[-0.3%]	0.4%(-11.2%)[-0.5%]
Na^+	1.1%(1.8%)[1.1%]	0.8%(-0.2%)[1.1%]	0.9%(-2.3%)[0.8%]
K^+	1.0%(-1.0%)[-0.1%]	0.3%(-3.8%)[0.0%]	0.4%(-5.7%)[0.0%]
Rb^+	0.3%(1.1%)[0.5%]	0.6%(-1.1%)[0.3%]	0.2%(-2.3%)[0.0%]
Cs^+	1.2%(0.8%)[0.7%]	0.7%(-1.5%)[1.0%]	0.0%(-4.5%)[0.8%]
Tl^+	0.4%(-9.8%)[-0.4%]	-0.3%(-12.0%)[-0.4%]	0.0%(-13.4%)[-0.1%]
Cu^+	-0.1%(-2.2%)[-0.4%]	0.5%(-2.8%)[-0.4%]	0.0%(-7.6%)[-0.8%]
Ag^+	-0.1%(-16.5%)[-0.8%]	-0.2%(-18.7%)[0.0%]	0.4%(-20.4%)[-0.6%]
NH_4^+	0.4%(-0.4%)[-0.4%]	-0.1%(-3.1%)[-0.3%]	1.0%(-4.8%)[0.4%]
H^+ (Zundel cation)	--(-31.4%)[0.0%]	--(-31.1%)[0.3%]	--(-35.9%)[-0.1%]
H^+ (Eigen cation)	--(-24.8%)[0.1%]	--(-24.5%)[0.1%]	--(-30.3%)[-0.2%]
H_3O^+	-0.1%(-31.3%)[-0.6%]	-0.6%(-32.8%)[0.8%]	0.2%(-33.7%)[-0.1%]
F^-	-0.5%(3.3%)[-0.3%]	0.0%(7.4%)[0.1%]	0.4%(9.6%)[-0.2%]
Cl^-	0.4%(4.8%)[0.0%]	0.0%(7.3%)[-0.7%]	0.4%(9.2%)[0.3%]
Br^-	0.5%(4.6%)[-0.1%]	0.4%(6.2%)[-0.7%]	-0.4%(7.9%)[-1.1%]
I^-	0.8%(5.5%)[0.3%]	0.3%(5.9%)[0.5%]	0.0%(8.3%)[-0.3%]
Average Value	0.4%(-6.4%)[0.0%]	0.2%(-7.1%)[0.1%]	0.3%(-8.6%)[-0.1%]
Standard Deviation	0.5%(12.7%)[0.5%]	0.4%(13.2%)[0.6%]	0.4%(14.9%)[0.5%]
UAE	0.5%(9.1%)[0.4%]	0.3%(10.4%)[0.4%]	0.3%(12.9%)[0.4%]

a. The first value in each cell is the percentage error for the HFE parameter set, the values in brackets are the percentage errors for the IOD parameter set while the values in the square brackets are the percentage errors for the 12-6-4 parameter set (which is introduced in the section 3 of the main text). There are no entries for some values because there are no corresponding parameters.

Table SI.9b. Percentage errors for the three parameter sets of monolvanet ions against the target IODs.[a]

	TIP3P	SPC/E	$TIP4P_{EW}$
Li^+	-6.3%(0.0%)[0.5%]	-6.7%(-0.5%)[0.5%]	-8.7%(1.4%)[0.5%]
Na^+	0.4%(0.0%)[0.4%]	-0.9%(0.0%)[0.0%]	-1.3%(0.9%)[0.0%]
K^+	-2.2%(-0.4%)[-0.4%]	-3.6%(-0.4%)[0.0%]	-3.9%(0.4%)[0.0%]
Rb^+	0.3%(-0.3%)[0.3%]	-1.4%(0.0%)[0.0%]	-2.1%(0.3%)[0.0%]
Cs^+	-1.0%(-0.3%)[0.0%]	-1.3%(0.0%)[0.3%]	-2.6%(0.0%)[0.0%]
Tl^+	-8.1%(-0.3%)[0.0%]	-9.8%(0.0%)[0.3%]	-10.5%(0.3%)[0.0%]
Cu^+	-1.6%(-0.5%)[-0.5%]	-2.1%(-0.5%)[-0.5%]	-27.8%(0.5%)[-0.5%]
Ag^+	-11.2%(-0.4%)[0.0%]	-12.9%(-0.4%)[0.0%]	-14.9%(0.4%)[0.0%]
NH_4^+	-1.1%(-0.4%)[0.4%]	-2.8%(-0.4%)[0.0%]	-3.9%(0.4%)[0.4%]
H^+ (Zundel cation)	--(-0.8%)[0.0%]	--(0.0%)[-0.8%]	--(0.8%)[0.8%]
H^+ (Eigen cation)	--(0.0%)[0.0%]	--(0.0%)[0.0%]	--(1.0%)[1.0%]
H_3O^+	-22.5%(-0.4%)[0.0%]	-23.6%(-0.4%)[0.0%]	-25.5%(0.4%)[0.0%]
F^-	3.0%(0.4%)[0.0%]	4.2%(0.0%)[0.0%]	5.3%(-0.4%)[0.0%]
Cl^-	3.8%(0.3%)[0.0%]	5.0%(0.0%)[0.0%]	5.3%(-0.3%)[0.0%]
Br^-	3.3%(0.0%)[0.0%]	4.5%(-0.3%)[0.0%]	5.6%(-0.3%)[0.0%]
I^-	4.1%(0.5%)[0.0%]	4.7%(-0.3%)[0.0%]	6.3%(-0.3%)[0.0%]
Average Value	-2.8%(-0.2%)[0.0%]	-3.3%(-0.2%)[0.0%]	-5.6%(0.3%)[0.1%]
Standard Deviation	7.3%(0.4%)[0.3%]	8.0%(0.2%)[0.3%]	11.0%(0.5%)[0.4%]
UAE	4.9%(0.3%)[0.2%]	6.0%(0.2%)[0.2%]	8.8%(0.5%)[0.2%]

a. The first value in each cell is the percentage error for the HFE parameter set, the values in brackets are the percentage errors for the IOD parameter set while the values in the square brackets are the percentage errors for the 12-6-4 parameter set (which is introduced in the section 3 of the main text). There are no entries for some values because there are no corresponding parameters.

Table SI.10a. Percent errors for the three parameter sets of divalent cations towards the target HFEs.[a]

	TIP3P	SPCE	$TIP4P_{EW}$	TIP4P
Be^{2+}	0.0%(-4.4%)[-17.9%]	-0.2%(-4.4%)[-17.5%]	0.1%(-7.0%)[-21.9%]	--(--)[-24.0%]
Cu^{2+}	0.2%(-5.3%)[-17.7%]	0.2%(-5.4%)[-17.7%]	0.1%(-8.4%)[-21.2%]	--(--)[-23.3%]
Ni^{2+}	0.0%(-5.3%)[-13.9%]	0.0%(-5.2%)[-13.7%]	-0.2%(-8.6%)[-17.5%]	--(--)[-19.5%]
Pt^{2+}	-0.1%(-5.3%)[--]	0.0%(-5.3%)[--]	-0.1%(-8.7%)[--]	--(--)[--]
Zn^{2+}	0.0%(-5.4%)[-14.4%]	0.0%(-5.5%)[-14.4%]	0.0%(-8.5%)[-18.3%]	--(--)[-20.1%]
Co^{2+}	-0.2%(-5.4%)[-13.3%]	-0.2%(-5.6%)[-13.2%]	0.2%(-8.9%)[-17.1%]	--(--)[-19.0%]
Pd^{2+}	0.1%(-5.5%)[--]	0.1%(-5.3%)[--]	-0.1%(-8.7%)[--]	--(--)[--]
Ag^{2+}	-0.2%(-5.6%)[--]	0.1%(-5.7%)[--]	-0.1%(-9.1%)[--]	--(--)[--]
Cr^{2+}	-0.1%(-5.6%)[-8.9%]	-0.1%(-5.7%)[-8.8%]	0.0%(-8.8%)[-12.9%]	--(--)[-15.0%]
Fe^{2+}	-0.1%(-5.7%)[-10.2%]	-0.1%(-5.6%)[-10.1%]	0.1%(-9.0%)[-14.0%]	--(--)[-16.0%]
Mg^{2+}	0.1%(-5.8%)[-8.5%]	0.0%(-5.6%)[-8.4%]	-0.2%(-9.4%)[-12.5%]	--(--)[-14.5%]
V^{2+}	-0.1%(-5.8%)[-14.5%]	-0.1%(-5.7%)[-14.7%]	-0.1%(-9.3%)[-18.3%]	--(--)[-19.9%]
Mn^{2+}	-0.2%(-5.8%)[-10.7%]	0.0%(-5.8%)[-10.8%]	-0.2%(-9.5%)[-14.5%]	--(--)[-16.4%]
Hg^{2+}	-0.2%(-5.8%)[-16.8%]	0.0%(-5.8%)[-17.7%]	-0.2%(-9.5%)[-20.3%]	--(--)[-21.7%]
Cd^{2+}	0.1%(-6.2%)[-12.8%]	-0.1%(-6.0%)[-13.3%]	0.0%(-9.7%)[-16.7%]	--(--)[-18.2%]
Yb^{2+}	-0.2%(-7.0%)[--]	-0.2%(-7.1%)[--]	0.1%(-11.3%)[--]	--(--)[--]
Ca^{2+}	0.1%(-7.0%)[-4.8%]	0.3%(-7.0%)[-5.3%]	0.0%(-11.3%)[-8.5%]	--(--)[-10.1%]
Sn^{2+}	0.1%(-7.0%)[-10.8%]	0.1%(-6.9%)[-11.6%]	0.0%(-11.1%)[-14.3%]	--(--)[-15.8%]
Pb^{2+}	0.1%(-7.2%)[--]	-0.1%(-7.3%)[--]	-0.3%(-11.5%)[--]	--(--)[--]
Eu^{2+}	0.1%(-7.6%)[--]	0.0%(-7.8%)[--]	0.0%(-12.2%)[--]	--(--)[--]
Sr^{2+}	0.0%(-7.6%)[-4.7%]	0.2%(-7.7%)[-5.5%]	-0.1%(-12.2%)[-8.5%]	--(--)[-9.7%]
Sm^{2+}	-0.1%(-7.8%)[--]	0.0%(-7.9%)[--]	0.1%(-12.3%)[--]	--(--)[--]
Ba^{2+}	0.2%(-8.6%)[-3.5%]	0.1%(-8.1%)[-4.6%]	0.1%(-13.5%)[-7.3%]	--(--)[-8.5%]
Ra^{2+}	0.2%(-8.6%)[--]	0.1%(-8.1%)[--]	0.1%(-13.5%)[--]	--(--)[--]
Average Value	0.0%(-6.3%)[-11.5%]	0.0%(-6.3%)[-11.7%]	0.0%(-10.1%)[-15.2%]	--(--)[-17.0%]
Standard Deviation	0.1%(1.1%)[4.5%]	0.1%(1.1%)[4.3%]	0.1%(1.8%)[4.5%]	--(--)[4.7%]

a. The first values in the cells are for the HFE parameter set, the values in parentheses are for the CM parameter set while the ones in square brackets are for the IOD parameter set. Some values are shown as dashes because we did not design IOD parameter set for some M(II) metal ions due to lack of the corresponding experimental values and we only designed the IOD parameter set for the TIP4P water model.

Table SI.10b. Percent errors for the three parameter sets of divalent cations towards the target IODs.[a]

	TIP3P	SPCE	$TIP4P_{EW}$	TIP4P
Be^{2+}	-31.7%(-27.5%)[-0.6%]	-31.1%(-26.9%)[-0.6%]	-47.9%(-29.9%)[0.6%]	---(---)[0.6%]
Cu^{2+}	-22.7%(-10.9%)[-0.5%]	-22.3%(-10.0%)[-0.5%]	-25.6%(-10.9%)[0.5%]	---(---)[0.0%]
Ni^{2+}	-19.9%(-6.8%)[-0.5%]	-19.4%(-6.8%)[-0.5%]	-22.3%(-7.3%)[0.5%]	---(---)[0.5%]
Zn^{2+}	-20.1%(-7.7%)[-0.5%]	-19.6%(-6.7%)[-0.5%]	-23.0%(-7.2%)[0.5%]	---(---)[0.5%]
Co^{2+}	-11.0%(-6.7%)[-0.5%]	-10.0%(-5.7%)[-0.5%]	-21.9%(-6.2%)[0.5%]	---(---)[0.5%]
Cr^{2+}	-6.7%(-2.9%)[-0.5%]	-6.3%(-2.4%)[-0.5%]	-11.5%(-2.9%)[0.5%]	---(---)[0.5%]
Fe^{2+}	-8.1%(-4.3%)[-0.5%]	-7.1%(-3.8%)[-0.5%]	-10.9%(-3.8%)[0.5%]	---(---)[0.0%]
Mg^{2+}	-6.7%(-2.9%)[-0.5%]	-6.2%(-2.4%)[-0.5%]	-9.6%(-1.9%)[0.5%]	---(---)[0.0%]
V^{2+}	-11.8%(-7.7%)[0.0%]	-11.3%(-7.2%)[-0.9%]	-14.0%(-7.2%)[0.5%]	---(---)[2.3%]
Mn^{2+}	-8.2%(-4.6%)[-0.5%]	-8.2%(-4.1%)[-0.5%]	-10.5%(-3.7%)[0.5%]	---(---)[1.4%]
Hg^{2+}	-16.6%(-13.3%)[0.0%]	-16.6%(-12.9%)[-0.4%]	-18.7%(-12.4%)[0.4%]	---(---)[0.4%]
Cd^{2+}	-12.6%(-8.7%)[-0.4%]	-12.2%(-8.7%)[-0.9%]	-14.8%(-8.3%)[0.4%]	---(---)[0.4%]
Ca^{2+}	-5.3%(1.2%)[-0.4%]	-6.1%(0.8%)[-0.4%]	-10.6%(2.8%)[0.4%]	---(---)[0.0%]
Sn^{2+}	-9.9%(-4.2%)[-0.4%]	-11.1%(-4.6%)[-0.4%]	-14.9%(-3.1%)[0.4%]	---(---)[0.4%]
Sr^{2+}	-4.5%(2.3%)[-0.4%]	-4.9%(1.5%)[-0.8%]	-6.8%(3.8%)[0.4%]	---(---)[0.4%]
Ba^{2+}	-3.2%(3.9%)[-0.4%]	-3.9%(2.5%)[-0.4%]	-5.7%(6.0%)[0.4%]	---(---)[0.4%]
Average Value	-12.4%(-6.3%)[-0.4%]	-12.3%(-6.1%)[-0.6%]	-16.8%(-5.8%)[0.5%]	---(---)[0.5%]
Standard Deviation	7.8%(7.3%)[0.2%]	7.6%(6.9%)[0.2%]	10.2%(8.2%)[0.1%]	---(---)[0.6%]

a. The first values in the cells are for the HFE parameter set, the values in parentheses are for the CM parameter set while the ones in square brackets are for the IOD parameter set. Because of limited experimental values, only 16 M(II) cations are shown in the table. Some values are shown as dashes because we only designed the IOD parameter set for the TIP4P water model.

Table SI.11. The estimated errors and estimated percent errors for the 12-6 HFE and IOD parameter sets of the trivalent and tetravalent ions.[a]

	TIP3P		SPC/E		$TIP4P_{EW}$	
	HFE set	IOD set	HFE set	IOD set	HFE set	IOD set
Al^{3+}	-0.59(-31.4%)	180.9(-16.7%)	-0.57(-30.3%)	177.0(-16.4%)	-0.78(-41.5%)	216.5(-20.0%)
Fe^{3+}	-0.54(-26.6%)	163.0(-16.0%)	-0.52(-25.6%)	160.3(-15.7%)	-0.71(-35.0%)	194.9(-19.1%)
Cr^{3+}	-0.27(-13.8%)	81.5(-8.5%)	-0.26(-13.3%)	78.0(-8.1%)	-0.42(-21.4%)	115.3(-12.0%)
In^{3+}	-0.44(-20.5%)	129.6(-13.6%)	-0.42(-19.5%)	127.6(-13.4%)	-0.58(-27.0%)	158.5(-16.7%)
Tl^{3+}	-0.51(-22.9%)	150.2(-15.8%)	-0.50(-22.4%)	148.6(-15.7%)	-0.66(-29.6%)	177.3(-18.7%)
Y^{3+}	-0.22(-9.3%)	62.7(-7.6%)	-0.21(-8.9%)	62.0(-7.5%)	-0.33(-14.0%)	86.6(-10.5%)
La^{3+}	-0.12(-4.8%)	33.3(-4.4%)	-0.12(-4.8%)	33.6(-4.5%)	-0.21(-8.3%)	54.7(-7.3%)
Ce^{3+}	-0.20(-7.8%)	54.4(-7.1%)	-0.20(-7.8%)	54.9(-7.2%)	-0.29(-11.4%)	75.0(-9.8%)
Pr^{3+}	-0.23(-9.1%)	62.5(-8.1%)	-0.22(-8.7%)	63.2(-8.1%)	-0.33(-13.0%)	83.5(-10.8%)
Nd^{3+}	-0.19(-7.7%)	52.2(-6.7%)	-0.18(-7.3%)	52.1(-6.6%)	-0.29(-11.7%)	74.0(-9.4%)
Sm^{3+}	-0.20(-8.2%)	54.8(-6.9%)	-0.19(-7.8%)	54.6(-6.9%)	-0.30(-12.3%)	77.2(-9.7%)
Eu^{3+}	-0.24(-9.8%)	65.8(-8.2%)	-0.23(-9.4%)	65.6(-8.2%)	-0.34(-13.9%)	88.4(-11.0%)
Gd^{3+}	-0.19(-7.9%)	53.0(-6.6%)	-0.18(-7.5%)	52.4(-6.5%)	-0.29(-12.1%)	76.6(-9.5%)
Tb^{3+}	-0.22(-9.2%)	61.7(-7.6%)	-0.21(-8.8%)	61.2(-7.5%)	-0.32(-13.3%)	85.2(-10.5%)
Dy^{3+}	-0.21(-8.9%)	59.5(-7.3%)	-0.20(-8.4%)	58.8(-7.2%)	-0.32(-13.5%)	83.2(-10.2%)
Er^{3+}	-0.26(-11.0%)	73.4(-8.8%)	-0.25(-10.6%)	72.7(-8.7%)	-0.37(-15.7%)	97.3(-11.6%)
Tm^{3+}	-0.27(-11.4%)	78.2(-9.3%)	-0.26(-11.0%)	77.5(-9.2%)	-0.39(-16.5%)	102.1(-12.2%)
Lu^{3+}	-0.25(-10.7%)	72.6(-8.6%)	-0.24(-10.3%)	71.7(-8.5%)	-0.37(-15.8%)	97.3(-11.6%)
Average Value	-0.29(-12.8%)	82.7(-9.3%)	-0.28(-12.4%)	81.8(-9.2%)	-0.41(-18.1%)	108.0(-12.3%)
Standard Deviation	0.14(7.4%)	42.7(3.6%)	0.13(7.2%)	41.6(3.5%)	0.16(9.2%)	46.4(3.7%)
Hf^{4+}	-0.70(-32.4%)	297.7(-17.9%)	-0.67(-31.0%)	296.1(-17.8%)	-0.89(-41.2%)	342.1(-20.6%)
Zr^{4+}	-0.63(-28.8%)	268.2(-16.5%)	-0.61(-27.9%)	266.7(-16.4%)	-0.81(-37.0%)	311.5(-19.2%)
Ce^{4+}	-0.49(-20.2%)	202.4(-13.8%)	-0.48(-19.8%)	204.1(-14.0%)	-0.63(-26.0%)	238.6(-16.3%)
U^{4+}	-0.73(-30.2%)	307.6(-19.6%)	-0.72(-29.8%)	309.3(-19.7%)	-0.90(-37.2%)	343.8(-21.9%)
Pu^{4+}	-0.59(-24.7%)	248.0(-16.3%)	-0.58(-24.3%)	249.0(-16.4%)	-0.75(-31.4%)	284.9(-18.7%)
Th^{4+}	-0.34(-13.9%)	142.1(-10.2%)	-0.34(-13.9%)	143.9(-10.4%)	-0.47(-19.2%)	177.0(-12.7%)
Average Value	-0.58(-25.0%)	244.3(-15.7%)	-0.57(-24.5%)	244.9(-15.8%)	-0.74(-32.0%)	283.0(-18.2%)
Standard Deviation	0.15(7.0%)	62.7(3.3%)	0.14(6.6%)	61.8(3.2%)	0.17(8.2%)	65.1(3.3%)

a. The first values in the cells are for the estimated errors, the values in parentheses are for the estimated percent errors.

Table SI.12a. The simulated HFE values of the 12-6-4 parameter space scanning for the divalent cations in the TIP3P water model. The X axis is κ (Å^{-2}) while the Y axis is $R_{min}/2$ (Å).[a]

	0	1	2	3	4	5	6
0.8	-627.0	-626.9	-626.4	-626.2	-625.8	-625.4	-625.5
0.9	-573.6	-574.0	-575.0	-575.6	-576.7	-576.9	-577.8
1.0	-531.4	-533.2	-534.1	-535.3	-536.0	-537.1	-537.6
1.1	-499.6	-503.0	-506.9	-510.9	-516.1	-520.9	-525.3
1.2	-461.7	-472.2	-482.1	-493.1	-502.7	-512.8	-523.5
1.3	-434.5	-455.9	-478.1	-501.1	-524.9	-551.9	-577.9
1.4	-399.7	-440.9	-484.0	-529.2	-577.3	-626.7	-678.2
1.5	-369.6	-433.4	-503.2	-579.3	-661.1	-746.9	-839.0
1.6	-344.8	-445.0	-557.7	-684.6	-821.4	-971.9	-1131.2
1.7	-327.5	-468.3	-636.5	-828.5	-1041.7	-1274.5	-1524.1
1.8	-306.1	-498.2	-734.8	-1012.6	-1323.9	-1658.9	-2029.8
1.9	-291.7	-542.6	-872.6	-1263.6	-1708.5	-2197.6	-2730.0
2.0	-276.0	-599.2	-1033.5	-1553.8	-2147.8	-2810.1	-3526.7
2.1	-262.9	-663.6	-1212.7	-1865.5	-2639.6	-3384.2	-4272.5
2.2	-251.1	-731.8	-1398.5	-2210.3	-3142.7	-4181.0	-5311.8
2.3	-239.8	-810.1	-1625.7	-2622.2	-3765.4	-5038.3	-6422.9

a. Units of the HFE values are kcal/mol.

Table SI.12b. The simulated HFE values of the 12-6-4 parameter space scanning for the divalent cations in the SPC/E water model. The X axis is κ ($Å^{-2}$) while the Y axis is $R_{min}/2$ (Å).[a]

	0	1	2	3	4	5	6
0.8	-632.2	-631.6	-629.9	-631.5	-630.5	-629.9	-629.7
0.9	-575.7	-577.0	-578.1	-579.3	-579.4	-580.4	-580.7
1.0	-534.7	-535.9	-537.3	-538.5	-539.1	-540.1	-541.0
1.1	-501.7	-504.9	-509.5	-514.7	-518.6	-523.3	-528.7
1.2	-463.2	-470.4	-481.9	-492.9	-503.0	-515.0	-524.9
1.3	-435.4	-457.2	-481.0	-503.5	-527.0	-553.8	-580.9
1.4	-399.4	-441.7	-486.7	-532.6	-580.8	-632.3	-685.0
1.5	-368.4	-433.3	-504.6	-582.0	-665.2	-752.7	-845.7
1.6	-342.6	-444.3	-558.9	-688.4	-829.1	-980.3	-1143.1
1.7	-324.1	-467.7	-639.6	-835.0	-1052.4	-1288.8	-1542.5
1.8	-302.3	-498.6	-740.8	-1022.2	-1327.9	-1676.1	-2050.9
1.9	-287.5	-545.1	-879.3	-1275.7	-1727.1	-2223.6	-2762.1
2.0	-272.5	-600.9	-1042.5	-1571.7	-2175.8	-2846.2	-3574.1
2.1	-259.6	-666.8	-1225.1	-1882.3	-2666.3	-3432.3	-4330.8
2.2	-247.3	-737.7	-1418.3	-2242.9	-3187.5	-4237.8	-5385.4
2.3	-235.5	-817.9	-1649.0	-2657.5	-3814.0	-5106.6	-6514.8

a. Units of the HFE values are kcal/mol.

Table SI.12c. The simulated HFE values of the 12-6-4 parameter space scanning for the divalent cations in the TIP_{EW} water model. The X axis is κ ($Å^{-2}$) while the Y axis is $R_{min}/2$ (Å).[a]

	0	1	2	3	4	5	6
0.8	-586.2	-585.8	-584.9	-585.5	-585.6	-584.6	-583.7
0.9	-537.4	-538.3	-538.9	-539.8	-540.7	-540.9	-541.8
1.0	-502.2	-504.3	-505.1	-506.3	-506.4	-507.8	-509.0
1.1	-473.0	-476.4	-480.9	-484.6	-489.7	-494.4	-498.9
1.2	-440.2	-450.6	-460.5	-471.4	-480.0	-491.8	-501.3
1.3	-414.5	-437.4	-459.9	-482.2	-507.8	-533.9	-561.2
1.4	-382.4	-424.8	-467.9	-514.5	-563.2	-613.8	-667.2
1.5	-354.0	-418.0	-491.0	-569.1	-651.5	-742.2	-834.9
1.6	-331.1	-433.2	-549.5	-679.6	-822.2	-976.3	-1141.4
1.7	-313.9	-459.2	-633.8	-832.4	-1052.9	-1294.3	-1552.2
1.8	-294.0	-492.2	-738.5	-1025.3	-1347.6	-1692.1	-2074.0
1.9	-280.3	-540.9	-883.7	-1287.4	-1747.0	-2252.6	-2800.9
2.0	-265.1	-600.6	-1052.3	-1591.3	-2205.3	-2887.5	-3630.6
2.1	-253.1	-669.8	-1239.4	-1927.6	-2717.6	-3577.0	-4532.0
2.2	-241.6	-741.9	-1431.5	-2270.3	-3232.0	-4301.0	-5466.2
2.3	-231.2	-824.0	-1670.4	-2697.5	-3878.8	-5193.5	-6624.5

a. Units of the HFE values are kcal/mol.

Table SI.13a. The simulated IOD and CN values of the 12-6-4 parameter space scanning for the divalent cations in the TIP3P water model. The X axis is κ ($Å^{-2}$) while Y axis is $R_{min}/2$ (Å). The number before the slash is the IOD value while the one after is the CN value.[a]

	0	1	2	3	4	5	6
0.8	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0
0.9	1.13/2.0	1.13/2.0	1.13/2.0	1.13/2.0	1.13/2.0	1.13/2.0	1.13/2.0
1.0	1.40/3.0	1.40/3.0	1.40/3.0	1.40/3.0	1.39/3.0	1.39/3.0	1.39/3.0
1.1	1.58/4.0	1.57/4.0	1.57/4.0	1.57/4.0	1.57/4.0	1.56/4.0	1.56/4.0
1.2	1.86/6.0	1.85/6.0	1.85/6.0	1.84/6.0	1.83/5.9	1.82/6.0	1.81/5.9
1.3	1.97/6.0	1.95/6.0	1.93/6.0	1.91/6.0	1.90/6.0	1.89/6.0	1.87/6.0
1.4	2.08/6.0	2.05/6.0	2.02/6.0	1.99/6.0	1.97/6.0	1.94/6.0	1.92/6.0
1.5	2.28/7.1	2.22/7.1	2.18/7.2	2.14/7.2	2.11/7.2	2.08/7.1	2.05/7.1
1.6	2.44/8.0	2.35/8.0	2.28/8.0	2.23/8.0	2.18/8.0	2.15/8.0	2.11/8.0
1.7	2.56/8.3	2.46/8.9	2.38/9.0	2.31/9.0	2.26/9.0	2.21/9.0	2.17/9.0
1.8	2.69/8.9	2.54/9.0	2.44/9.4	2.39/10.0	2.33/10.0	2.28/10.0	2.24/10.0
1.9	2.80/9.1	2.63/10.0	2.57/12.0	2.48/12.0	2.41/12.0	2.36/12.0	2.25/10.0
2.0	2.92/9.5	2.74/12.0	2.60/12.0	2.50/12.0	2.43/12.0	2.37/12.0	2.32/12.0
2.1	3.03/9.9	2.79/12.0	2.63/12.0	2.53/12.0	2.45/12.0	2.39/12.0	2.34/12.0
2.2	3.14/10.4	2.84/12.0	2.75/14.0	2.56/12.0	2.48/12.0	2.42/12.0	2.37/12.0
2.3	3.25/11.2	2.95/14.3	2.79/14.8	2.69/14.9	2.57/14.0	2.53/14.5	2.47/14.0

a. Units of the IOD values are Å.

Table SI.13b. The simulated IOD and CN values of the 12-6-4 parameter space scanning for the divalent cations in the SPC/E water model. The X axis is κ ($Å^{-2}$) while Y axis is $R_{min}/2$ (Å). The number before the slash is the IOD value while the one after is the CN value.[a]

	0	1	2	3	4	5	6
0.8	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0
0.9	1.13/2.0	1.13/2.0	1.13/2.0	1.13/2.0	1.13/2.0	1.13/2.0	1.13/2.0
1.0	1.40/3.0	1.40/3.0	1.40/3.0	1.40/3.0	1.40/3.0	1.40/3.0	1.40/3.0
1.1	1.58/4.0	1.58/4.0	1.58/4.0	1.57/4.0	1.57/4.0	1.57/4.0	1.57/4.0
1.2	1.87/6.0	1.86/6.0	1.85/6.0	1.84/6.0	1.83/5.8	1.82/5.8	1.81/5.5
1.3	1.97/6.0	1.95/6.0	1.94/6.0	1.92/6.0	1.91/6.0	1.89/6.0	1.88/6.0
1.4	2.09/6.0	2.05/6.0	2.02/6.0	2.00/6.0	1.97/6.0	1.95/6.0	1.93/6.0
1.5	2.26/6.7	2.21/6.7	2.17/6.9	2.14/7.0	2.10/6.9	2.08/7.0	2.05/7.0
1.6	2.44/7.9	2.36/8.0	2.29/8.0	2.24/8.0	2.19/8.0	2.15/8.0	2.12/8.0
1.7	2.56/8.1	2.46/8.8	2.38/9.0	2.32/9.0	2.26/9.0	2.22/9.0	2.18/9.0
1.8	2.69/8.7	2.54/9.0	2.43/9.0	2.37/9.4	2.33/9.9.0	2.28/10.0	2.24/10.0
1.9	2.81/9.0	2.64/10.0	2.58/12.0	2.49/12.0	2.42/12.0	2.31/10.0	2.26/10.0
2.0	2.92/9.3	2.75/12.0	2.61/12.0	2.51/12.0	2.43/12.0	2.38/12.0	2.33/12.0
2.1	3.03/9.8	2.80/12.0	2.64/12.0	2.53/12.0	2.46/12.0	2.40/12.0	2.35/12.0
2.2	3.14/10.1	2.85/12.0	2.68/12.0	2.57/12.0	2.49/12.0	2.43/12.0	2.38/12.0
2.3	3.25/10.6	2.96/14.3	2.79/14.5	2.69/14.8	2.58/14.0	2.46/12.0	2.47/14.0

a. Units of the IOD values are Å.

Table SI.13c. The simulated IOD and CN values of the 12-6-4 parameter space scanning for the divalent cations in the TIP4P$_{EW}$ water model. The X axis is κ (Å^{-2}) while Y axis is $R_{min}/2$ (Å). The number before the slash is the IOD value while the one after is the CN value.[a]

	0	1	2	3	4	5	6
0.8	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0	0.83/1.0
0.9	1.15/2.0	1.15/2.0	1.15/2.0	1.15/2.0	1.15/2.0	1.15/2.0	1.15/2.0
1.0	1.42/3.0	1.42/3.0	1.42/3.0	1.42/3.0	1.42/3.0	1.41/3.0	1.41/3.0
1.1	1.60/4.0	1.60/4.0	1.59/4.0	1.59/4.0	1.59/4.0	1.59/4.0	1.58/4.0
1.2	1.88/6.0	1.88/6.0	1.87/6.0	1.86/6.0	1.85/6.0	1.84/6.0	1.83/5.8
1.3	1.99/6.0	1.97/6.0	1.95/6.0	1.93/6.0	1.92/6.0	1.91/6.0	1.89/6.0
1.4	2.10/6.0	2.07/6.0	2.04/6.0	2.01/6.0	1.98/6.0	1.96/6.0	1.94/6.0
1.5	2.29/7.0	2.24/7.1	2.20/7.1	2.16/7.2	2.12/7.2	2.09/7.1	2.06/7.0
1.6	2.46/8.0	2.37/8.0	2.30/8.0	2.24/8.0	2.20/8.0	2.16/8.0	2.12/8.0
1.7	2.58/8.2	2.48/8.9	2.39/9.0	2.32/9.0	2.27/9.0	2.22/9.0	2.18/9.0
1.8	2.71/8.9	2.55/9.1	2.45/9.3	2.39/9.8	2.34/10.0	2.29/10.0	2.24/10.0
1.9	2.83/9.2	2.65/10.4	2.58/12.0	2.49/12.0	2.42/12.0	2.32/10.5	2.26/10.0
2.0	2.94/9.6	2.76/12.0	2.61/12.0	2.51/12.0	2.44/12.0	2.38/12.0	2.33/12.0
2.1	3.06/10.0	2.80/12.0	2.64/12.0	2.54/12.0	2.46/12.0	2.40/12.0	2.35/12.0
2.2	3.17/10.5	2.85/12.0	2.68/12.0	2.57/12.0	2.49/12.0	2.47/13.0	2.38/12.0
2.3	3.27/11.0	2.96/14.2	2.72/12.0	2.61/12.0	2.52/12.0	2.52/14.0	2.41/12.0

a. Units of the IOD values are Å.

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