## **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<sup>1</sup> 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<sup>2</sup>, 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<sup>3+</sup> 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<sup>3</sup> 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<sup>2</sup> 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  $2 \text{ ps}^{-1}$  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<sup>4</sup> was used to constrain bonds involving hydrogen atoms and the three-point SHAKE<sup>5</sup> 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).



Diffusion coefficient of different parameter sets for Al<sup>3+</sup> (Exp.0.541)

**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.

Water model	Q(O)  or  Q(M) (e)	Q(H) (e)	<i>r</i> (О-Н) (Å)	H-О-Н (°)	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 <sub>Ew</sub>	-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

**Table S1.** Parameters for the Eight Different Water Models<sup>a</sup>

"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.

			Triv	alent Metal	Ion			Tetra	avalent Meta	l Ion	
R <sub>min</sub> ,	٤ <sub>M</sub>		<b>C</b> 4	(kcal/mol*.	Å4)			$C_4$	(kcal/mol*.	Å <sup>4</sup> )	
м/2 (Å)	(kcal/mol)	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

**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<sup>*ab*</sup>

<sup>*b*</sup>At low  $R_{min,M}/2$  and high C<sub>4</sub> 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<sub>4</sub> combinations.

			Triv	alent Metal	Ion			Tetr	avalent Meta	l Ion	
R <sub>min</sub> ,	٤ <sub>M</sub>		<b>C</b> 4	(kcal/mol*.	Å4)			<b>C</b> <sub>4</sub>	(kcal/mol*.	Å4)	
м/2 (Å)	(kcal/mol)	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

**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  $Model^{ab}$ 

<sup>*a*</sup>Here "N/A" means the simulation job failed. These points were not used in the curve fittings. <sup>*b*</sup>At low  $R_{min,M}/2$  and high C<sub>4</sub> 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<sub>4</sub> combinations.

			Triv	alent Metal	Ion			Tetr	avalent Meta	l Ion	
R <sub>min</sub> ,	٤ <sub>M</sub>		<b>C</b> 4	(kcal/mol*.	Å4)			<b>C</b> 4	(kcal/mol*.	Å4)	
м/2 (Å)	(kcal/mol)	0	125	250	375	500	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

**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<sup>*ab*</sup>

<sup>*b*</sup>At low  $R_{min,M}/2$  and high C<sub>4</sub> 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<sub>4</sub> combinations.

			Triv	alent Metal	Ion			Tetr	avalent Meta	l Ion	
R <sub>min</sub> ,	٤ <sub>M</sub>		C4	(kcal/mol*.	Å4)			C4	(kcal/mol*.	Å4)	
м/2 (Å)	(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

**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<sup>*ab*</sup>

<sup>*a*</sup>Here "N/A" means the simulation job failed. These points were not used in the curve fittings. <sup>*b*</sup>At low  $R_{min,M}/2$  and high C<sub>4</sub> 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<sub>4</sub> combinations.

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		C4	=0	C4=	:125	C4=	250	C4=	:375	C4=	:500
$R_{min,M}/2$	ε <sub>M</sub>	kcal/m	ol*Å <sup>4</sup>	kcal/m	nol*Å4	kcal/m	ol*Å <sup>4</sup>	kcal/n	nol*Å4	kcal/n	nol*Å <sup>4</sup>
(Å)	(kcal/mol)	IOD	CN	IOD	CN	IOD	CN	IOD	CN	IOD	CN
		(Å)	CIV	(Å)	cn	(Å)	CIV	(Å)	cn	(Å)	ch
0.9	0.0000062	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
23	0.63803333	3.14	12.0	3.12	12.0	3.11	12.0	3.09	12.0	3.08	12.0
2.5	0.00000000		1210	5.12	12.0	0.11	12.0	2.07		0.00	
2.3	0.000000000	C4	=0	C4=	:250	C4=	500	C4=	750	C4=	1000
Rmin,M/2	ε <sub>M</sub>	C4 kcal/m	=0 ol*Å <sup>4</sup>	C4= kcal/m	=250 nol*Å <sup>4</sup>	C4= kcal/m	500 101*Å <sup>4</sup>	C4= kcal/m	750 nol*Å <sup>4</sup>	C4= kcal/m	1000 nol*Å <sup>4</sup>
R <sub>min,M</sub> /2 (Å)	ε <sub>M</sub> (kcal/mol)	C4 kcal/m IOD	$=0$ $ol^{*}Å^{4}$ $CN$	C4= kcal/m IOD	250 nol*Å <sup>4</sup>	C4= kcal/m IOD	500 ol*Å <sup>4</sup>	C4= kcal/m IOD	750 nol*Å <sup>4</sup>	C4= kcal/m IOD	1000 nol*Å <sup>4</sup>
R <sub>min,M</sub> /2 (Å)	٤ <sub>M</sub> (kcal/mol)	C4 kcal/m IOD (Å)	=0 lol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	250 nol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	500 ol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	750 nol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	1000 nol*Å <sup>4</sup> CN
R <sub>min,M</sub> /2 (Å) 0.9	ε <sub>M</sub> (kcal/mol)	C4 kcal/m IOD (Å) 1.06	$=0$ $ol*Å^4$ $CN$ $2.0$	C4= kcal/m IOD (Å) N/A	250 nol*Å <sup>4</sup> CN N/A	C4= kcal/m IOD (Å) N/A	500 aol*Å <sup>4</sup> CN N.A	C4= kcal/m IOD (Å) N/A	=750 nol*Å <sup>4</sup> CN N/A	C4= kcal/m IOD (Å) N/A	1000 nol*Å <sup>4</sup> CN N/A
R <sub>min,M</sub> /2 (Å) 0.9 1.0	ε <sub>M</sub> (kcal/mol) 0.00000062 0.00001422	C4 kcal/m IOD (Å) 1.06 1.32		C4= kcal/m IOD (Å) N/A 1.13	250 nol*Å <sup>4</sup> CN N/A 1.8	C4= kcal/m IOD (Å) N/A 1.07	500 nol*Å <sup>4</sup> CN N.A 2.0	C4= kcal/m IOD (Å) N/A N/A	750 nol*Å <sup>4</sup> CN N/A N/A	C4= kcal/m IOD (Å) N/A N/A	1000 nol*Å <sup>4</sup> CN N/A N/A
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1	ε <sub>M</sub> (kcal/mol) 0.00000062 0.00001422 0.00016377	C4 kcal/m IOD (Å) 1.06 1.32 1.48		C4= kcal/m IOD (Å) N/A 1.13 1.43	250 nol*Å <sup>4</sup> CN N/A 1.8 4.0	C4= kcal/m IOD (Å) N/A 1.07 1.38	500 tol*Å <sup>4</sup> CN N.A 2.0 4.0	C4= kcal/m IOD (Å) N/A N/A 1.35	750 nol*Å <sup>4</sup> CN N/A N/A 4.0	C4= kcal/m IOD (Å) N/A N/A 1.32	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377 0.00110429	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75		C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71	2250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50	500 nol*Å <sup>4</sup> CN N.A 2.0 4.0 4.0 4.0	C4= kcal/m IOD (Å) N/A N/A 1.35 1.47	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83		C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79	$ \frac{-250}{\text{nol}^* \text{Å}^4} \\ \underline{\text{CN}} \\ \underline{\text{N/A}} \\ 1.8 \\ 4.0 \\ 6.0 \\ 6.0 \\ 6.0 $	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75	500 101*Å <sup>4</sup> CN N.A 2.0 4.0 4.0 4.0 6.0	C4= kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99		C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90	-250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0 6.0 6.0 6.0	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86	500 101*Å <sup>4</sup> CN N.A 2.0 4.0 4.0 4.0 6.0 6.0	C4= kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.82	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99 2.18		C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14	-250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0 6.0 6.0 8.0	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86 2.11	500 101*Å <sup>4</sup> CN N.A 2.0 4.0 4.0 4.0 6.0 6.0 8.0	C4= kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.82 2.08	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1 8.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81 2.06	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6	$\frac{\epsilon_{M}}{(\text{kcal/mol})}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99 2.18 2.30		C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25	250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0 6.0 6.0 6.0 8.0 7.1	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86 2.11 2.21	$\begin{array}{r} 500\\ 500\\ \text{sol}*\text{\AA}^4\\ \hline \\ \hline$	C4= kcal/m IOD (Å) N/A 1.35 1.47 1.72 1.82 2.08 2.18	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1 8.0 8.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81 2.06 2.16	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 6.0 8.0 8.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7	$\frac{\epsilon_{M}}{(\text{kcal/mol})}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493 0.13818331	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99 2.18 2.30 2.41	$ \begin{array}{c}         =0 \\         =0$	C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37	$ \frac{1200}{1001 \times 10^{-250}} = 250 \\ \frac{1200}{1001 \times 10^{-2}} = 1200 \\ \frac{1200}{1001 \times 10^{-2}} = 120$	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86 2.11 2.21 2.34	$\begin{array}{r} 500\\ 500\\ \text{sol}*\text{\AA}^4\\ \hline \\ \hline$	C4= kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.82 2.08 2.18 2.32	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1 8.0 8.0 9.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81 2.06 2.16 2.29	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8	$\frac{\epsilon_{M}}{(\text{kcal/mol})}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493 0.13818331 0.21312875	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99 2.18 2.30 2.41 2.54	$ \begin{array}{c}         =0 \\         =0$	C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51	250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0 6.0 6.0 6.0 8.0 7.1 9.0 10.0	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86 2.11 2.21 2.34 2.48	500 101*Å <sup>4</sup> CN N.A 2.0 4.0 4.0 6.0 6.0 8.0 8.2 9.0 10.0	C4= kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.82 2.08 2.18 2.32 2.46	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1 8.0 8.0 9.0 10.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81 2.06 2.16 2.29 2.44	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9	$\frac{\epsilon_{M}}{(\text{kcal/mol})}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493 0.13818331 0.21312875 0.29896986	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99 2.18 2.30 2.41 2.54 2.71	$ \begin{array}{c}                                     $	C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51 2.68	250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0 6.0 6.0 6.0 6.0 8.0 7.1 9.0 10.0 12.0	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86 2.11 2.21 2.34 2.48 2.65	500 101*Å <sup>4</sup> CN N.A 2.0 4.0 4.0 6.0 6.0 8.0 8.2 9.0 10.0 12.0	C4= kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.82 2.08 2.18 2.32 2.46 2.63	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1 8.0 8.0 9.0 10.0 12.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81 2.06 2.16 2.29 2.44 2.60	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493 0.13818331 0.21312875 0.29896986 0.38943250	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99 2.18 2.30 2.41 2.54 2.71 2.78	$\begin{array}{c} = 0 \\ = 0 \\ = 0 \\ = 0 \\ = 1 \\ \hline \\ CN \\ \hline \\ 2.0 \\ 3.0 \\ 4.0 \\ 6.0 \\ 6.0 \\ 6.0 \\ 6.1 \\ 8.0 \\ 8.9 \\ 9.1 \\ 10.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ \end{array}$	C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51 2.68 2.75	250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0 6.0 6.0 6.0 6.0 8.0 7.1 9.0 10.0 12.0 12.0	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86 2.11 2.21 2.34 2.48 2.65 2.73	$\begin{array}{r} 500\\ 500\\ \text{sol}*\text{\AA}^4\\ \hline \\ \hline$	C4= kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.82 2.08 2.18 2.32 2.46 2.63 2.70	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1 8.0 8.0 9.0 10.0 12.0 12.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81 2.06 2.16 2.29 2.44 2.60 2.68	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1	$\frac{\epsilon_{M}}{(\text{kcal/mol})}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493 0.13818331 0.21312875 0.29896986 0.38943250 0.47874242	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99 2.18 2.30 2.41 2.54 2.71 2.78 2.86	$\begin{array}{c} =0\\ =0\\ =0\\ \text{ol}^*\text{Å}^4\\ \hline \\ \hline$	C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51 2.68 2.75 2.84	250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0 6.0 6.0 6.0 6.0 8.0 7.1 9.0 10.0 12.0 12.0 12.0	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86 2.11 2.21 2.34 2.48 2.65 2.73 2.81	$\begin{array}{r} 500\\ 500\\ \text{sol} * \text{\AA}^4\\ \hline \\ \hline$	C4= kcal/m IOD (Å) N/A 1.35 1.47 1.72 1.82 2.08 2.18 2.32 2.46 2.63 2.70 2.79	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1 8.0 8.0 9.0 10.0 12.0 12.0 12.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81 2.06 2.16 2.29 2.44 2.60 2.68 2.77	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0 12.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2	$\frac{\epsilon_{M}}{(\text{kcal/mol})}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493 0.13818331 0.21312875 0.29896986 0.38943250 0.47874242 0.56252208	C4 kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 1.99 2.18 2.30 2.41 2.54 2.71 2.78 2.86 2.95	$\begin{array}{c} =0\\ =0\\ =0\\ =0\\ =0\\ =0\\ =0\\ =0\\ =0\\ =0\\$	C4= kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51 2.68 2.75 2.84 2.92	250 nol*Å <sup>4</sup> CN N/A 1.8 4.0 6.0 6.0 6.0 6.0 6.0 8.0 7.1 9.0 10.0 12.0 12.0 12.0 12.0	C4= kcal/m IOD (Å) N/A 1.07 1.38 1.50 1.75 1.86 2.11 2.21 2.34 2.48 2.65 2.73 2.81 2.90	$\begin{array}{r} 500\\ 500\\ \text{sol}*\text{Å}^4\\ \hline \\ \hline$	C4= kcal/m IOD (Å) N/A 1.35 1.47 1.72 1.82 2.08 2.18 2.32 2.46 2.63 2.70 2.79 2.87	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.1 8.0 8.0 9.0 10.0 12.0 12.0 12.0 12.0	C4= kcal/n IOD (Å) N/A N/A 1.32 1.44 1.69 1.81 2.06 2.16 2.29 2.44 2.60 2.68 2.77 2.85	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0 12.0 12.0 12.0

**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<sup>*a*</sup>

und 100	in valent (00	juoni) n	Ictui Io	10  m  co	njuneti			, mater i	mouci		
		C4	=0	C4=	125	C4=	250	C4=	375	C4=	500
$R_{min,M}/2$	ε <sub>M</sub>	kcal/m	ol*Å <sup>4</sup>	kcal/m	nol*Å <sup>4</sup>	kcal/m	iol*Å <sup>4</sup>	kcal/n	nol*Å <sup>4</sup>	kcal/m	iol*Å <sup>4</sup>
(Å)	(kcal/mol)	IOD	CN	IOD	CN	IOD	CN	IOD	CN	IOD	CN
		(Å)	CIV	(Å)	CIV	(Å)	CIV	(Å)	CIV	(Å)	CIV
0.9	0.0000062	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
23	0.63803333	3.17	12.0	3 1 5	12.0	3.14	12.0	3.12	12.0	3.11	12.0
2.5	0.0000000000		12.0	5.15	12.0	0.1	12.0		12.0		
2.5	0.05005555	C4	=0	C4=	250	C4=	500	C4=	750	C4=	1000
Rmin,M/2	ε <sub>M</sub>	C4 kcal/m	=0 ol*Å <sup>4</sup>	C4= kcal/m	250 nol*Å <sup>4</sup>	C4= kcal/m	500 101*Å <sup>4</sup>	C4= kcal/m	=750 nol*Å <sup>4</sup>	C4= kcal/m	1000 nol*Å <sup>4</sup>
R <sub>min,M</sub> /2 (Å)	ε <sub>M</sub> (kcal/mol)	C4 kcal/m IOD	$=0$ $=0$ $=0^{*}Å^{4}$ $CN$	C4= kcal/m IOD	250 nol*Å <sup>4</sup>	C4= kcal/m IOD	500 ol*Å <sup>4</sup>	C4= kcal/m IOD	2750 nol*Å <sup>4</sup>	C4= kcal/m IOD	1000 nol*Å <sup>4</sup>
R <sub>min,M</sub> /2 (Å)	٤ <sub>M</sub> (kcal/mol)	C4 kcal/m IOD (Å)	=0 ol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	250 nol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	500 ol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	750 nol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	1000 nol*Å <sup>4</sup> CN
R <sub>min,M</sub> /2 (Å) 0.9	ε <sub>M</sub> (kcal/mol)	C4 kcal/m IOD (Å) 1.09	=0 ol*Å <sup>4</sup> CN 2.0	C4= kcal/m IOD (Å) 1.01	250 nol*Å <sup>4</sup> CN 2.0	C4= kcal/m IOD (Å) N/A	500 aol*Å <sup>4</sup> CN N/A	C4= kcal/m IOD (Å) N/A	=750 nol*Å <sup>4</sup> CN N/A	C4= kcal/m IOD (Å) N/A	1000 nol*Å <sup>4</sup> CN N/A
2.3 R <sub>min,M</sub> /2 (Å) 0.9 1.0	ε <sub>M</sub> (kcal/mol) 0.00000062 0.00001422	C4 kcal/m IOD (Å) 1.09 1.35		C4= kcal/m IOD (Å) 1.01 N/A	250 nol*Å <sup>4</sup> CN 2.0 N/A	C4= kcal/m IOD (Å) N/A N/A	500 aol*Å <sup>4</sup> CN N/A N/A	C4= kcal/m IOD (Å) N/A N/A	750 nol*Å <sup>4</sup> CN N/A N/A	C4= kcal/m IOD (Å) N/A N/A	1000 aol*Å <sup>4</sup> CN N/A N/A
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377	C4 kcal/m IOD (Å) 1.09 1.35 1.52		C4= kcal/m IOD (Å) 1.01 N/A 1.46	250 nol*Å <sup>4</sup> CN 2.0 N/A 4.0	C4= kcal/m IOD (Å) N/A N/A 1.42	500 aol*Å <sup>4</sup> CN N/A N/A 4.0	C4= kcal/m IOD (Å) N/A N/A 1.38	750 nol*Å <sup>4</sup> CN N/A N/A 4.0	C4= kcal/m IOD (Å) N/A N/A N/A	1000 aol*Å <sup>4</sup> CN N/A N/A N/A
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377 0.00110429	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79		C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74	2250 nol*Å <sup>4</sup> CN 2.0 N/A 4.0 6.0	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53	500 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0	C4= kcal/m IOD (Å) N/A N/A 1.38 1.49	E750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47	1000 1001*Å <sup>4</sup> CN N/A N/A N/A 4.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87		C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82	$ \frac{250}{\text{nol}*Å^4} $ CN 2.0 N/A 4.0 6.0 6.0	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79	500 sol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0	C4= kcal/m IOD (Å) N/A N/A 1.38 1.49 1.76	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73	1000 1001*Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97	$ \begin{array}{r} = 0 \\ = 0 \\ = 0 \\ = 0 \\ \hline \\ 0 \\ = 1 \\ \hline \\ 0 \\ = 0 \\ \hline \\ 0 \\ 0 \\ \hline \\ 0 \\ 0 \\ \hline \\ 0 \\ 0 \\$	C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93	$ \frac{250}{\text{nol}*Å^4} $ CN 2.0 N/A 4.0 6.0 6.0 6.0	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90	500 sol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0	C4= kcal/m IOD (Å) N/A N/A 1.38 1.49 1.76 1.86	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84	1000 1001*Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5	ε <sub>M</sub> (kcal/mol) 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97 2.22		C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93 2.18	$ \frac{250}{\text{nol}*Å^4} \\  \hline  CN \\  \hline  2.0 \\  N/A \\  4.0 \\  6.0 \\  6.0 \\  6.0 \\  8.0 \\  \hline $	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90 2.15	500 sol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0	C4= kcal/m IOD (Å) N/A N/A 1.38 1.49 1.76 1.86 2.12	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84 2.10	1000 1001*Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0 8.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ \end{array}$	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97 2.22 2.32	$ \begin{array}{c}                                     $	C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93 2.18 2.28	$ \frac{250}{\text{nol}*\text{Å}^4} \\ \frac{\text{CN}}{2.0} \\ \text{N/A} \\ 4.0 \\ 6.0 \\ 6.0 \\ 6.0 \\ 8.0 \\ 8.1 $	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90 2.15 2.25	500 sol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0	C4= kcal/m IOD (Å) N/A 1.38 1.49 1.76 1.86 2.12 2.22	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84 2.10 2.19	1000 1001*Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0 8.0 8.0 8.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ \end{array}$	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97 2.22 2.32 2.44	$ \begin{array}{c}         =0 \\         =0$	C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93 2.18 2.28 2.41	$\begin{array}{c} 250\\ \text{nol}*Å^4\\ \hline \\ \text{CN}\\ \hline \\ 2.0\\ \text{N/A}\\ 4.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 8.0\\ 8.1\\ 9.0\\ \end{array}$	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90 2.15 2.25 2.38	500 sol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0	C4= kcal/m IOD (Å) N/A 1.38 1.49 1.76 1.86 2.12 2.22 2.35	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84 2.10 2.19 2.33	1000 1001*Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0 8.0 8.0 8.0 9.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \end{array}$	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97 2.22 2.32 2.44 2.67	$ \begin{array}{c}         =0 \\         =0$	C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93 2.18 2.28 2.41 2.55	$\begin{array}{c} 250\\ \text{nol}*Å^4\\ \hline \\ \text{CN}\\ \hline \\ 2.0\\ \text{N/A}\\ 4.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 8.0\\ 8.1\\ 9.0\\ 10.0\\ \end{array}$	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90 2.15 2.25 2.38 2.52	500 sol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0	C4= kcal/m IOD (Å) N/A 1.38 1.49 1.76 1.86 2.12 2.22 2.35 2.50	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84 2.10 2.19 2.33 2.47	1000 1001*Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \end{array}$	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97 2.22 2.32 2.44 2.67 2.74	$ \begin{array}{c}         =0 \\         =0$	C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93 2.18 2.28 2.41 2.55 2.72	$\begin{array}{c} 250\\ \text{nol}*Å^4\\ \hline \\ \text{CN}\\ \hline \\ 2.0\\ \text{N/A}\\ 4.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 8.0\\ 8.1\\ 9.0\\ 10.0\\ 12.0\\ \end{array}$	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90 2.15 2.25 2.38 2.52 2.69	500 500 500 500 500 500 N/A N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0 12.0	C4= kcal/m IOD (Å) N/A 1.38 1.49 1.76 1.86 2.12 2.22 2.35 2.50 2.67	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0 12.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84 2.10 2.19 2.33 2.47 2.64	1000 100 <sup>*</sup> Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ 0.38943250 \\ \end{array}$	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97 2.22 2.32 2.44 2.67 2.74 2.82	$ \begin{array}{c}         =0 \\         =0$	C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93 2.18 2.28 2.41 2.55 2.72 2.79	$\begin{array}{c} 250\\ \text{nol}*Å^4\\ \hline \\ \text{CN}\\ \hline \\ 2.0\\ \text{N/A}\\ 4.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 8.0\\ 8.1\\ 9.0\\ 10.0\\ 12.0\\ 12.0\\ 12.0\\ \end{array}$	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90 2.15 2.25 2.38 2.52 2.69 2.77	500 500 500 500 500 500 8.0 8.0 8.0 8.0 9.0 10.0 12.0 12.0	C4= kcal/m IOD (Å) N/A 1.38 1.49 1.76 1.86 2.12 2.22 2.35 2.50 2.67 2.74	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0 12.0 12.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84 2.10 2.19 2.33 2.47 2.64 2.72	1000 100 <sup>*</sup> Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ 0.38943250 \\ 0.47874242 \\ \end{array}$	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97 2.22 2.32 2.44 2.67 2.74 2.82 2.90	$\begin{array}{c} =0\\ =0\\ =0\\ =0\\ =0\\ =0\\ =12\\ \hline \\ CN\\ \hline \\ 2.0\\ 3.0\\ 4.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 8.5\\ 9.0\\ 12.0\\$	C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93 2.18 2.28 2.41 2.55 2.72 2.79 2.87	$\begin{array}{c} 250\\ \text{nol}*Å^4\\ \hline \\ \text{CN}\\ \hline \\ 2.0\\ \text{N/A}\\ 4.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 8.0\\ 8.1\\ 9.0\\ 10.0\\ 12.0\\ 12.0\\ 12.0\\ 12.0\\ 12.0\\ \end{array}$	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90 2.15 2.25 2.38 2.52 2.69 2.77 2.85	500 500 500 500 500 500 8.0 8.0 9.0 10.0 12.0 12.0 12.0	C4= kcal/m IOD (Å) N/A 1.38 1.49 1.76 1.86 2.12 2.22 2.35 2.50 2.67 2.74 2.82	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0 12.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84 2.10 2.19 2.33 2.47 2.64 2.72 2.80	1000 1000 101*Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0 12.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ 0.38943250 \\ 0.47874242 \\ 0.56252208 \end{array}$	C4 kcal/m IOD (Å) 1.09 1.35 1.52 1.79 1.87 1.97 2.22 2.32 2.44 2.67 2.74 2.82 2.90 2.98	$\begin{array}{c} =0\\ =0\\ =0\\ =0\\ =0\\ =0\\ =12\\ \hline \\ CN\\ \hline \\ 2.0\\ 3.0\\ 4.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 8.5\\ 9.0\\ 12.0\\$	C4= kcal/m IOD (Å) 1.01 N/A 1.46 1.74 1.82 1.93 2.18 2.28 2.41 2.55 2.72 2.79 2.87 2.96	$\begin{array}{c} 250\\ \text{nol}*Å^4\\ \hline \\ \text{CN}\\ \hline \\ 2.0\\ \text{N/A}\\ 4.0\\ 6.0\\ 6.0\\ 6.0\\ 6.0\\ 8.0\\ 8.1\\ 9.0\\ 10.0\\ 12.0$	C4= kcal/m IOD (Å) N/A N/A 1.42 1.53 1.79 1.90 2.15 2.25 2.38 2.52 2.69 2.77 2.85 2.93	500 500 500 500 500 500 8.0 8.0 9.0 10.0 12.0 12.0 12.0 12.0 12.0	C4= kcal/m IOD (Å) N/A 1.38 1.49 1.76 1.86 2.12 2.22 2.35 2.50 2.67 2.74 2.82 2.91	750 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0 12.0 12.0	C4= kcal/m IOD (Å) N/A N/A N/A 1.47 1.73 1.84 2.10 2.19 2.33 2.47 2.64 2.72 2.80 2.89	1000 1000 101*Å <sup>4</sup> CN N/A N/A N/A 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0 12.0 12.0

**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<sup>*a*</sup>

		Ć4	=0	C4=	:125	C4=	250	C4=	375	C4=	500
$R_{min,M}/2$	٤ <sub>M</sub>	kcal/m	ol*Å <sup>4</sup>	kcal/n	nol*Å <sup>4</sup>	kcal/m	ol*Å <sup>4</sup>	kcal/m	nol*Å <sup>4</sup>	kcal/n	nol*Å <sup>4</sup>
(Å)	(kcal/mol)	IOD	CN	IOD	GN	IOD	C) I	IOD	CD I	IOD	C) I
		(Å)	CN	(Å)	CN	(Å)	CN	(Å)	CN	(Å)	CN
0.9	0.0000062	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
		C4	=0	C4=	250	C4=	500	C4=	750	C4=	1000
							0		~ ~		<b>1 1 1</b>
$R_{min,M}/2$	ε <sub>M</sub>	kcal/m	ol*Å <sup>4</sup>	kcal/n	nol*Å4	kcal/m	iol*Å <sup>4</sup>	kcal/n	nol*Å <sup>4</sup>	kcal/n	nol*A4
R <sub>min,M</sub> /2 (Å)	ε <sub>M</sub> (kcal/mol)	kcal/m IOD	ol*Å <sup>4</sup>	kcal/m IOD	nol*Å <sup>4</sup>	kcal/m IOD	ol*Å <sup>4</sup>	kcal/m IOD	nol*Å <sup>4</sup>	kcal/m IOD	ON
R <sub>min,M</sub> /2 (Å)	ε <sub>M</sub> (kcal/mol)	kcal/m IOD (Å)	ol*Å <sup>4</sup> CN	kcal/m IOD (Å)	nol*Å <sup>4</sup> CN	kcal/m IOD (Å)	ol*Å <sup>4</sup> CN	kcal/m IOD (Å)	nol*Å <sup>4</sup> CN	kcal/m IOD (Å)	CN
R <sub>min,M</sub> /2 (Å) 0.9	ε <sub>M</sub> (kcal/mol) 0.00000062	kcal/m IOD (Å) 1.06	01*Å <sup>4</sup> CN 2.0	kcal/m IOD (Å) N/A	nol*Å <sup>4</sup> CN N/A	kcal/m IOD (Å) N/A	IOI*Å <sup>4</sup> CN N/A	kcal/m IOD (Å) N/A	nol*Å <sup>4</sup> CN N/A	kcal/m IOD (Å) N/A	CN N/A
R <sub>min,M</sub> /2 (Å) 0.9 1.0	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.00001422 \end{array}$	kcal/m IOD (Å) 1.06 1.32	ol*Å <sup>4</sup> CN 2.0 3.0	kcal/m IOD (Å) N/A 1.13	nol*Å <sup>4</sup> CN N/A 2.0	kcal/m IOD (Å) N/A N/A	CN N/A N/A	kcal/m IOD (Å) N/A N/A	nol*Å <sup>4</sup> CN N/A N/A	kcal/m IOD (Å) N/A 1.00	CN N/A 2.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1	ε <sub>M</sub> (kcal/mol) 0.00000062 0.00001422 0.00016377	kcal/m IOD (Å) 1.06 1.32 1.48	ol*Å <sup>4</sup> CN 2.0 3.0 4.0	kcal/m IOD (Å) N/A 1.13 1.43	nol*Å <sup>4</sup> CN N/A 2.0 4.0	kcal/m IOD (Å) N/A N/A 1.38	N/A N/A 4.0	kcal/m IOD (Å) N/A N/A 1.35	nol*Å <sup>4</sup> CN N/A N/A 4.0	kcal/m IOD (Å) N/A 1.00 1.32	N/A 2.0 4.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2	ε <sub>M</sub> (kcal/mol) 0.00000062 0.00001422 0.00016377 0.00110429	kcal/m IOD (Å) 1.06 1.32 1.48 1.75	ol*Å <sup>4</sup> CN           2.0           3.0           4.0           6.0	kcal/m IOD (Å) N/A 1.13 1.43 1.71	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0	kcal/m IOD (Å) N/A N/A 1.38 1.66	N/A N/A N/A 4.0 6.0	kcal/m IOD (Å) N/A N/A 1.35 1.47	N/A N/A N/A 4.0 4.0	kcal/m IOD (Å) N/A 1.00 1.32 1.44	N/A           2.0           4.0           4.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.00001422 0.00016377 0.00110429 0.00490301	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83	ol*Å <sup>4</sup> CN 2.0 3.0 4.0 6.0 6.0	kcal/n IOD (Å) N/A 1.13 1.43 1.71 1.79	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0	kcal/m IOD (Å) N/A 1.38 1.66 1.75	nol*Å <sup>4</sup> CN N/A N/A 4.0 6.0 6.0	kcal/m IOD (Å) N/A 1.35 1.47 1.72	nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69	N/A           2.0           4.0           6.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.00001422 0.00016377 0.00110429 0.00490301 0.01570749	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00		kcal/n IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0	kcal/m IOD (Å) N/A 1.38 1.66 1.75 1.86	N/A           N/A           N/A           6.0           6.0           6.0	kcal/m IOD (Å) N/A 1.35 1.47 1.72 1.83	nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80	N/A           2.0           4.0           4.0           6.0           6.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00 2.18	ol*Å4           CN           2.0           3.0           4.0           6.0           6.1           8.0	kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0	kcal/m IOD (Å) N/A N/A 1.38 1.66 1.75 1.86 2.11	N/A           N/A           N/A           6.0           6.0           6.0           6.0           6.0           6.0	kcal/n IOD (Å) N/A N/A 1.35 1.47 1.72 1.83 2.08	nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80 2.06	N/A           N/A           4.0           4.0           6.0           6.0           8.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00 2.18 2.30	ol*Å4           CN           2.0           3.0           4.0           6.0           6.1           8.0           8.9	kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0 8.6	kcal/m IOD (Å) N/A N/A 1.38 1.66 1.75 1.86 2.11 2.21	N/A           N/A           N/A           0.0           0.0           0.0           0.0           0.0           0.0           0.0           8.0           8.2	kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.83 2.08 2.18	nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.1	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80 2.06 2.15	N/A           N/A           4.0           4.0           6.0           8.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493 0.13818331	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00 2.18 2.30 2.41	ol*Å <sup>4</sup> CN 2.0 3.0 4.0 6.0 6.0 6.1 8.0 8.9 9.1	kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0 8.0 8.6 9.0	kcal/m IOD (Å) N/A N/A 1.38 1.66 1.75 1.86 2.11 2.21 2.34	N/A           N/A           N/A           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0	kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.83 2.08 2.18 2.32	nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.1 9.0	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80 2.06 2.15 2.29	N/A           N/A           2.0           4.0           6.0           6.0           8.0           9.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ \end{array}$	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00 2.18 2.30 2.41 2.63	ol*Å4           CN           2.0           3.0           4.0           6.0           6.1           8.0           8.9           9.1           12.0	kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0 8.0 8.6 9.0 10.0	kcal/m IOD (Å) N/A N/A 1.38 1.66 1.75 1.86 2.11 2.21 2.34 2.48	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.83 2.08 2.18 2.32 2.46	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80 2.06 2.15 2.29 2.43	N/A           N/A           2.0           4.0           6.0           6.0           8.0           9.0           10.0
Rmin,M/2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.00001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ \end{array}$	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00 2.18 2.30 2.41 2.63 2.70		kcal/m IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51 2.68	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0 8.0 8.6 9.0 10.0 12.0	kcal/m IOD (Å) N/A N/A 1.38 1.66 1.75 1.86 2.11 2.21 2.34 2.48 2.65	N/A           N/A           N/A           N/A           6.0           6.0           6.0           8.0           8.2           9.0           10.0           12.0	kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.83 2.08 2.18 2.32 2.46 2.62	nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.1 9.0 10.0 12.0	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80 2.06 2.15 2.29 2.43 2.60	N/A           N/A           2.0           4.0           6.0           6.0           8.0           9.0           10.0           12.0
Rmin.M/2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.00001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838 0.07934493 0.13818331 0.21312875 0.29896986 0.38943250	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00 2.18 2.30 2.41 2.63 2.70 2.78	$\begin{array}{c} \text{ol}^* \text{\AA}^4 \\ \hline \text{CN} \\ \hline 2.0 \\ 3.0 \\ 4.0 \\ 6.0 \\ 6.0 \\ 6.1 \\ 8.0 \\ 8.9 \\ 9.1 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \end{array}$	kcal/n IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51 2.68 2.75	nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0 8.0 8.6 9.0 10.0 12.0 12.0	kcal/m IOD (Å) N/A N/A 1.38 1.66 1.75 1.86 2.11 2.21 2.34 2.48 2.65 2.73	N/A           N/A           N/A           N/A           6.0           6.0           6.0           8.0           8.2           9.0           10.0           12.0	kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.83 2.08 2.18 2.32 2.46 2.62 2.70	nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0 8.1 9.0 10.0 12.0 12.3	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80 2.06 2.15 2.29 2.43 2.60 2.68	N/A           N/A           2.0           4.0           6.0           6.0           8.0           9.0           10.0           12.0           12.0
Rmin.M/2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.00001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ 0.38943250 \\ 0.47874242 \\ \end{array}$	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00 2.18 2.30 2.41 2.63 2.70 2.78 2.86	$\begin{array}{c} \text{ol}^* \text{\AA}^4 \\ \hline \text{CN} \\ \hline 2.0 \\ 3.0 \\ 4.0 \\ 6.0 \\ 6.0 \\ 6.1 \\ 8.0 \\ 8.9 \\ 9.1 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \end{array}$	kcal/n IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51 2.68 2.75 2.84	N/A           N/A           2.0           4.0           6.0           6.0           8.0           8.6           9.0           10.0           12.0           12.0           12.0	kcal/m IOD (Å) N/A N/A 1.38 1.66 1.75 1.86 2.11 2.21 2.34 2.48 2.65 2.73 2.81	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.83 2.08 2.18 2.32 2.46 2.62 2.70 2.79	N/A           N/A           N/A           N/A           4.0           6.0           6.0           8.0           8.1           9.0           10.0           12.0           12.3           12.0	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80 2.06 2.15 2.29 2.43 2.60 2.68 2.76	N/A           N/A           2.0           4.0           6.0           6.0           8.0           9.0           10.0           12.0           12.0           12.0
$\begin{array}{c} R_{min,M}/2 \\ ({\rm \AA}) \\ \hline \\ 0.9 \\ 1.0 \\ 1.1 \\ 1.2 \\ 1.3 \\ 1.4 \\ 1.5 \\ 1.6 \\ 1.7 \\ 1.8 \\ 1.9 \\ 2.0 \\ 2.1 \\ 2.2 \\ \end{array}$	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.00001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ 0.38943250 \\ 0.47874242 \\ 0.56252208 \\ \end{array}$	kcal/m IOD (Å) 1.06 1.32 1.48 1.75 1.83 2.00 2.18 2.30 2.41 2.63 2.70 2.78 2.86 2.95	$\begin{array}{c} \text{ol}^* \text{\AA}^4 \\ \hline \text{CN} \\ \hline 2.0 \\ 3.0 \\ 4.0 \\ 6.0 \\ 6.0 \\ 6.1 \\ 8.0 \\ 8.9 \\ 9.1 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \end{array}$	kcal/n IOD (Å) N/A 1.13 1.43 1.71 1.79 1.90 2.14 2.25 2.37 2.51 2.68 2.75 2.84 2.92	N/A           N/A           2.0           4.0           6.0           6.0           6.0           8.0           8.6           9.0           10.0           12.0           12.0           12.0           12.0	kcal/m IOD (Å) N/A N/A 1.38 1.66 1.75 1.86 2.11 2.21 2.34 2.48 2.65 2.73 2.81 2.90	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	kcal/m IOD (Å) N/A N/A 1.35 1.47 1.72 1.83 2.08 2.18 2.32 2.46 2.62 2.70 2.79 2.87	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	kcal/n IOD (Å) N/A 1.00 1.32 1.44 1.69 1.80 2.06 2.15 2.29 2.43 2.60 2.68 2.76 2.85	

**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<sup>*a*</sup>

una ret		C4	=0	C4=	:125	C4=	250	C4=	375	C4=	500
$R_{min,M}/2$	٤ <sub>M</sub>	kcal/m	ol*Å <sup>4</sup>	kcal/n	nol*Å <sup>4</sup>	kcal/m	ol*Å <sup>4</sup>	kcal/m	nol*Å <sup>4</sup>	kcal/n	nol*Å <sup>4</sup>
(Å)	(kcal/mol)	IOD	CD I	IOD	GN	IOD	CDI	IOD	CD I	IOD	GNI
		(Å)	CN	(Å)	CN	(Å)	CN	(Å)	CN	(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
		C4	=0	C4=	250	C4=	500	C4=	750	C4=	1000
Rmin,M/2	ε <sub>M</sub>	C4 kcal/m	=0 iol*Å <sup>4</sup>	C4= kcal/m	=250 nol*Å <sup>4</sup>	C4= kcal/m	500 101*Å <sup>4</sup>	C4= kcal/m	750 101*Å <sup>4</sup>	C4= kcal/m	1000 101*Å <sup>4</sup>
R <sub>min,M</sub> /2 (Å)	ε <sub>M</sub> (kcal/mol)	C4 kcal/m IOD	=0 tol*Å <sup>4</sup>	C4= kcal/m IOD	250 nol*Å <sup>4</sup>	C4= kcal/m IOD	500 ol*Å <sup>4</sup>	C4= kcal/m IOD	750 101*Å <sup>4</sup>	C4= kcal/m IOD	1000 nol*Å <sup>4</sup>
R <sub>min,M</sub> /2 (Å)	ε <sub>M</sub> (kcal/mol)	C4 kcal/m IOD (Å)	=0 ol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	250 nol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	500 ol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	750 nol*Å <sup>4</sup> CN	C4= kcal/m IOD (Å)	1000 nol*Å <sup>4</sup> CN
R <sub>min,M</sub> /2 (Å) 0.9	ε <sub>M</sub> (kcal/mol) 0.00000062	C4 kcal/m IOD (Å) 1.08	=0 nol*Å <sup>4</sup> CN 2.0	C4= kcal/m IOD (Å) N/A	250 nol*Å <sup>4</sup> CN N/A	C4= kcal/m IOD (Å) 0.94	500 tol*Å <sup>4</sup> CN 2.0	C4= kcal/m IOD (Å) N/A	750 nol*Å <sup>4</sup> CN N/A	C4= kcal/m IOD (Å) N/A	1000 nol*Å <sup>4</sup> CN N/A
R <sub>min,M</sub> /2 (Å) 0.9 1.0	ε <sub>M</sub> (kcal/mol) 0.00000062 0.00001422	C4 kcal/m IOD (Å) 1.08 1.34	$     =0 \\     =0 \\     =0 \\     = \hat{A}^{4} \\     CN \\     = 2.0 \\     = 3.0   $	C4= kcal/m IOD (Å) N/A 1.14	250 nol*Å <sup>4</sup> CN N/A 2.0	C4= kcal/m IOD (Å) 0.94 1.08	500 tol*Å <sup>4</sup> CN 2.0 2.0	C4= kcal/m IOD (Å) N/A 1.04	750 nol*Å <sup>4</sup> CN N/A 2.0	C4= kcal/m IOD (Å) N/A N/A	1000 nol*Å <sup>4</sup> CN N/A N/A
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1	ε <sub>M</sub> (kcal/mol) 0.00000062 0.00001422 0.00016377	C4 kcal/m IOD (Å) 1.08 1.34 1.50		C4= kcal/m IOD (Å) N/A 1.14 1.44	250 nol*Å <sup>4</sup> CN N/A 2.0 4.0	C4= kcal/m IOD (Å) 0.94 1.08 1.40	500 tol*Å <sup>4</sup> CN 2.0 2.0 4.0	C4= kcal/m IOD (Å) N/A 1.04 1.36	750 nol*Å <sup>4</sup> CN N/A 2.0 4.0	C4= kcal/m IOD (Å) N/A N/A 1.33	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2	$\frac{\epsilon_{M}}{(\text{kcal/mol})}$ 0.00000062 0.0001422 0.00016377 0.00110429	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77	$     =0 \\     =0 * Å^{4} \\     \hline                               $	C4= kcal/m IOD (Å) N/A 1.14 1.44 1.72	250 nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48	750 nol*Å <sup>4</sup> CN N/A 2.0 4.0 4.0	C4= kcal/n IOD (Å) N/A 1.33 1.45	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85	$     =0 \\     =0^{*} Å^{4} \\     \hline         CN \\         2.0 \\         3.0 \\         4.0 \\         6.0 \\         6.0 \\         6.0     $	C4= kcal/n IOD (Å) N/A 1.14 1.44 1.72 1.80	250 nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73	750 nol*Å <sup>4</sup> CN N/A 2.0 4.0 4.0 4.0 6.0	C4= kcal/n IOD (Å) N/A N/A 1.33 1.45 1.71	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4	$\frac{\epsilon_{M}}{(kcal/mol)}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01	$     =0 \\     =0^{*} Å^{4} \\     \hline         CN \\         2.0 \\         3.0 \\         4.0 \\         6.0 \\         6.0 \\         6.0 \\         6.0     $	C4= kcal/n IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91	250 nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85	750 nol*Å <sup>4</sup> CN N/A 2.0 4.0 4.0 6.0 6.0	C4= kcal/n IOD (Å) N/A 1.33 1.45 1.71 1.82	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0
R <sub>min,M</sub> /2 (Å) 0.9 1.0 1.1 1.2 1.3 1.4 1.5	$\frac{\epsilon_{M}}{(\text{kcal/mol})}$ 0.00000062 0.0001422 0.00016377 0.00110429 0.00490301 0.01570749 0.03899838	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01 2.20	$     =0 \\         iol*Å4            $	C4= kcal/m IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91 2.16	250 nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 8.0	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88 2.13		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85 2.10	750 nol*Å <sup>4</sup> CN N/A 2.0 4.0 4.0 6.0 6.0 8.0	C4= kcal/n IOD (Å) N/A 1.33 1.45 1.71 1.82 2.07	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 8.0
$\begin{array}{c} R_{\min,M}/2 \\ ({\rm \AA}) \\ \hline 0.9 \\ 1.0 \\ 1.1 \\ 1.2 \\ 1.3 \\ 1.4 \\ 1.5 \\ 1.6 \\ \end{array}$	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ \end{array}$	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01 2.20 2.31	$     =0 \\     iol*Å4     CN     2.0     3.0     4.0     6.0     6.0     6.0     8.0     8.8     $	C4= kcal/m IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91 2.16 2.27	250 nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0 8.4	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88 2.13 2.23		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85 2.10 2.20	750 nol*Å <sup>4</sup> CN N/A 2.0 4.0 4.0 6.0 6.0 8.0 8.0 8.0	C4= kcal/n IOD (Å) N/A 1.33 1.45 1.71 1.82 2.07 2.17	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 6.0 8.0 8.0 8.0
$\begin{array}{c} R_{\min,M}/2 \\ ({\rm \AA}) \\ \hline 0.9 \\ 1.0 \\ 1.1 \\ 1.2 \\ 1.3 \\ 1.4 \\ 1.5 \\ 1.6 \\ 1.7 \\ \end{array}$	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ \end{array}$	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01 2.20 2.31 2.43	$     =0 \\     iol*Å4     CN     2.0     3.0     4.0     6.0     6.0     6.0     8.0     8.8     9.2     $	C4= kcal/m IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91 2.16 2.27 2.39	250 nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0 8.4 9.0	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88 2.13 2.23 2.36		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85 2.10 2.20 2.33	750 101*Å <sup>4</sup> CN N/A 2.0 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0	C4= kcal/n IOD (Å) N/A 1.33 1.45 1.71 1.82 2.07 2.17 2.31	1000 nol*Å <sup>4</sup> CN N/A N/A 4.0 4.0 6.0 6.0 6.0 8.0 8.0 8.0 9.0
$\begin{array}{c} R_{\min,M}/2 \\ ({\rm \AA}) \\ \hline \\ 0.9 \\ 1.0 \\ 1.1 \\ 1.2 \\ 1.3 \\ 1.4 \\ 1.5 \\ 1.6 \\ 1.7 \\ 1.8 \\ \end{array}$	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \end{array}$	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01 2.20 2.31 2.43 2.65	=0 tol*Å <sup>4</sup> CN 2.0 3.0 4.0 6.0 6.0 6.0 6.0 8.0 8.8 9.2 12.0	C4= kcal/m IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91 2.16 2.27 2.39 2.61	250 nol*Å <sup>4</sup> CN N/A 2.0 4.0 6.0 6.0 6.0 6.0 8.0 8.4 9.0 11.6	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88 2.13 2.23 2.36 2.58		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85 2.10 2.20 2.33 2.48	750 101*Å <sup>4</sup> CN N/A 2.0 4.0 4.0 6.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0	C4= kcal/n IOD (Å) N/A 1.33 1.45 1.71 1.82 2.07 2.17 2.31 2.45	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0
$\begin{array}{c} R_{\min,M}/2 \\ ({\rm \AA}) \\ \hline \\ 0.9 \\ 1.0 \\ 1.1 \\ 1.2 \\ 1.3 \\ 1.4 \\ 1.5 \\ 1.6 \\ 1.7 \\ 1.8 \\ 1.9 \\ \end{array}$	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ \end{array}$	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01 2.20 2.31 2.43 2.65 2.72	=0 tol*Å <sup>4</sup> CN 2.0 3.0 4.0 6.0 6.0 6.0 8.0 8.8 9.2 12.0 12.0	C4= kcal/m IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91 2.16 2.27 2.39 2.61 2.69	$\begin{array}{c} 250 \\ nol^* \mathring{A}^4 \\ \hline \\ CN \\ \hline \\ N/A \\ 2.0 \\ 4.0 \\ 6.0 \\ 6.0 \\ 6.0 \\ 6.0 \\ 6.0 \\ 8.0 \\ 8.4 \\ 9.0 \\ 11.6 \\ 12.0 \\ \end{array}$	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88 2.13 2.23 2.36 2.58 2.67		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85 2.10 2.20 2.33 2.48 2.64	750 101*Å <sup>4</sup> CN N/A 2.0 4.0 4.0 6.0 6.0 8.0 8.0 8.0 9.0 10.0 12.0	C4= kcal/n IOD (Å) N/A 1.33 1.45 1.71 1.82 2.07 2.17 2.31 2.45 2.62	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0
$\begin{array}{c} R_{\min,M}/2 \\ ({\rm \AA}) \\ \hline \\ 0.9 \\ 1.0 \\ 1.1 \\ 1.2 \\ 1.3 \\ 1.4 \\ 1.5 \\ 1.6 \\ 1.7 \\ 1.8 \\ 1.9 \\ 2.0 \\ \end{array}$	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ 0.38943250 \\ \end{array}$	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01 2.20 2.31 2.43 2.65 2.72 2.80	=0 tol*Å <sup>4</sup> CN 2.0 3.0 4.0 6.0 6.0 6.0 8.0 8.8 9.2 12.0 12.0 12.0 12.0	C4= kcal/m IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91 2.16 2.27 2.39 2.61 2.69 2.77	$\begin{array}{c} 250 \\ nol^* \mathring{A}^4 \\ \hline \\ $	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88 2.13 2.23 2.36 2.58 2.67 2.74		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85 2.10 2.20 2.33 2.48 2.64 2.72	$\begin{array}{c} 750 \\ 1001^* \text{\AA}^4 \\ \hline \text{CN} \\ \hline \text{N/A} \\ 2.0 \\ 4.0 \\ 4.0 \\ 4.0 \\ 6.0 \\ 6.0 \\ 8.0 \\ 8.0 \\ 8.0 \\ 9.0 \\ 10.0 \\ 12.0 \\ 12.0 \\ 12.0 \end{array}$	C4= kcal/m IOD (Å) N/A 1.33 1.45 1.71 1.82 2.07 2.17 2.31 2.45 2.62 2.70	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0
$\begin{array}{c} R_{\min,M}/2 \\ ({\rm \AA}) \\ \hline \\ 0.9 \\ 1.0 \\ 1.1 \\ 1.2 \\ 1.3 \\ 1.4 \\ 1.5 \\ 1.6 \\ 1.7 \\ 1.8 \\ 1.9 \\ 2.0 \\ 2.1 \\ \end{array}$	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ 0.38943250 \\ 0.47874242 \\ \end{array}$	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01 2.20 2.31 2.43 2.65 2.72 2.80 2.88	=0 tol*Å <sup>4</sup> CN 2.0 3.0 4.0 6.0 6.0 6.0 6.0 8.0 8.8 9.2 12.0 12.0 12.0 12.0 12.0	C4= kcal/n IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91 2.16 2.27 2.39 2.61 2.69 2.77 2.85	$\begin{array}{c} 250 \\ nol^* \mathring{A}^4 \\ \hline \\ $	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88 2.13 2.23 2.36 2.58 2.67 2.74 2.83		C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85 2.10 2.20 2.33 2.48 2.64 2.72 2.80	$\begin{array}{c} 750 \\ 1001^* \text{\AA}^4 \\ \hline \text{CN} \\ \hline \text{N/A} \\ 2.0 \\ 4.0 \\ 4.0 \\ 4.0 \\ 6.0 \\ 6.0 \\ 8.0 \\ 9.0 \\ 10.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \end{array}$	C4= kcal/m IOD (Å) N/A 1.33 1.45 1.71 1.82 2.07 2.17 2.31 2.45 2.62 2.70 2.78	1000 nol*Å <sup>4</sup> CN N/A 4.0 4.0 6.0 6.0 8.0 8.0 9.0 10.0 12.0 12.0 12.0
$\begin{array}{c} R_{\min,M}/2 \\ ({\rm \AA}) \\ \hline 0.9 \\ 1.0 \\ 1.1 \\ 1.2 \\ 1.3 \\ 1.4 \\ 1.5 \\ 1.6 \\ 1.7 \\ 1.8 \\ 1.9 \\ 2.0 \\ 2.1 \\ 2.2 \end{array}$	$\begin{array}{c} \epsilon_{M} \\ (kcal/mol) \\ \hline 0.00000062 \\ 0.0001422 \\ 0.00016377 \\ 0.00110429 \\ 0.00490301 \\ 0.01570749 \\ 0.03899838 \\ 0.07934493 \\ 0.13818331 \\ 0.21312875 \\ 0.29896986 \\ 0.38943250 \\ 0.47874242 \\ 0.56252208 \\ \end{array}$	C4 kcal/m IOD (Å) 1.08 1.34 1.50 1.77 1.85 2.01 2.20 2.31 2.43 2.65 2.72 2.80 2.88 2.96	=0 tol*Å <sup>4</sup> CN 2.0 3.0 4.0 6.0 6.0 6.0 6.0 8.0 8.8 9.2 12.0 12.0 12.0 12.0 12.0 12.0	C4= kcal/n IOD (Å) N/A 1.14 1.44 1.72 1.80 1.91 2.16 2.27 2.39 2.61 2.69 2.77 2.85 2.94	$\begin{array}{c} 250 \\ nol^* \mathring{A}^4 \\ \hline \\ $	C4= kcal/m IOD (Å) 0.94 1.08 1.40 1.51 1.77 1.88 2.13 2.23 2.36 2.58 2.67 2.74 2.83 2.91	$\begin{array}{c} 500\\ \text{ol}^* \text{\AA}^4\\ \hline \\ \hline$	C4= kcal/m IOD (Å) N/A 1.04 1.36 1.48 1.73 1.85 2.10 2.20 2.33 2.48 2.64 2.72 2.80 2.89	$\begin{array}{c} 750 \\ 1001^* \text{\AA}^4 \\ \hline \text{CN} \\ \hline \text{N/A} \\ 2.0 \\ 4.0 \\ 4.0 \\ 4.0 \\ 6.0 \\ 6.0 \\ 8.0 \\ 9.0 \\ 10.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \\ 12.0 \end{array}$	C4= kcal/m IOD (Å) N/A 1.33 1.45 1.71 1.82 2.07 2.17 2.31 2.45 2.62 2.70 2.78 2.87	$\begin{array}{c} 1000\\ 1000\\ 101^{*} \mathring{A}^{4}\\ \hline \\ \hline$

**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<sup>*a*</sup>

	OF	PC3		O	PC		TIP3	P-FB		TIP4P-FB			
	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	
$\mathrm{Fe}^{3+}$	-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 <sup>3+</sup>	-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 <sup>3+</sup>	-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	
$\mathrm{Sm}^{\mathrm{3+}}$	-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	
$\mathrm{Gd}^{3+}$	-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	
$\mathrm{Er}^{3+}$	-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 <sup>3+</sup>	-839.8	2.03	6.0	-840.5	2.00	6.0	-838.4	2.01	6.0	-841.7	1.97	6.0	
$\mathrm{Hf}^{4+}$	-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 S4.** Calculated HFE, IOD, and CN Values for the 12-6 HFE Parameter Set for the Four New Water Models (Parameters in Table 2).

	OF	PC3		0	PC		TIP	3P-FB		TIP	4P-FB	
	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 <sup>3+</sup>	-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 <sup>3+</sup>	-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 <sup>3+</sup>	-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 <sup>3+</sup>	-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 <sup>3+</sup>	-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
$\mathrm{Sm}^{\mathrm{3+}}$	-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
$\mathrm{Gd}^{3+}$	-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 <sup>3+</sup>	-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 <sup>3+</sup>	-775.2	2.33	8.2	-758.7	2.33	8.0	-767.1	2.33	8.4	-753.5	2.33	8.1
$\mathrm{Hf}^{4+}$	-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
$\mathrm{U}^{4+}$	-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 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									
$Al^{3+}$	-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 <sup>3+</sup>	-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 <sup>3+</sup>	-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 <sup>3+</sup>	-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
$\mathrm{Sm}^{3+}$	-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
$\mathrm{Gd}^{3+}$	-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
$\mathrm{Er}^{3+}$	-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
$\mathrm{Hf}^{4+}$	-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
$\mathrm{U}^{4+}$	-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 S6.** Calculated HFE, IOD, and CN Values for the 12-6-4 Parameter Set for the Four New Water Models (Parameters in Table 4).

Diffusivity coefficients of the and creation of the conjunction with the of carbon history									
	$Al^{3+}$	$Cr^{3+}$							
Parameter Set	Diffusion coefficient $(10^{-5} \text{ cm}^2/\text{s})$	Parameter Set	Diffusion coefficient $(10^{-5} \text{ cm}^2/\text{s})$						
12-6 HFE	0.619±0.110	12-6 HFE	$0.592 \pm 0.099$						
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 <sup>6</sup>	0.541	Experiment <sup>6</sup>	0.595						

**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

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