Supporting Information for:

Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model

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Table S1. Density determined using the AMOEBA14 and AMOEBA03 models for temperatures ranging from 249.15 Kelvin to 373.15 Kelvin at 1 atm. Units are kg/m^3.

Temp	Expt.	AMOEBA 14	AMOEBA03
249.15	990.5	989.5 ± 1.1	960.5 ± 3.6
253.15	993.5	993.2 ± 0.9	973.1 ± 2.0
257.15	995.8	996.5 ± 0.7	980.5 ± 1.1
261.15	997.5	998.6 ± 0.5	986.2 ± 0.8
265.15	998.6	999.9 ± 0.5	991.0 ± 0.6
269.15	999.4	1000.7 ± 0.4	995.0 ± 0.5
273.15	999.8	1001.3 ± 0.4	998.0 ± 0.4
277.15	1000.0	1001.5 ± 0.3	1000.0 ± 0.4
281.15	999.8	1001.3 ± 0.3	1001.0 ± 0.3
285.15	999.5	1000.8 ± 0.3	1001.5 ± 0.3
289.15	998.9	1000.1 ± 0.3	1001.6 ± 0.3
293.15	998.2	999.1 ± 0.2	1001.3 ± 0.2
298.15	997.0	997.9 ± 0.2	1000.7 ± 0.2
301.15	996.2	997.1 ± 0.2	1000.1 ± 0.2
305.15	995.0	996.0 ± 0.2	999.1 ± 0.2
309.15	993.7	994.7 ± 0.2	997.8 ± 0.2
313.15	992.2	993.3 ± 0.2	996.2 ± 0.2
317.15	990.6	991.7 ± 0.2	994.3 ± 0.2
321.15	988.9	989.9 ± 0.2	992.2 ± 0.2
325.15	987.1	987.9 ± 0.2	990.0 ± 0.2
329.15	985.2	985.7 ± 0.2	987.7 ± 0.2
333.15	983.2	983.4 ± 0.2	985.3 ± 0.2
337.15	981.1	981.1 ± 0.2	982.7 ± 0.2
341.15	978.9	978.6 ± 0.2	979.9 ± 0.2
345.15	976.6	975.9 ± 0.2	976.9 ± 0.2
349.15	974.2	973.1 ± 0.2	973.9 ± 0.2
353.15	971.8	970.3 ± 0.2	970.8 ± 0.2
357.15	969.3	967.4 ± 0.2	967.6 ± 0.2
361.15	966.7	964.3 ± 0.2	964.1 ± 0.2
365.15	964.0	961.2 ± 0.2	960.5 ± 0.2
369.15	961.2	958.0 ± 0.2	956.7 ± 0.2
373.15	958.4	954.8 ± 0.2	952.8 ± 0.3

Table S2. Enthalpy of vaporization determined using the AMOEBA14 and AMOEBA03 models for temperatures ranging from 249.15 Kelvin to 373.15 Kelvin at 1 atm. Units are kcal/mol.

Temp.	Expt.	AMOEBA14	AMOEBA03
249.15	46.103	47.239 ± 0.065	47.095 ± 0.094
253.15	45.919	46.974 ± 0.055	46.632 ± 0.056
257.15	45.740	46.716 ± 0.048	46.282 ± 0.039
261.15	45.565	46.473 ± 0.046	45.967 ± 0.036
265.15	45.393	46.246 ± 0.046	45.668 ± 0.035
269.15	45.223	46.024 ± 0.046	45.369 ± 0.034
273.15	45.053	45.809 ± 0.046	45.081 ± 0.035
277.15	44.884	45.598 ± 0.045	44.805 ± 0.035
281.15	44.714	45.389 ± 0.045	44.541 ± 0.034
285.15	44.544	45.175 ± 0.045	44.288 ± 0.034
289.15	44.374	44.958 ± 0.044	44.043 ± 0.033
293.15	44.203	44.741 ± 0.044	43.802 ± 0.032
298.15	43.989	44.475 ± 0.044	43.502 ± 0.032
301.15	43.861	44.316 ± 0.045	43.320 ± 0.032
305.15	43.689	44.106 ± 0.046	43.078 ± 0.033
309.15	43.517	43.904 ± 0.047	42.840 ± 0.033
313.15	43.345	43.709 ± 0.047	42.607 ± 0.034
317.15	43.172	43.511 ± 0.047	42.375 ± 0.035
321.15	42.999	43.305 ± 0.047	42.142 ± 0.035
325.15	42.826	43.097 ± 0.048	41.910 ± 0.035
329.15	42.652	42.894 ± 0.048	41.678 ± 0.035
333.15	42.476	42.692 ± 0.048	41.450 ± 0.035
337.15	42.300	42.486 ± 0.048	41.228 ± 0.035
341.15	42.123	42.272 ± 0.048	41.005 ± 0.035
345.15	41.943	42.055 ± 0.049	40.781 ± 0.035
349.15	41.762	41.841 ± 0.049	40.559 ± 0.036
353.15	41.580	41.632 ± 0.050	40.337 ± 0.036
357.15	41.396	41.430 ± 0.051	40.113 ± 0.037
361.15	41.210	41.227 ± 0.053	39.881 ± 0.039
365.15	41.024	41.019 ± 0.058	39.648 ± 0.042
369.15	40.837	40.806 ± 0.067	39.415 ± 0.047
373.15	40.652	40.591 ± 0.077	39.181 ± 0.055

Table S3. Thermal expansion coefficient determined using the AMOEBA14 and AMOEBA03 models for temperatures ranging from 249.15 K to 373.15 K at 1 atm. Units are 10^{-4} K^{-1}.

Temp.	Expt.	AMOEBA14	AMOEBA03
249.15	-8.877	-9.152 ± 2.488	-46.628 ± 12.614
253.15	-6.606	-9.097 ± 2.017	-23.434 ± 6.649
257.15	-4.874	-6.872 ± 1.528	-16.216 ± 3.260
261.15	-3.506	-4.099 ± 1.189	-13.155 ± 2.044
265.15	-2.395	-2.520 ± 1.024	-11.041 ± 1.623
269.15	-1.469	-1.784 ± 0.900	-9.027 ± 1.303
273.15	-0.680	-0.967 ± 0.779	-6.348 ± 1.035
277.15	0.003	-0.053 ± 0.691	-3.636 ± 0.845
281.15	0.604	0.795 ± 0.630	-1.726 ± 0.720
285.15	1.141	1.633 ± 0.564	-0.655 ± 0.628
289.15	1.626	2.265 ± 0.498	0.134 ± 0.549
293.15	2.068	2.445 ± 0.457	0.904 ± 0.482
298.15	2.572	2.416 ± 0.428	1.726 ± 0.415
301.15	2.853	2.582 ± 0.411	2.183 ± 0.387
305.15	3.206	3.051 ± 0.389	2.874 ± 0.370
309.15	3.539	3.513 ± 0.372	3.653 ± 0.370
313.15	3.853	3.836 ± 0.362	4.388 ± 0.367
317.15	4.152	4.236 ± 0.353	4.989 ± 0.353
321.15	4.438	4.828 ± 0.343	5.427 ± 0.338
325.15	4.712	5.359 ± 0.333	5.703 ± 0.327
329.15	4.975	5.647 ± 0.325	5.974 ± 0.318
333.15	5.231	5.866 ± 0.318	6.411 ± 0.307
337.15	5.478	6.207 ± 0.313	6.941 ± 0.298
341.15	5.719	6.630 ± 0.310	7.367 ± 0.293
345.15	5.954	6.987 ± 0.310	7.616 ± 0.293
349.15	6.185	7.215 ± 0.312	7.830 ± 0.294
353.15	6.411	7.412 ± 0.316	8.187 ± 0.296
357.15	6.633	7.704 ± 0.321	8.680 ± 0.299
361.15	6.853	8.056 ± 0.332	9.199 ± 0.309
365.15	7.071	8.317 ± 0.356	9.688 ± 0.330
369.15	7.287	8.407 ± 0.398	10.105 ± 0.367
373.15	7.501	8.369 ± 0.454	10.437 ± 0.418

Table S4. Isothermal compressibility determined using the AMOEBA14 and AMOEBA03 models for temperatures ranging from 249.15 K to 373.15 K at 1 atm. Units are 10^{-6} bar^{-1}.

Temp	Expt.	AMOEBA14	AMOEBA03
249.15	67.985	65.373 ± 5.070	160.222 ± 27.616
253.15	63.996	65.066 ± 4.149	118.122 ± 14.617
257.15	60.783	61.819 ± 3.127	104.895 ± 7.348
261.15	58.116	58.027 ± 2.351	98.056 ± 4.755
265.15	55.851	55.527 ± 1.980	91.552 ± 3.731
269.15	53.893	53.806 ± 1.755	86.138 ± 2.952
273.15	52.176	52.072 ± 1.527	81.446 ± 2.363
277.15	50.653	50.469 ± 1.348	77.030 ± 1.940
281.15	49.288	49.163 ± 1.235	73.512 ± 1.655
285.15	48.056	48.108 ± 1.115	71.061 ± 1.465
289.15	46.934	47.417 ± 0.988	69.278 ± 1.292
293.15	45.892	47.049 ± 0.910	67.803 ± 1.130
298.15	45.247	46.577 ± 0.872	66.105 ± 0.965
301.15	44.943	46.171 ± 0.845	65.162 ± 0.904
305.15	44.622	45.639 ± 0.791	64.136 ± 0.879
309.15	44.390	45.260 ± 0.742	63.491 ± 0.888
313.15	44.239	44.988 ± 0.712	63.150 ± 0.879
317.15	44.162	44.877 ± 0.695	62.923 ± 0.839
321.15	44.153	45.046 ± 0.675	62.697 ± 0.796
325.15	44.209	45.339 ± 0.651	62.532 ± 0.772
329.15	44.324	45.551 ± 0.636	62.612 ± 0.766
333.15	44.496	45.747 ± 0.634	63.003 ± 0.763
337.15	44.723	46.060 ± 0.644	63.546 ± 0.759
341.15	45.003	46.501 ± 0.658	63.980 ± 0.755
345.15	45.333	47.018 ± 0.666	64.160 ± 0.751
349.15	45.714	47.632 ± 0.667	64.226 ± 0.743
353.15	46.143	48.421 ± 0.668	64.509 ± 0.736
357.15	46.621	49.337 ± 0.674	65.251 ± 0.744
361.15	47.148	50.194 ± 0.698	66.518 ± 0.787
365.15	47.722	50.889 ± 0.752	68.277 ± 0.873
369.15	48.346	51.520 ± 0.839	70.342 ± 0.999
373.15	49.019	52.246 ± 0.952	72.489 ± 1.162

Table S5. Isobaric heat capacity determined using the AMOEBA14 and AMOEBA03 models for temperatures ranging from 249.15 K to 373.15 K at 1 atm. Units are cal mol^{-1} K^{-1}.

Temp.	Expt.	AMOEBA14	AMOEBA03
249.15	19.177	23.689 ± 2.010	42.263 ± 8.351
253.15	18.777	23.745 ± 1.658	30.878 ± 4.336
257.15	18.532	23.081 ± 1.252	27.610 ± 2.023
261.15	18.380	22.014 ± 0.953	26.255 ± 1.231
265.15	18.280	21.341 ± 0.822	25.821 ± 1.032
269.15	18.210	20.992 ± 0.748	25.589 ± 0.845
273.15	18.157	20.658 ± 0.691	24.812 ± 0.649
277.15	18.115	20.454 ± 0.649	24.114 ± 0.531
281.15	18.080	20.519 ± 0.611	23.431 ± 0.474
285.15	18.052	20.770 ± 0.576	22.755 ± 0.445
289.15	18.030	20.925 ± 0.548	22.386 ± 0.425
293.15	18.015	20.732 ± 0.525	22.252 ± 0.406
298.15	18.002	20.482 ± 0.498	22.359 ± 0.389
301.15	17.998	20.425 ± 0.482	22.405 ± 0.382
305.15	17.995	20.087 ± 0.465	22.182 ± 0.376
309.15	17.995	19.513 ± 0.460	21.855 ± 0.373
313.15	17.996	19.334 ± 0.458	21.691 ± 0.368
317.15	17.999	19.713 ± 0.454	21.591 ± 0.358
321.15	18.002	20.039 ± 0.448	21.595 ± 0.345
325.15	18.006	19.857 ± 0.441	21.616 ± 0.333
329.15	18.011	19.509 ± 0.433	21.369 ± 0.325
333.15	18.018	19.535 ± 0.422	20.985 ± 0.320
337.15	18.026	19.930 ± 0.409	20.824 ± 0.318
341.15	18.035	20.237 ± 0.399	20.840 ± 0.318
345.15	18.046	20.178 ± 0.396	20.760 ± 0.320
349.15	18.058	19.811 ± 0.398	20.611 ± 0.321
353.15	18.071	19.339 ± 0.402	20.647 ± 0.319
357.15	18.086	19.060 ± 0.407	20.886 ± 0.318
361.15	18.101	19.141 ± 0.419	21.060 ± 0.325
365.15	18.117	19.397 ± 0.446	21.024 ± 0.350
369.15	18.134	19.547 ± 0.493	20.928 ± 0.396
373.15	18.151	19.505 ± 0.558	21.075 ± 0.461

Table S6. Dielectric constant determined using the AMOEBA14 and AMOEBA03 models for temperatures ranging from 249.15 K to 373.15 K at 1 atm.

Temp.	Expt.	AMOEBA14	AMOEBA03
249.15	98.650	97.737 ± 7.876	121.234 ± 11.002
253.15	96.580	95.578 ± 5.816	115.714 ± 7.315
257.15	94.683	94.541 ± 4.643	111.897 ± 5.229
261.15	92.898	93.602 ± 4.124	110.050 ± 4.030
265.15	91.186	92.808 ± 3.694	109.014 ± 3.364
269.15	89.525	92.249 ± 3.398	107.758 ± 2.991
273.15	87.903	91.219 ± 3.202	106.083 ± 2.748
277.15	86.311	89.491 ± 2.921	103.973 ± 2.501
281.15	84.749	87.585 ± 2.571	101.347 ± 2.225
285.15	83.213	85.704 ± 2.254	98.525 ± 1.998
289.15	81.705	83.697 ± 1.996	95.856 ± 1.808
293.15	80.223	81.622 ± 1.785	93.335 ± 1.605
298.15	78.409	79.396 ± 1.597	90.395 ± 1.379
301.15	77.339	78.390 ± 1.529	88.835 ± 1.288
305.15	75.935	77.276 ± 1.473	86.965 ± 1.204
309.15	74.556	76.081 ± 1.416	85.206 ± 1.135
313.15	73.200	74.611 ± 1.332	83.368 ± 1.067
317.15	71.869	72.889 ± 1.225	81.256 ± 0.992
321.15	70.560	70.958 ± 1.114	78.936 ± 0.901
325.15	69.275	68.958 ± 1.017	76.686 ± 0.808
329.15	68.012	67.152 ± 0.941	74.669 ± 0.737
333.15	66.772	65.670 ± 0.880	72.815 ± 0.690
337.15	65.555	64.407 ± 0.827	70.990 ± 0.653
341.15	64.359	63.233 ± 0.780	69.187 ± 0.616
345.15	63.184	62.104 ± 0.739	67.522 ± 0.578
349.15	62.030	60.962 ± 0.702	66.075 ± 0.541
353.15	60.897	59.704 ± 0.665	64.771 ± 0.505
357.15	59.784	58.286 ± 0.632	63.442 ± 0.473
361.15	58.691	56.811 ± 0.610	61.976 ± 0.454
365.15	57.617	55.435 ± 0.618	60.418 ± 0.462
369.15	56.561	54.223 ± 0.665	58.913 ± 0.502
373.15	55.522	53.142 ± 0.746	57.562 ± 0.568

Table S7. Second virial coefficient of water. AMOEBA14 and AMOEBA03 results are shown for the classical value, $B_{cl}(T)$, as well as the translational and rotational quantum corrections, ΔB_{trans} and ΔB_{rot}. The overall value, B(T), is the sum of the three terms.

Temp. (K)	Expt.	AMOEBA03				AMOEBA14			
		$B_{cl}(T)$	ΔB_{trans}	ΔB_{rot}	B(T)	$B_{cl}(T)$	ΔB_{trans}	ΔB_{rot}	B(T)
298	-1.158	-1.2013	0.0301	0.3738	-0.7974	-1.0689	0.0245	0.3089	-0.7356
310	-0.966	-0.9866	0.0224	0.2755	-0.6888	-0.8941	0.0185	0.2371	-0.6385
323	-0.816	-0.7982	0.0160	0.2016	-0.5806	-0.7323	0.0137	0.1723	-0.5462
336	-0.696	-0.6679	0.0120	0.1533	-0.5025	-0.6142	0.0103	0.1318	-0.4721
360	-0.526	-0.6615	0.0121	0.1507	-0.4988	-0.4533	0.0065	0.0837	-0.3631
380	-0.428	-0.3876	0.0053	0.0656	-0.3167	-0.3653	0.0046	0.0594	-0.3013
400	-0.356	-0.3198	0.0039	0.0478	-0.2681	-0.2991	0.0034	0.0437	-0.2520
423	-0.275	-0.2573	0.0028	0.0345	-0.2200	-0.2479	0.0025	0.0319	-0.2135
448	-0.240	-0.2128	0.0020	0.0250	-0.1857	-0.2014	0.0018	0.0232	-0.1764
473	-0.201	-0.1755	0.0015	0.0188	-0.1552	-0.1688	0.0014	0.0178	-0.1496
523	-0.150	-0.1255	0.0009	0.0113	-0.1133	-0.1210	0.0009	0.0108	-0.1093
573	-0.116	-0.0932	0.0006	0.0074	-0.0852	-0.0907	0.0006	0.0072	-0.0829
673	-0.074	-0.0559	0.0003	0.0037	-0.0518	-0.0543	0.0003	0.0037	-0.0504
773	-0.050	-0.0351	0.0002	0.0022	-0.0327	-0.0341	0.0002	0.0022	-0.0317

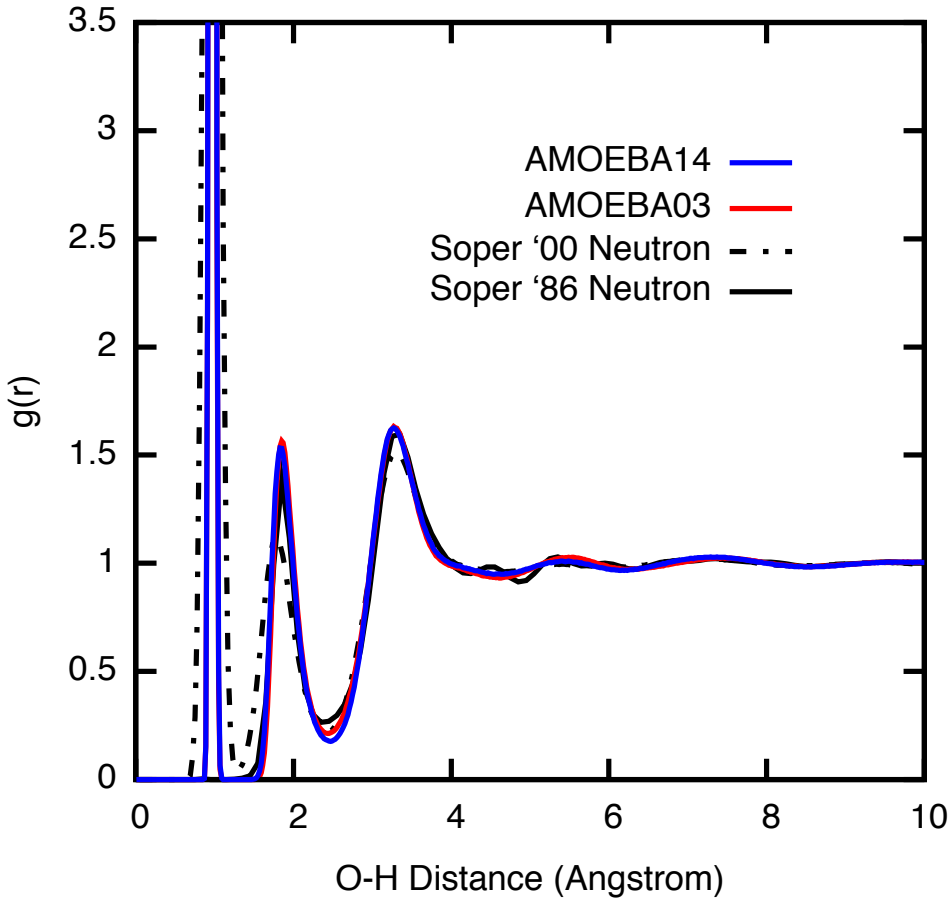

Figure S1. The water O-H radial distribution functions at 298K for AMOEBA03, AMOEBA14 and iAMOEBA compared against experimental values.

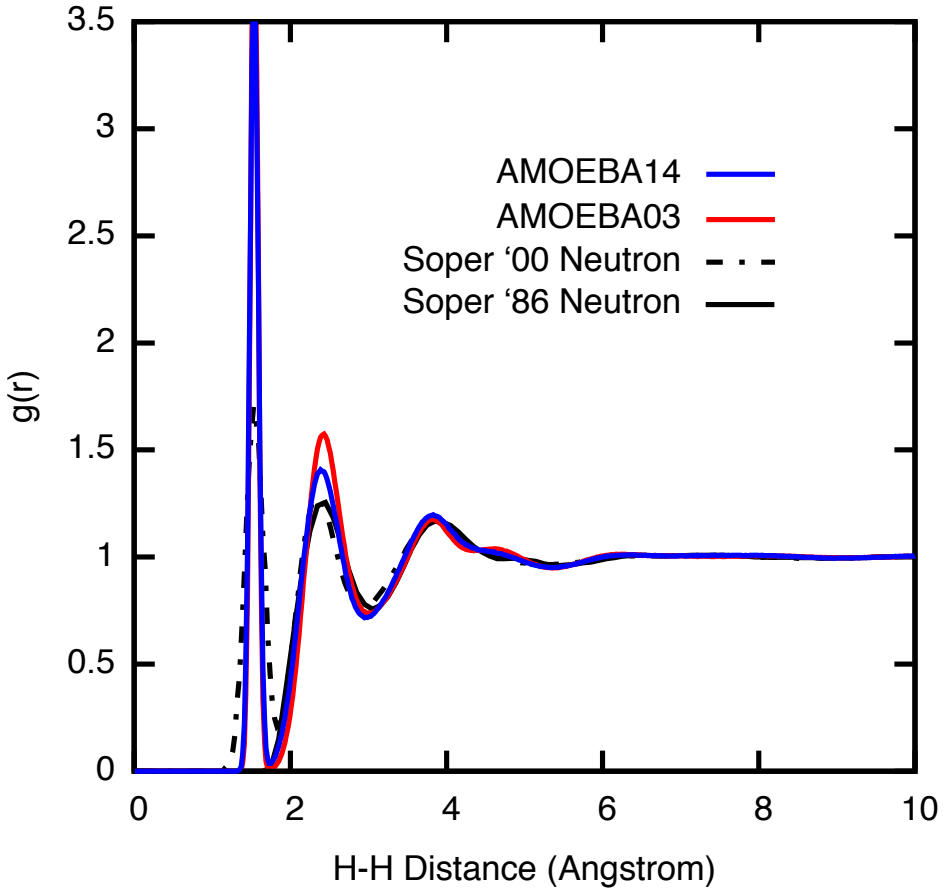

Figure S2. The water H-H radial distribution functions at 298K for AMOEBA03, AMOEBA14 and iAMOEBA compared against experimental values.