

Comparison of Frozen-Density Embedding and Discrete Reaction Field Solvent Models for Molecular Properties

Supplementary Material

Christoph R. Jacob^{a,1}, Johannes Neugebauer^{a,2}, Lasse Jensen^{b,3},
and Lucas Visscher^{a,4}

^aVrije Universiteit Amsterdam,
Department of Theoretical Chemistry, Faculty of Sciences,
De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands

^bNorthwestern University, Department of Chemistry,
2145 Sheridan Road, Evanston, IL 60208-3113, USA

¹E-Mail: jacob@few.vu.nl

²E-Mail: jneugeb@chem.vu.nl

³E-Mail: l.jensen@chem.northwestern.edu

⁴E-Mail: visscher@chem.vu.nl

In this supplementary material the coordinates of the water cluster used in our calculations are given. These coordinates are also given in XYZ format in a separate file.

Table I: Structure of the water cluster used in the calculations. Water molecule no. 1 is considered as the solute, all other water molecules form the solvent shell. All coordinates are given in atomic units.

no.	atom	x	y	z
H2O 1 (solute)	O	0.000000	0.000000	0.000000
	H	-1.430143	0.000000	1.107393
	H	1.430143	0.000000	1.107393
H2O 2	O	-11.380487	-11.810553	-4.515226
	H	-13.104750	-11.837668	-3.969549
	H	-10.510887	-12.853302	-3.320214
H2O 3	O	-1.116350	9.119186	-3.230948
	H	-2.822701	9.717028	-3.180632
	H	-0.123780	10.538183	-2.708611
H2O 4	O	4.469332	-0.503788	2.210877
	H	4.273576	-2.085090	3.066884
	H	5.919073	-0.737018	1.154734
H2O 5	O	-16.969012	-3.658353	-10.785713
	H	-15.708245	-4.239962	-9.626497
	H	-16.478149	-4.360802	-12.378572
H2O 6	O	-10.765608	-4.163577	0.518032
	H	-9.161169	-3.986232	-0.298001
	H	-11.974842	-3.796368	-0.775990
H2O 7	O	-6.554233	-9.202975	-11.231254
	H	-8.153008	-9.653539	-10.515367
	H	-6.907141	-7.749987	-12.249029
H2O 8	O	-14.167136	-6.558132	-6.629574
	H	-13.746900	-8.312032	-6.766757
	H	-15.432937	-6.495366	-5.339073
H2O 9	O	-1.012338	-6.537375	-20.632283
	H	0.513578	-7.016737	-19.787667
	H	-2.258470	-6.487215	-19.322236
H2O 10	O	-7.973723	4.333816	8.858697
	H	-7.392102	2.717043	9.423808
	H	-7.341341	4.477733	7.170217
H2O 11	O	1.687680	-11.293163	-2.876367
	H	1.520004	-11.659990	-4.639576
	H	0.925644	-9.664791	-2.678150
H2O 12	O	1.091846	-1.698117	-18.817171
	H	2.072153	-2.343258	-20.193534
	H	0.133987	-3.119028	-18.238291
H2O 13	O	-13.852587	-1.513172	-3.428477
	H	-13.345617	-1.909473	-5.118894
	H	-15.318869	-2.533446	-3.144505
H2O 14	O	5.289604	-6.812668	-13.105858
	H	7.017082	-6.621785	-12.604893
	H	4.346712	-5.977920	-11.807499
H2O 15	O	-11.474072	-10.907083	-9.440850
	H	-11.216113	-12.454404	-10.341316

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Table I: Structure of the water cluster used in the calculations.
(continued)

no.	atom	x	y	z
	H	-11.176343	-11.335919	-7.709076
H20 16	O	-1.645921	-11.435233	1.480980
	H	-0.305579	-10.473635	0.739090
	H	-1.729938	-12.940685	0.481912
H20 17	O	-7.324684	-5.018181	4.387749
	H	-8.818370	-4.730291	3.409176
	H	-7.759228	-6.389106	5.484707
H20 18	O	5.208797	-6.838506	3.691461
	H	5.265790	-6.685119	1.890125
	H	6.391621	-5.607189	4.288426
H20 19	O	-1.248954	-6.977509	-2.931094
	H	-2.378328	-6.595798	-1.570801
	H	-0.212881	-5.503091	-3.086752
H20 20	O	6.737491	-0.260656	-6.588501
	H	6.563017	-2.046802	-6.813946
	H	8.299250	0.148296	-7.404129
H20 21	O	5.306243	-5.543095	-6.435993
	H	3.812800	-6.090722	-7.296991
	H	6.651899	-6.435270	-7.251355
H20 22	O	-5.722143	-7.593764	-5.609892
	H	-5.637663	-7.499595	-7.414214
	H	-3.997351	-7.514256	-5.071046
H20 23	O	-4.964121	4.323349	-3.258997
	H	-6.269194	5.559506	-3.058294
	H	-3.431140	5.226291	-2.933039
H20 24	O	-10.942326	0.554379	-13.182449
	H	-9.993651	2.083341	-13.366497
	H	-12.257983	0.686448	-14.416622
H20 25	O	-9.296367	5.399236	-12.624634
	H	-7.787172	5.399698	-11.627680
	H	-8.713677	5.570734	-14.328348
H20 26	O	2.976413	-12.445061	3.626050
	H	3.661096	-10.770921	3.633077
	H	1.221490	-12.215013	3.253348
H20 27	O	-7.520338	-2.709606	-16.431855
	H	-8.541435	-2.016582	-15.109485
	H	-8.126184	-1.911147	-17.937510
H20 28	O	-1.697017	-2.043822	-8.206757
	H	-1.169362	-0.432664	-8.837102
	H	-0.636639	-2.337826	-6.771227
H20 29	O	5.301322	-9.560473	8.452236
	H	5.273862	-8.617631	6.908901
	H	4.550179	-8.455453	9.671374
H20 30	O	5.994893	-5.843987	-1.278668
	H	6.104997	-5.948817	-3.081019
	H	7.022977	-4.420655	-0.844212
H20 31	O	-8.499334	6.307303	1.262069
	H	-9.264138	5.216347	0.038764
	H	-9.841307	6.720288	2.402303

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Table I: Structure of the water cluster used in the calculations.
(continued)

no.	atom	x	y	z
H20 32	O	1.422658	7.151005	-6.702457
	H	0.491241	7.745308	-5.270377
	H	2.872433	6.334866	-5.992772
H20 33	O	1.165723	-15.863273	-8.030117
	H	-0.439795	-16.566458	-8.476687
	H	1.270245	-14.330699	-8.985039
H20 34	O	-1.891948	-10.635521	-8.584698
	H	-2.788156	-10.717519	-10.153669
	H	-2.907785	-11.590556	-7.432498
H20 35	O	1.303221	-6.546667	-9.290668
	H	0.041454	-7.803822	-8.975882
	H	0.439986	-4.972917	-9.067680
H20 36	O	-4.108004	-6.593872	-16.433977
	H	-4.900894	-8.114135	-17.009918
	H	-5.447950	-5.380612	-16.369714
H20 37	O	-5.920829	-3.031071	-2.510728
	H	-5.780713	-4.560880	-3.465523
	H	-6.212676	-1.747908	-3.751655
H20 38	O	-5.199834	-12.826876	-4.968785
	H	-6.704703	-13.433268	-5.768310
	H	-5.429549	-11.035455	-4.870672
H20 39	O	-4.897867	5.501788	-16.517711
	H	-4.966749	7.305860	-16.407434
	H	-3.227631	5.077951	-15.967930
H20 40	O	-17.578987	-4.993467	-2.976815
	H	-18.763866	-3.841942	-2.240855
	H	-17.398663	-6.306119	-1.745551
H20 41	O	-3.507768	-17.323802	-10.104425
	H	-4.401931	-18.633085	-10.974960
	H	-4.539511	-16.949532	-8.666715
H20 42	O	-10.819116	-4.666408	-11.144871
	H	-11.621851	-4.882964	-9.538538
	H	-10.609156	-2.877364	-11.308649
H20 43	O	-6.392055	0.017935	-6.732485
	H	-5.821253	1.226250	-5.513574
	H	-4.874902	-0.728020	-7.375433
H20 44	O	-11.305055	0.463797	-8.250657
	H	-9.642271	0.806743	-7.626859
	H	-11.198970	0.791091	-10.026384
H20 45	O	9.003924	1.260468	-13.978052
	H	8.872950	1.029481	-12.188897
	H	7.294256	1.453383	-14.536089
H20 46	O	1.143175	-2.768263	-3.930866
	H	2.949704	-2.781020	-3.842132
	H	0.628498	-1.739396	-2.535113
H20 47	O	-5.215466	-0.716794	1.975589
	H	-5.881933	-1.357545	0.420969
	H	-5.825941	-1.861509	3.235957
H20 48	O	-5.420316	3.662969	4.478819

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Table I: Structure of the water cluster used in the calculations.
(continued)

no.	atom	x	y	z
	H	-6.477342	4.753711	3.496698
	H	-5.283871	2.154314	3.490422
H20 49	O	-10.890417	3.434227	-2.589015
	H	-11.048283	1.963519	-3.630016
	H	-12.483474	3.562677	-1.742108
H20 50	O	-5.775320	11.853646	-3.101847
	H	-7.420972	11.268971	-2.631136
	H	-5.594935	13.436445	-2.245230
H20 51	O	4.649786	3.675426	-3.783517
	H	5.304643	2.161377	-4.525409
	H	3.400168	3.100409	-2.609040
H20 52	O	-1.567977	3.410131	-9.464615
	H	-0.626486	4.692285	-8.603650
	H	-1.229765	3.700123	-11.217641
H20 53	O	-5.851145	5.947899	-8.752976
	H	-4.364364	4.937406	-8.952908
	H	-5.233574	7.643906	-8.635724
H20 54	O	-5.554133	-7.923600	0.255548
	H	-4.383273	-9.288435	0.450223
	H	-6.017695	-7.479952	1.946662
H20 55	O	-10.801479	4.924607	-18.428256
	H	-9.467731	4.114450	-19.342775
	H	-12.082856	3.656860	-18.278348
H20 56	O	11.847656	6.046520	-5.603357
	H	12.238224	7.542818	-4.665204
	H	10.145164	6.293731	-6.161919
H20 57	O	1.386876	-3.561002	5.147103
	H	2.355859	-2.845564	6.496475
	H	2.259942	-5.087064	4.722284
H20 58	O	9.401772	-2.164511	0.065934
	H	9.991916	-0.603357	-0.631284
	H	10.908492	-3.099727	0.421948
H20 59	O	-3.306352	-3.510754	7.521433
	H	-1.821452	-3.757766	6.518615
	H	-4.649775	-4.184206	6.514825
H20 60	O	-3.837669	11.000091	-8.559487
	H	-3.743740	10.833060	-6.760914
	H	-4.874396	12.458209	-8.825323
H20 61	O	-8.922772	7.515155	-5.130050
	H	-7.642411	6.796305	-6.186229
	H	-9.987510	6.119163	-4.695168
H20 62	O	-0.328799	4.856437	-14.284939
	H	-0.201219	6.618156	-13.895513
	H	1.105589	4.519547	-15.334042
H20 63	O	-2.881192	-21.161439	-13.737737
	H	-1.096481	-20.881550	-13.827486
	H	-3.127888	-22.768721	-14.529801
H20 64	O	4.084301	-17.323502	4.721371
	H	4.024131	-15.518279	4.625782

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Table I: Structure of the water cluster used in the calculations.
(continued)

no.	atom	x	y	z
	H	2.369362	-17.818926	5.013133
H20 65	O	-12.718566	7.205589	4.460795
	H	-14.459983	7.694157	4.479549
	H	-11.909749	8.368875	5.585145
H20 66	O	3.646309	-5.777295	11.936169
	H	4.697699	-5.280697	13.321648
	H	1.980190	-5.852159	12.636189
H20 67	O	-11.582902	-8.009770	-14.717441
	H	-11.154532	-6.961783	-13.306835
	H	-13.310143	-7.607206	-15.072634
H20 68	O	-22.691319	-4.602067	-11.338511
	H	-22.222728	-6.122623	-12.198693
	H	-21.135451	-3.704676	-11.125083
H20 69	O	5.964801	4.513703	3.703328
	H	5.242917	3.066218	2.893848
	H	4.736155	5.002020	4.937653
H20 70	O	4.568726	15.366721	-5.272902
	H	6.232086	14.724941	-5.577752
	H	4.568871	17.006212	-6.036872
H20 71	O	-19.420245	0.101012	-13.928108
	H	-18.314059	-1.071686	-13.107913
	H	-20.713212	0.433367	-12.707714
H20 72	O	4.028370	-8.180716	-24.036693
	H	5.655114	-8.965853	-24.130736
	H	3.080163	-9.236467	-22.915141
H20 73	O	-16.598416	-12.079831	-3.027250
	H	-16.867920	-10.478507	-2.230559
	H	-17.759278	-12.096643	-4.414224
H20 74	O	-7.269666	11.013178	-13.834325
	H	-8.505325	11.789160	-12.765409
	H	-5.999216	12.281927	-14.052995
H20 75	O	14.926078	0.729892	-0.880692
	H	14.684685	0.444233	0.888972
	H	13.432629	1.604655	-1.406033
H20 76	O	-10.249930	-15.511937	-12.567035
	H	-10.815693	-16.802050	-11.432530
	H	-8.811185	-16.233598	-13.392143
H20 77	O	6.153774	-6.810349	-18.378764
	H	5.668826	-7.601311	-16.826092
	H	7.802388	-6.142320	-18.051056
H20 78	O	3.767930	-11.873194	-12.000036
	H	5.530167	-12.150411	-12.298787
	H	3.520657	-10.115534	-12.347993
H20 79	O	4.238655	2.169696	-16.376549
	H	3.035930	0.926934	-16.906250
	H	5.028606	2.717325	-17.908757
H20 80	O	-14.682710	0.723814	-16.713445
	H	-15.146156	-0.558170	-17.902276
	H	-16.240331	1.191942	-15.922083

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Table I: Structure of the water cluster used in the calculations.
(continued)

no.	atom	x	y	z
H20 81	O	-8.561719	-1.140463	-21.112374
	H	-7.247272	0.101638	-21.143972
	H	-7.967236	-2.456681	-22.201292
H20 82	O	3.098039	-19.304371	-4.729504
	H	4.475918	-18.539272	-3.842004
	H	2.316059	-17.936405	-5.617626
H20 83	O	-11.481971	-2.627730	8.985770
	H	-12.101806	-1.963577	7.421708
	H	-12.537150	-4.058240	9.320165
H20 84	O	-15.326832	4.993788	0.715203
	H	-16.282312	3.624938	1.411545
	H	-14.247077	5.525334	2.065452
H20 85	O	4.699246	-3.093313	-22.212181
	H	4.440050	-3.027219	-24.001044
	H	4.907824	-4.853023	-21.849556
H20 86	O	5.481254	-14.871569	-2.300088
	H	6.047926	-15.537002	-0.716527
	H	4.081237	-13.810067	-1.870262
H20 87	O	7.716927	7.491705	-0.281469
	H	7.150103	7.474634	1.436088
	H	6.704471	6.239325	-1.104914
H20 88	O	-0.099717	10.178584	-12.503376
	H	1.433197	10.526454	-11.608532
	H	-1.386487	10.226881	-11.233150
H20 89	O	0.174031	-13.358407	-17.219676
	H	-1.538844	-13.329107	-16.639346
	H	1.160370	-13.516676	-15.711807
H20 90	O	-12.876200	-6.358544	5.051406
	H	-11.965607	-7.839829	5.549600
	H	-12.072332	-5.826137	3.521071
H20 91	O	10.374968	3.013642	-1.655659
	H	10.560607	4.591509	-0.791103
	H	10.505729	3.439678	-3.408650
H20 92	O	-10.546723	11.487361	-1.141891
	H	-10.877949	9.851362	-1.838584
	H	-11.173553	12.643663	-2.383515
H20 93	O	16.771883	5.466609	-7.085057
	H	15.059461	5.871879	-6.666781
	H	17.622371	5.393421	-5.490410
H20 94	O	3.754576	11.312079	-9.304066
	H	3.860035	12.752060	-8.214609
	H	3.061607	10.005879	-8.262327
H20 95	O	-12.292259	3.567992	15.558774
	H	-11.551327	2.039891	14.936268
	H	-13.884710	3.052567	16.244353
H20 96	O	-6.101086	-22.917487	-8.300376
	H	-4.397045	-23.519612	-8.227759
	H	-6.818520	-23.760124	-9.731051
H20 97	O	-16.474111	-10.067162	-10.990268

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Table I: Structure of the water cluster used in the calculations.
(continued)

no.	atom	x	y	z
	H	-16.578248	-8.410626	-11.709038
	H	-14.818169	-10.647783	-11.428810
H20 98	O	-19.797465	-9.667636	-6.291155
	H	-19.300393	-9.924126	-8.011247
	H	-20.691509	-8.095379	-6.307792
H20 99	O	-5.173425	-12.712808	-15.395169
	H	-6.298381	-11.960539	-16.595231
	H	-5.886872	-12.300065	-13.785131
H20 100	O	-0.985868	2.698559	-21.389839
	H	-2.772036	2.967797	-21.483095
	H	-0.804981	1.203452	-20.388080
H20 101	O	-6.036941	3.692122	-20.942100
	H	-6.140711	5.167311	-21.983556
	H	-5.389533	4.295973	-19.364820
H20 102	O	8.569219	-3.794649	6.339855
	H	9.506348	-2.259850	6.534192
	H	9.732419	-5.097931	6.808897
H20 103	O	1.629116	13.174149	-1.603484
	H	2.665934	13.034467	-0.127990
	H	2.665646	14.042581	-2.804738
H20 104	O	-1.793830	17.039669	-2.196744
	H	-0.532014	15.757285	-2.009931
	H	-1.427261	17.806463	-3.793377
H20 105	O	-7.668774	-18.374941	-6.401296
	H	-8.484260	-18.612928	-4.804446
	H	-7.099663	-20.026682	-6.869747
H20 106	O	10.403971	-3.097182	-22.166270
	H	8.729735	-2.493265	-21.844084
	H	11.118126	-1.873647	-23.290782
H20 107	O	-15.303927	1.380876	7.300949
	H	-14.621806	2.684838	8.352603
	H	-16.432204	0.470603	8.382603
H20 108	O	8.586125	-8.600562	-9.057275
	H	8.704894	-9.813191	-10.394065
	H	8.628559	-9.589696	-7.543539
H20 109	O	16.039129	1.515730	-10.242663
	H	15.156300	2.196577	-11.666967
	H	16.442450	2.957886	-9.228217
H20 110	O	-15.024905	4.616965	-7.229413
	H	-13.962813	5.310923	-8.518586
	H	-14.288548	3.008246	-6.853399
H20 111	O	-3.380516	-15.912024	-1.000610
	H	-4.224096	-15.041860	-2.343283
	H	-1.903827	-16.614472	-1.773616
H20 112	O	-15.260480	6.494595	-20.095316
	H	-13.528983	6.244390	-19.636073
	H	-15.477693	5.509412	-21.596587
H20 113	O	-18.039071	-8.431035	0.810660
	H	-19.833632	-8.649203	0.751210

continued on following page

Table I: Structure of the water cluster used in the calculations.
(continued)

no.	atom	x	y	z
	H	-17.604252	-8.725105	2.541566
H20 114	O	-1.661337	-24.854339	-7.595623
	H	-0.939126	-26.256071	-6.709540
	H	-2.163790	-25.538535	-9.192807
H20 115	O	-13.114116	4.624061	10.656335
	H	-12.770748	4.110898	12.356437
	H	-11.486048	4.717060	9.873819
H20 116	O	-12.415589	11.848047	-6.994473
	H	-11.301689	10.449792	-6.719341
	H	-12.471242	12.035666	-8.792606
H20 117	O	-6.990293	15.098132	-9.148407
	H	-8.451163	15.701720	-10.027681
	H	-7.148884	15.784283	-7.482385
H20 118	O	-12.346254	10.561505	-12.238735
	H	-11.449595	8.995109	-12.357032
	H	-12.498223	11.126656	-13.950194
H20 119	O	11.408034	-1.036518	-9.303117
	H	13.124194	-0.467289	-9.351673
	H	11.316250	-2.308130	-10.586145
H20 120	O	-5.118967	-0.122532	11.023945
	H	-3.926824	1.229469	10.874032
	H	-4.376584	-1.485876	10.095644
H20 121	O	-9.994751	-0.336500	13.264888
	H	-8.344874	0.245731	12.806086
	H	-10.596101	-1.198962	11.793113
H20 122	O	-2.302168	10.694993	2.997228
	H	-1.936063	10.018308	1.360264
	H	-4.049229	11.156282	2.916163
H20 123	O	13.022958	-5.274418	1.238475
	H	14.310326	-4.634833	0.140659
	H	13.911509	-5.785673	2.728668
H20 124	O	7.566591	6.942112	-9.525069
	H	8.221679	5.879240	-10.833788
	H	6.672251	8.244973	-10.405006
H20 125	O	-2.177550	7.035558	6.401299
	H	-2.965508	5.658517	5.532698
	H	-2.216268	8.400625	5.215265
H20 126	O	9.007883	12.608974	-5.620298
	H	10.262452	11.860688	-4.553663
	H	7.974532	11.220878	-6.146567
H20 127	O	-1.447855	-3.724807	-24.991095
	H	0.236826	-4.371453	-25.114711
	H	-1.920641	-4.018898	-23.270174
H20 128	O	-7.648252	12.615523	3.065177
	H	-7.811671	14.380621	3.424765
	H	-8.836893	12.312229	1.735993