Supporting Information for:

Improved Density Functionals for Water

Erin E. Dahlke and Donald G. Truhlar

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Table S1: Accurate Binding Energies, D_e , for Water Data Set

	Structure	E_{bind} (kcal/mol)
Literature structures		
Dimers	Non-planar Open Cs	4.99
	Open C1	4.47
	Planar Open Cs	4.42
	Cyclic Ci	4.29
	Cyclic C2	4.04
	Cyclic C2h	4.00
	Triply Hydrogen Bonded Cs	3.18
	Doubly Bifurcated C2h	1.42
	Non-planar Bifurcated C2v	3.20
	Planar Bifurcated C2v	2.28
Trimers	C1 Global Min	15.76
	C3 Local Min	14.99
	C3h 3rd order SP	14.51
	C1 -> C1 TS	15.53
	C1 -> C3 TS	14.98
	Bifurcated TS	13.61
Simulation structures		
	ice XI dimer 1	3.72
	Ice XI dimer 2	4.57
	Ice VIII 0GPa	4.46
	Ice VIII 10GPa	3.87
	Ice VIII 20GPa	2.70
	Ice VIII 30GPa	1.42
	Ice VIII 40GPa	0.07
	Ice VIII 50GPa	-1.30
	Ice VIII 60GPa	-2.64
	Ice VIII 70GPa	-4.01
	gemc.323K	3.40
	gemc.373K	3.37
	gemc.423K	3.03
	gemc.473K	0.28
	gemc.523K	1.67
	npt	3.70
	nvt	4.60
	vapor.523K	0.11
Trimers	gemc.323K	7.04
	nvt	7.05

Table S2 Cartesian Coordinates (Å) of Dimers and Trimers in Water Data Set

	X	Y	Z
Non-planar Open Cs			
O	-0.06678738	-1.48970563	0.00000000
O	0.06228850	1.41602459	0.00000000
H	0.82307378	-1.84440824	0.00000000
H	0.05551587	-0.53228359	0.00000000
H	-0.40360261	1.77303160	-0.75915711
H	-0.40360261	1.77303160	0.75915711
Open C1			
O	-1.50604100	-0.05258106	-0.01780256
O	1.41789540	0.00414561	-0.03710306
H	-1.85434194	0.76071661	0.34925063
H	-0.55245021	0.08732087	-0.05164801
H	1.72177917	-0.75686874	0.46175864
H	2.08394725	0.67753690	0.11203050
Planar Open Cs			
O	-1.51122083	-0.05948516	0.00000000
O	1.41745246	0.01939109	0.00000000
H	-1.90652981	0.81295215	0.00000000
H	-0.56170288	0.10615140	0.00000000
H	1.76899889	-0.87278107	0.00000000
H	2.18740547	0.58999940	0.00000000
Cyclic Ci			
O	-1.41076608	0.00000000	0.00000000
O	1.41076608	0.00000000	0.00000000
H	-2.05607452	-0.26389789	0.65768661
H	-0.75682695	-0.70491146	0.00000000
H	2.05607452	0.26389789	-0.65768661
H	0.75682695	0.70491146	0.00000000
Cyclic C2			
O	1.39602972	0.04797206	0.02965124
O	-1.39602972	-0.04797206	0.02965124
H	2.19208810	-0.23478001	-0.42246539
H	0.78984700	-0.69407169	-0.04812121
H	-2.19208810	0.23478001	-0.42246539
H	-0.78984700	0.69407169	-0.04812121
Cyclic C2h			
O	-1.37983193	0.00000000	0.00000000
O	1.37983193	0.00000000	0.00000000
H	-2.25349784	-0.39266515	0.00000000
H	-0.77067457	-0.74320134	0.00000000
H	2.25349784	0.39266515	0.00000000
H	0.77067457	0.74320134	0.00000000

Triply Hydrogen Bonded Cs

O	1.41599488	-0.03438578	0.00000000
O	-1.52519007	0.01945205	0.00000000
H	2.36105615	-0.19732864	0.00000000
H	1.33525209	0.92186537	0.00000000
H	-0.98165088	-0.24376384	0.74584440
H	-0.98165088	-0.24376384	-0.74584440

Doubly Bifurcated C2h

O	-1.64689866	0.00000000	0.00000000
O	1.64689866	0.00000000	0.00000000
H	-1.33202355	0.50625151	-0.75154947
H	-1.33202355	0.50625151	0.75154947
H	1.33202355	-0.50625151	-0.75154947
H	1.33202355	-0.50625151	0.75154947

Non-planar Bifurcated C2v

O	0.00000000	0.00000000	1.57157753
O	0.00000000	0.00000000	-1.43789934
H	0.74333689	0.00000000	0.96486888
H	-0.74333689	0.00000000	0.96486888
H	0.00000000	-0.75802673	-2.02565354
H	0.00000000	0.75802673	-2.02565354

Planar Bifurcated C2v

O	0.00000000	0.00000000	1.65746310
O	0.00000000	0.00000000	-1.52383794
H	-0.74483845	0.00000000	1.05334639
H	0.74483845	0.00000000	1.05334671
H	0.75624625	0.00000000	-2.11371028
H	-0.75624625	0.00000000	-2.11371028

Monomer (literature dimers)

O	0.00000000	0.00000000	-0.06594358
H	0.00000000	-0.75632601	0.52328614
H	0.00000000	0.75632601	0.52328614

C1 Global Min

O	-1.29572900	-0.95160800	-0.09291200
O	-0.17985000	1.59421700	0.10931100
O	1.47640600	-0.63643100	-0.08296100
H	2.03102400	-1.07162500	0.56968600
H	0.61080600	-1.07953700	-0.02731400
H	-1.96138700	-1.20309400	0.55250500
H	-1.21807400	0.01749300	-0.02194400
H	-0.09348600	2.24083000	-0.59629500
H	0.62449900	1.04651500	0.05585300

C3 Local Min			
O	-0.97062300	1.28313900	-0.06639300
O	1.59654300	0.19901400	-0.06639300
O	-0.62592000	-1.48215400	-0.06639300
H	0.00000000	1.24131200	-0.00152600
H	1.07500800	-0.62065600	-0.00152600
H	-1.07500800	-0.62065600	-0.00152600
H	-1.23973000	1.98391000	0.53266900
H	2.33798200	0.08168300	0.53266900
H	-1.09825200	-2.06559300	0.53266900

C3h 3rd order SP			
O	-0.97025900	1.27328300	0.00000000
O	1.58782500	0.20362700	0.00000000
O	-0.61756600	-1.47691000	0.00000000
H	0.00000000	1.29071700	0.00000000
H	1.11779300	-0.64535800	0.00000000
H	-1.11779300	-0.64535800	0.00000000
H	-1.25625700	2.18902200	0.00000000
H	2.52387700	-0.00656100	0.00000000
H	-1.26762100	-2.18246200	0.00000000

C1 -> C1 TS			
O	-1.33318500	-0.86225400	-0.00704100
O	-0.06900500	1.60824300	0.10374700
O	1.43759600	-0.74221000	-0.09791500
H	-1.24502900	0.10664800	0.01666300
H	0.67529900	0.98163200	0.03928700
H	0.55897200	-1.15617200	-0.06723900
H	-2.27321600	-1.05381000	0.00743000
H	0.07131800	2.23769200	-0.60861600
H	1.92940200	-1.14622600	0.62214700

C1 -> C3 TS			
O	1.56396900	-0.41304200	-0.07624400
O	-1.11510100	-1.13635100	-0.02318800
O	-0.42896600	1.55503100	-0.07425300
H	0.79233300	-0.99991400	-0.00405500
H	-1.23947600	-0.17223200	0.01883600
H	0.44806500	1.13361600	-0.02783500
H	2.19197300	-0.73863300	0.57370800
H	-1.94565500	-1.52976800	0.25296800
H	-0.40645900	2.26182900	0.57585400

Bifurcated TS			
O	-1.59759200	-0.34607500	0.03003700
O	0.50434800	1.51328500	-0.08199300
O	1.16093600	-1.22198200	-0.00114500
H	-1.11102900	0.49554600	0.02721300
H	1.00843000	0.68341500	-0.00262300
H	0.58178500	-1.41709300	0.74515300
H	-2.51774200	-0.10721600	-0.10691000
H	0.93467700	2.13670900	0.50869300
H	0.56235000	-1.35318800	-0.74672700

Monomer (literature dimers)			
O	-0.09307200	0.00000000	-0.07206400
H	-0.09114700	0.00000000	0.88679400
H	0.83572600	0.00000000	-0.31027900

ice XI dimer 1			
O	0.00000000	0.00000000	0.00000000
O	-2.19162000	1.27574000	-0.89313000
H	0.00000000	-0.00958000	1.00098000
H	0.00000000	-0.95543000	-0.29865000
H	-1.38985000	0.78213000	-0.55290000
H	-2.99340000	0.78213000	-0.55290000

Ice XI dimer 2			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.01267000	2.68853000
H	0.00000000	-0.00958000	1.00098000
H	0.00000000	-0.95543000	-0.29865000
H	0.80177000	0.50628000	3.02876000
H	-0.80177000	0.50628000	3.02876000

Ice VIII 0GPa			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	2.40640000	-1.73746000
H	0.00000000	-0.78336000	-0.59566000
H	0.00000000	0.78336000	-0.59566000
H	0.78336000	2.40640000	-2.33312000
H	-0.78336000	2.40640000	-2.33312000

Ice VIII 10GPa			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	2.20753000	-1.58334000
H	0.00000000	-0.79510000	-0.59792000
H	0.00000000	0.79510000	-0.59792000
H	0.79510000	2.20753000	-2.18125000
H	-0.79510000	2.20753000	-2.18125000

Ice VIII 20GPa			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	2.12273000	-1.51869000
H	0.00000000	-0.80334000	-0.59969000
H	0.00000000	0.80334000	-0.59969000
H	0.80334000	2.12273000	-2.11839000
H	-0.80334000	2.12273000	-2.11839000

Ice VIII 30GPa			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	2.06736000	-1.47639000
H	0.00000000	-0.81100000	-0.60171000
H	0.00000000	0.81100000	-0.60171000
H	0.81100000	2.06736000	-2.07810000
H	-0.81100000	2.06736000	-2.07810000

Ice VIII 40GPa			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	2.02539000	-1.44418000
H	0.00000000	-0.81851000	-0.60393000
H	0.00000000	0.81851000	-0.60393000
H	0.81851000	2.02539000	-2.04810000
H	-0.81851000	2.02539000	-2.04810000

Ice VIII 50GPa			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	1.99169000	-1.41844000
H	0.00000000	-0.82599000	-0.60637000
H	0.00000000	0.82599000	-0.60637000
H	0.82599000	1.99169000	-2.02481000
H	-0.82599000	1.99169000	-2.02481000

Ice VIII 60GPa			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	1.96427000	-1.39690000
H	0.00000000	-0.83473000	-0.60971000
H	0.00000000	0.83473000	-0.60971000
H	0.83473000	1.96427000	-2.00661000
H	-0.83473000	1.96427000	-2.00661000

Ice VIII 70GPa			
O	0.00000000	0.00000000	0.00000000
O	0.00000000	1.94015000	-1.37811000
H	0.00000000	-0.84385000	-0.61337000
H	0.00000000	0.84385000	-0.61337000
H	0.84385000	1.94015000	-1.99148000
H	-0.84385000	1.94015000	-1.99148000

gemc.323K			
O	7.67305842	6.85715850	4.14317433
O	8.64038451	8.92755991	5.64321380
H	8.15448430	7.49748703	4.78216323
H	8.16250423	7.18901213	3.33820281
H	9.57435146	9.06719999	5.52465042
H	8.50254235	8.95990303	6.61111398
gemc.373K			
O	7.88102402	3.88419447	7.51393046
O	10.18759900	5.29078086	6.67345352
H	7.29929257	3.97264215	8.22309719
H	7.80735703	2.91980795	7.33386725
H	9.64852226	4.76047568	7.37304051
H	9.49897518	5.92150529	6.36422820
gemc.423K			
O	7.32522844	8.02331859	5.22217221
O	9.33149787	9.36227724	6.63880055
H	7.88007402	8.66714763	5.67829385
H	7.81884964	7.42909467	4.63351837
H	9.93809186	8.76378624	6.12306479
H	9.41279010	9.04401171	7.56465124
gemc.473K			
O	4.33883243	6.49640410	3.68364894
O	5.26273987	4.33503166	5.21789064
H	3.53722871	6.45702740	3.16350132
H	4.09974413	7.07545678	4.43248186
H	5.45585285	5.20836358	4.88998109
H	4.49849554	4.35812118	5.80908706
gemc.523K			
O	9.30973464	2.03418719	8.90971516
O	10.46869371	3.50349801	6.68401460
H	8.99213319	1.65293146	8.13578924
H	8.68067311	2.74681513	9.14807531
H	10.16440888	2.90468155	7.42051130
H	10.10335961	4.34599172	6.93657602
NpT			
O	8.30224932	4.37317392	9.27567534
O	9.76736171	3.55462152	11.54371071
H	7.36976031	4.63397758	9.49435972
H	8.14556336	3.59838880	8.70086332
H	9.48635173	4.30739641	12.13787924
H	9.51043301	3.88735513	10.64278609

NVT			
O	4.43533449	4.96524530	5.51101477
O	3.59822431	3.03426778	3.58399289
H	3.94967987	5.17811727	6.35394029
H	4.38670813	5.75579963	4.86282537
H	3.78763416	3.56974543	4.44339376
H	4.31143596	3.25708298	2.95076363
vapor.523K			
O	5.22737913	8.91279090	3.98701155
O	0.46054907	8.97609348	9.54540165
H	4.82296246	8.06041363	3.78752392
H	5.95108990	8.80596317	4.58804630
H	1.03449303	9.00137685	8.79061650
H	0.68531125	9.73007360	10.08030412
gemc.323K			
O	6.23994376	8.10970045	10.01133347
O	8.54618301	9.26081138	8.68417435
O	7.05916455	7.20569271	12.68992973
H	5.75004492	8.98926738	9.70649318
H	5.74065987	7.43595417	9.47156692
H	8.44040112	10.20658347	9.03744861
H	7.91861719	8.67460573	9.26891412
H	6.25821669	7.49993357	13.18100091
H	6.97412174	7.70888394	11.83774905
NVT			
O	8.01960878	7.06705174	0.73836496
O	10.46884930	6.84899521	2.01763511
O	8.76081787	9.92930756	0.67903432
H	7.47338913	7.78312869	1.04797298
H	7.53685748	6.22543465	0.70923966
H	10.68394601	5.96516628	2.32760560
H	9.50195534	6.74492384	1.70035643
H	9.16960086	9.20001128	1.06489688
H	8.43429508	9.81707054	-0.21056248

Table S3: Dimers and Trimers Included in W7 Representative Data Set^a

Dimers	
	Non-planar Open
	Cs
	Cyclic C2h
	dimer.nvt
	dimer.vapor.523K
	50GPa
Trimers	
	trimer.nvt
	C3 Local Min

^aAccurate binding energies and cartesian coordinates can be found in Table S1 and S2 respectively.