Supporting Information for:

Assessment of the Pairwise Additive Approximation and Evaluation of Many-Body Terms for Small Water Clusters: a Comparison of Density Functional Theory and Higher Level ab Initio Calculations

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Table S1: Cartesian Coordinates (Å) of Structures in Small Data Set[a]

		BTS	
O(3)[b]	-1.59759200	-0.34607500	0.03003700
O(1)	0.50434800	1.51328500	-0.08199300
O(2)	1.16093600	-1.22198200	-0.00114500
H(3)	-1.11102900	0.49554600	0.02721300
H(1)	1.00843000	0.68341500	-0.00262300
H(2)	0.58178500	-1.41709300	0.74515300
H(3)	-2.51774200	-0.10721600	-0.10691000
H(1)	0.93467700	2.13670900	0.50869300
H(2)	0.56235000	-1.35318800	-0.74672700
		C1C1TS	
O(3)	-1.33318500	-0.86225400	-0.00704100
O(1)	-0.06900500	1.60824300	0.10374700
O(2)	1.43759600	-0.74221000	-0.09791500
H(3)	-1.24502900	0.10664800	0.01666300
H(1)	0.67529900	0.98163200	0.03928700
H(2)	0.55897200	-1.15617200	-0.06723900
H(3)	-2.27321600	-1.05381000	0.00743000
H(1)	0.07131800	2.23769200	-0.60861600
H(2)	1.92940200	-1.14622600	0.62214700
		C1C3TS	
O(3)	1.56396900	-0.41304200	-0.07624400
O(1)	-1.11510100	-1.13635100	-0.02318800
O(2)	-0.42896600	1.55503100	-0.07425300
H(3)	0.79233300	-0.99991400	-0.00405500
H(1)	-1.23947600	-0.17223200	0.01883600
H(2)	0.44806500	1.13361600	-0.02783500
H(3)	2.19197300	-0.73863300	0.57370800
H(1)	-1.94565500	-1.52976800	0.25296800
H(2)	-0.40645900	2.26182900	0.57585400
		C1GM	
O(2)	-1.29572900	-0.95160800	-0.09291200
O(1)	-0.17985000	1.59421700	0.10931100
O(3)	1.47640600	-0.63643100	-0.08296100
H(3)	2.03102400	-1.07162500	0.56968600
H(3)	0.61080600	-1.07953700	-0.02731400
H(2)	-1.96138700	-1.20309400	0.55250500
H(2)	-1.21807400	0.01749300	-0.02194400
H(1)	-0.09348600	2.24083000	-0.59629500
H(1)	0.62449900	1.04651500	0.05585300

C3LM

O(3)	-0.97062300	1.28313900	-0.06639300
O(1)	1.59654300	0.19901400	-0.06639300
O(2)	-0.62592000	-1.48215400	-0.06639300
H(3)	0.00000000	1.24131200	-0.00152600
H(1)	1.07500800	-0.62065600	-0.00152600
H(2)	-1.07500800	-0.62065600	-0.00152600
H(3)	-1.23973000	1.98391000	0.53266900
H(1)	2.33798200	0.08168300	0.53266900
H(2)	-1.09825200	-2.06559300	0.53266900

C3h3rdOSP

O(3)	-0.97025900	1.27328300	0.00000000
O(1)	1.58782500	0.20362700	0.00000000
O(2)	-0.61756600	-1.47691000	0.00000000
H(3)	0.00000000	1.29071700	0.00000000
H(1)	1.11779300	-0.64535800	0.00000000
H(2)	-1.11779300	-0.64535800	0.00000000
H(3)	-1.25625700	2.18902200	0.00000000
H(1)	2.52387700	-0.00656100	0.00000000
H(2)	-1.26762100	-2.18246200	0.00000000

G323

O(1)	6.23994376	8.10970045	10.01133347
H(1)	5.75004492	8.98926738	9.70649318
H(1)	5.74065987	7.43595417	9.47156692
O(2)	8.54618301	9.26081138	8.68417435
H(2)	8.44040112	10.20658347	9.03744861
H(2)	7.91861719	8.67460573	9.26891412
O(3)	7.05916455	7.20569271	12.68992973
H(3)	6.25821669	7.49993357	13.18100091
H(3)	6.97412174	7.70888394	11.83774905

NVT

O(1)	8.01960878	7.06705174	0.73836496
H(1)	7.47338913	7.78312869	1.04797298
H(1)	7.53685748	6.22543465	0.70923966
O(2)	10.46884930	6.84899521	2.01763511
H(2)	10.68394601	5.96516628	2.32760560
H(2)	9.50195534	6.74492384	1.70035643
O(3)	8.76081787	9.92930756	0.67903432
H(3)	9.16960086	9.20001128	1.06489688
H(3)	8.43429508	9.81707054	-0.21056248

BT1

O(1)	0.19278976	1.42397606	0.43019842
H(1)	-0.55814613	1.60716714	-0.23346195
H(1)	-0.49888105	1.07873702	1.06592157
O(2)	1.90701795	1.12473986	5.94521487
H(2)	2.03717862	1.25802381	4.99114881
H(2)	2.39979827	1.88739820	6.35098216
O(3)	5.29189778	2.64884858	1.99291425
H(3)	5.14044079	2.69704585	1.06024362
H(3)	6.22546494	2.31356850	2.12368698
O(4)	2.76554720	1.84822499	3.02985393
H(4)	2.34387915	1.87101269	2.16595250
H(4)	3.70718189	1.82421758	2.91334192

BT2

O(1)	-0.06106900	1.46290200	0.54771200
O(2)	-1.82143600	-0.27140400	-0.84096700
O(3)	0.07172300	-1.17816900	1.16186600
O(4)	1.92717000	-0.14839100	-0.80223500
H(1)	-0.02461100	2.17040600	1.19333300
H(1)	-0.00972200	0.62163200	1.04878200
H(4)	1.41250300	0.64239200	-0.59148900
H(2)	-1.49115400	0.57561900	-0.51131600
H(3)	0.82056300	-1.21457200	0.54892900
H(3)	-0.69276000	-1.30746300	0.58491400
H(4)	1.79587100	-0.28478600	-1.74229100
H(2)	-2.74179400	-0.12272400	-1.06186900

CT1

O(1)	0.18714253	5.39094115	7.97964946
H(1)	-0.81836668	5.43396152	7.85101761
H(1)	0.44130361	6.26655819	8.25535220
O(2)	2.57383965	6.10354438	11.62826523
H(2)	2.39561135	6.49341758	10.75945208
H(2)	1.75339557	6.40101060	12.09876398
O(3)	1.36982683	3.56522908	9.74001368
H(3)	0.89638939	4.21515778	9.14152756
H(3)	1.89278121	4.06006471	10.38787626
O(4)	1.26898892	8.02917257	8.29597896
H(4)	1.84374524	7.95142152	7.50363143
H(4)	0.45007301	8.42274723	7.94658635

CT2

O(1)	1.37496300	1.37496300	0.00734300
O(2)	1.37496300	-1.37496300	-0.00734300
O(3)	-1.37496300	-1.37496300	0.00734300

O(4)	-1.37496300	1.37496300	-0.00734300
H(2)	0.40676100	-1.50874300	0.01120900
H(3)	-1.50874300	-0.40676100	-0.01120900
H(4)	-0.40676100	1.50874300	0.01120900
H(1)	1.50874300	0.40676100	-0.01120900
H(1)	1.88998100	1.68877900	0.75224200
H(3)	-1.88998100	-1.68877900	0.75224200
H(2)	1.68877900	-1.88998100	-0.75224200
H(4)	-1.68877900	1.88998100	-0.75224200

LT1

O(1)	6.55842230	8.32774426	3.31500455
H(1)	7.00560043	9.03329128	3.84716864
H(1)	7.15237932	8.20184692	2.51510429
O(2)	5.72133103	5.15240281	3.60518000
H(2)	5.83796389	4.57241844	2.86261246
H(2)	5.96124466	6.07157041	3.59323011
O(3)	6.32271367	3.30427190	6.13877398
H(3)	5.63094856	3.74267189	6.73556493
H(3)	6.24408221	3.74625468	5.27847130
O(4)	8.16687002	2.22311537	7.78655152
H(4)	9.12087238	2.14065384	7.43135674
H(4)	7.56444744	2.46300879	7.05971115

LT2

H(4)	0.00000000	-0.00958000	1.00098000
H(4)	0.00000000	-0.95543000	-0.29865000
H(3)	0.80177000	0.50628000	3.02876000
H(3)	-0.80177000	0.50628000	3.02876000
H(2)	-2.19162000	1.29799000	4.58264000
H(2)	-2.19162000	2.24384000	3.28301000
H(1)	-1.38985000	0.78213000	6.61042000
H(1)	-2.99340000	0.78213000	6.61042000
O(4)	0.00000000	0.00000000	0.00000000
O(3)	0.00000000	0.01267000	2.68853000
O(2)	-2.19162000	1.28841000	3.58166000
O(1)	-2.19162000	1.27574000	6.27019000

P

O(1)	11.21653815	7.98047448	9.93683874
H(1)	11.82738860	8.68456039	10.27850674
H(1)	10.36560430	8.36488416	10.10859931
O(2)	8.89851139	11.66560493	10.43418090
H(2)	9.76813312	12.07885020	10.27207301
H(2)	8.99891389	11.75431830	11.43650604
O(3)	6.68985797	7.82408659	10.87320881

H(3)	6.23751680	8.65683708	11.14248267
H(3)	6.25616079	7.20182860	10.20130525
O(4)	9.16876897	9.67686775	7.61008750
H(4)	9.84650086	10.36114219	7.55325810
H(4)	8.88116542	9.29098545	8.46336165
O(5)	8.81031903	9.06455490	10.13682749
H(5)	8.84708613	10.15841354	10.31927326
H(5)	8.02534770	8.46997543	10.29694750

[a] Small data set corresponds to structures listed in Table 1 of text.

[b] Numbers in parentheses correspond to monomer numbers used in Table S-2.

Table S2: Weizmann-1 Binding Energies (kcal/mol) for Large Data Set

Structure	Monomers[a]	Dimers	Trimers	Tetramers	Binding Energy
BTS	1,2,3,4	1,2,3			14.15
BTS_1d[b]	1,2				4.53
BTS_2d	2,3				3.31
BTS_3d	1,3				4.60
C1C1TS	1,2,3,4	1,2,3			16.13
C1C1TS_1d	1,2				4.81
C1C1TS_2d	2,3				4.37
C1C1TS_3d	1,3				4.63
C1C3TS	1,2,3,4	1,2,3			15.56
C1C3TS_1d	1,2				4.52
C1C3TS_2d	2,3				4.41
C1C3TS_3d	1,3				4.35
C1GM	1,2,3,4	1,2,3			16.39
C1GM_1d	1,2				4.78
C1GM_2d	2,3				4.38
C1GM_3d	1,3				4.76
C3LM	1,2,3,4	1,2,3			15.59
C3LM_1d	1,2				4.42
C3LM_2d	2,3				4.42
C3LM_3d	1,3				4.42
C3h3rdOSP	1,2,3,4	1,2,3			15.00
C3h3rdOSP_1d	1,2				4.34

C3h3rdOSP_2d	2,3			4.34
C3h3rdOSP_3d	1,3			4.34
G323	1,2,3	1,2,3		7.04
G323_1d	2,3			-0.95
G323_2d	1,3			4.09
G323_3d	1,2			4.36
NVT	1,2,3	1,2,3		7.05
NVT_1d	2,3			0.58
NVT_2d	1,3			2.77
NVT_3d	1,2			3.81
BT1	1,2,3,4	1,2,3,4,5,6	1,2,3,4	10.72
BT1_1tri[b]	2,3,4	1,2,3		8.07
BT1_2tri	1,3,4	1,4,5		4.80
BT1_3tri	1,2,4	2,4,6		7.08
BT1_4tri	1,2,3	3,5,6		0.93
BT1_1d	3,4			2.75
BT1_2d	2,4			4.23
BT1_3d	2,3			0.60
BT1_4d	1,4			2.26
BT1_5d	1,3			-0.05
BT1_6d	1,2			0.37
CT1	1,2,3,4	1,2,3,4,5,6	1,2,3,4	11.55
CT1_1tri	2,3,4	1,2,3		4.88
CT1_2tri	1,3,4	1,4,5		8.95
CT1_3tri	1,2,4	2,4,6		4.43
CT1_4tri	1,2,3	3,5,6		5.23
CT1_1d	3,4			0.86

CT1_2d	2,4			1.84
CT1_3d	2,3			2.14
CT1_4d	1,4			3.36
CT1_5d	1,3			4.31
CT1_6d	1,2			-0.61
LT1	1,2,3,4	1,2,3,4,5,6	1,2,3,4	13.02
LT1_1tri	2,3,4	1,2,3		8.78
LT1_2tri	1,3,4	1,4,5		4.38
LT1_3tri	1,2,4	2,4,6		3.74
LT1_4tri	1,2,3	3,5,6		7.95
LT1_1d	3,4			3.80
LT1_2d	2,4			0.34
LT1_3d	2,3			3.96
LT1_4d	1,4			0.07
LT1_5d	1,3			0.42
LT1_6d	1,2			3.30
BT2	1,2,3,4	1,2,3,4,5,6	1,2,3,4	23.57
BT2_1tri	1,2,3	1,2,4		14.76
BT2_2tri	1,2,4	1,3,5		8.11
BT2_3tri	1,3,4	2,3,6		14.65
BT2_4tri	2,3,4	4,5,6		6.83
BT2_1d	1,2			4.35
BT2_2d	1,3			4.32
BT2_3d	1,4			4.71
BT2_4d	2,3			4.17
BT2_5d	2,4			-0.54
BT2_6d	3,4			3.68

CT2	1,2,3,4	1,2,3,4,5,6	1,2,3,4		28.62
CT2_1tri	1,2,3	1,2,4			12.58
CT2_2tri	1,2,4	1,3,5			12.58
CT2_3tri	1,3,4	2,3,6			12.58
CT2_4tri	2,3,4	4,5,6			12.58
CT2_1d	1,2				4.75
CT2_2d	1,3				1.62
CT2_3d	1,4				4.75
CT2_4d	2,3				4.75
CT2_5d	2,4				1.62
CT2_6d	3,4				4.75
LT2	1,2,3,4	1,2,3,4,5,6	1,2,3,4		18.31
LT2_1tri	2,3,4	1,2,3			10.74
LT2_2tri	1,3,4	1,4,5			5.77
LT2_3tri	1,2,4	2,4,6			5.61
LT2_4tri	1,2,3	3,5,6			10.97
LT2_1d	3,4				4.57
LT2_2d	2,4				0.93
LT2_3d	2,3				3.72
LT2_4d	1,4				0.02
LT2_5d	1,3				1.06
LT2_6d	1,2				4.57
Pentamer	1,2,3,4,5	1,2,3,4,5,6,7,8,9,10	1,2,3,4,5,6,7,8,9,10	1,2,3,4,5	17.84
P_1tet[b]	1,2,3,4	1,2,3,5,6,8	1,2,4,7		1.19
P_2tet	1,2,3,5	1,2,4,5,7,9	1,3,5,8		13.28
P_3tet	1,2,4,5	1,3,4,6,7,10	2,3,6,9		14.02
P_4tet	1,3,4,5	2,3,4,8,9,10	4,5,6,10		10.31
P_5tet	2,3,4,5	5,6,7,8,9,10	7,8,9,10		12.92
P_1tri	1,2,3	1,2,5			1.22

P_2tri	1,2,4	1,3,6	-0.52
P_3tri	1,2,5	1,4,7	11.78
P_4tri	1,3,4	2,3,8	0.29
P_5tri	1,3,5	2,4,9	8.01
P_6tri	1,4,5	3,4,10	3.26
P_7tri	2,3,4	5,6,8	1.55
P_8tri	2,3,5	5,7,9	5.39
P_9tri	2,4,5	6,7,10	11.14
P_10tri	3,4,5	8,9,10	7.58
P_1d	1,2		0.57
P_2d	1,3		0.71
P_3d	1,4		-1.50
P_4d	1,5		3.34
P_5d	2,3		-0.05
P_6d	2,4		0.50
P_7d	2,5		6.03
P_8d	3,4		1.11
P_9d	3,5		2.47
P_10	4,5		2.61

[a] monomer number refers to those given in Table S1

[b] *n*d, *n*tri, and *n*tet refer to the n^{th} consituent dimer, trimer and tetramer respectively.