Supporting Information

The lowest-energy structures of water clusters $(H_2O)_{11}$ and $(H_2O)_{13}$

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Reference 42.

Reference 45.

Table S1: Electronic energies (in a.u.), zero-point energies (ZPE in a.u.) and relative energies (in kcal/mol) of the lowest-lying clusters within each family of $(H_2O)_{11}$ and $(H_2O)_{13}$ based on B3LYP/6-311+G(d,p) level of theory. The bold-faced values correspond to the lowest-energy isomers at the B3LYP level of theory.

Table S2: The xyz-coordinates for **515-a**, **43'4** [$(H_2O)_{11}$] and **4414** [$(H_2O)_{13}$] isomers are tabulated.

Reference 42

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

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Kendall, R.A.; Aprà, E.; Bernholdt, D.E.; Bylaska, E.J.; Dupuis, M.; Fann, G.I.; Harrison, R.J.; Ju, J.; Nichols, J.A.; Nieplocha, J.; Straatsma, T.P.; Windus, T.L.; Wong, A.T. *Comput. Phys. Commun.* **2000**, *128*, 260.

Table S1

Clusters	B3LYP/6-311+G(d,p) (a.u.)	ZPE (a.u.)	ΔE(B3LYP+ZPE) (kcal/mol)
$(H_20)_{11}$			
515-a	-841.219538	0.280154	**0.002**
43'4	-841.217078	0.280595	1.822
55'1	-841.219726	0.280340	**0.000**
44'3'	-841.216466	0.280820	2.347
44'12	-841.217247	0.279899	1.279
bow-tie	-841.215211	0.279642	2.396
41141	-841.213258	0.278821	3.106
41114	-841.217148	0.278872	0.696
515-b	-841.218042	0.280126	0.922
$(H_20)_{13}$			
4414	-994.174479	0.333315	0.531
454-a	-994.174829	0.333473	0.411
445	-994.174635	0.333343	0.451
454-b	-994.173737	0.333856	1.336
515+2	-994.174573	0.332763	0.126
43'4+2	-994.172981	0.332261	0.810
41141+2	-994.173152	0.331643	0.315
616-a	-994.173793	0.331782	**0.000**
616-b	-994.173508	0.331815	0.199

Table S2

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515-a

O	2.23761292	-2.07665757	-0.57266217	1
H	2.71942882	-2.87852864	-0.79653341	1
H	1.28281871	-2.33270292	-0.45284883	1
O	-2.02595184	-1.03364042	-1.79428526	2
H	-1.44184833	-0.24379693	-2.00846510	2
H	-2.33006353	-1.38061245	-2.63897873	2
O	-0.38064147	2.67183180	0.14580603	3
H	-0.93691860	2.11867398	0.77413245	3
H	-0.74224792	3.56321268	0.17719103	3
O	-1.81187587	1.13879669	1.72906306	4
H	-2.57188799	0.74866165	1.25061134	4
H	-1.29633552	0.38087898	2.06455073	4
O	-0.34392055	-2.54071388	-0.06448563	5
H	-0.48060913	-2.12980081	0.80817408	5
H	-0.95907736	-2.09492682	-0.67769148	5
O	-0.46745219	1.03053309	-2.24912986	6
H	0.48559022	0.78653736	-2.28264900	6
H	-0.52747912	1.68797415	-1.53429061	6
O	-0.21258104	-1.09523671	2.42175691	7
H	-0.25693970	-1.50104341	3.29316062	7
H	0.74048307	-0.84613751	2.27175850	7
O	2.29764409	-0.47133614	1.76708018	8
H	2.48392137	-1.06469686	1.01574323	8
H	2.36584020	0.43021246	1.40310996	8
O	2.27853290	2.04122280	0.41062119	9
H	1.35282190	2.37610166	0.36249427	9
H	2.83415869	2.78882747	0.65145992	9
O	-3.76155958	-0.03838221	0.13413973	10
H	-3.26008557	-0.45469597	-0.59768121	10
H	-4.42360163	-0.67627651	0.41435213	10
O	2.21424657	0.40136109	-2.00145678	11
H	2.30722768	-0.49592526	-1.63386460	11
H	2.46237234	0.99583534	-1.27531471	11

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43'4

o	1.92505127	-2.04798431	-1.40440686	1
H	2.64058782	-2.51595653	-1.84488942	1
H	1.88139718	-1.13738744	-1.79661449	1
O	-0.85464742	2.72482765	-0.47526144	2
H	0.11475097	2.79185187	-0.56625335	2
H	-1.10254701	1.93091033	-0.97714020	2
O	1.47355334	-1.62482719	1.43058431	3
H	1.75566066	-1.83657621	0.52439863	3
H	0.58767782	-2.01602054	1.51936928	3
O	1.46105425	0.41607168	-2.34430527	4
H	0.49421658	0.47738344	-2.36668100	4
H	1.74632888	1.11925523	-1.72623761	4
O	-0.86663989	-2.37009892	-1.44424256	5
H	0.10220916	-2.45684350	-1.52448642	5
H	-1.06883118	-2.64121028	-0.52899539	5
O	-1.27357921	-2.54148462	1.33654542	6
H	-1.71714404	-3.18704184	1.89468144	6
H	-1.80983294	-1.70756174	1.36564528	6
O	-2.56603202	-0.20862955	1.08262003	7
H	-2.18348977	0.54051884	1.58009852	7
H	-2.44185700	0.02291518	0.14936268	7
O	-1.54698736	0.17704410	-1.78371084	8
H	-2.17315785	0.22188141	-2.51433417	8
H	-1.31055791	-0.79081100	-1.68027322	8
O	-1.20616530	2.03535194	2.09278776	9
H	-1.57222669	2.70824461	2.67481665	9
H	-1.13091655	2.43624016	1.18842343	9
O	1.54980522	1.09759204	1.89186310	10
H	0.65845440	1.34353546	2.18962375	10
H	1.54810653	0.11771843	1.79542129	10
O	1.93570795	2.34604152	-0.38985900	11
H	2.67215369	2.96323209	-0.34789154	11
H	1.88299010	1.87967822	0.49761419	11

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4414

O	-0.0940	-0.0180	-1.9160	1
O	-2.9760	0.2060	-1.9290	2
O	2.1830	-2.6800	-0.0780	3
O	2.6650	-0.7580	2.0210	4
O	2.6180	-0.8700	-2.0220	5
O	-0.1750	1.9300	0.1240	6
O	-0.5680	-2.0690	-0.1100	7
O	-0.1060	-0.1970	1.8930	8
O	2.2290	3.2310	-0.1150	9
O	-2.9880	0.0530	1.9570	10
O	-2.9720	2.1170	-0.0480	11
O	-3.3690	-1.8310	0.0650	12
O	3.6040	0.8290	0.1040	13
H	-0.0130	0.7520	-1.3160	1
H	0.8130	-0.2270	-2.2090	1
H	-3.2080	-0.5960	-1.4280	2
H	-2.0610	0.0730	-2.2310	2
H	2.4140	-2.2070	0.7430	3
H	1.2160	-2.7830	-0.0400	3
H	3.0580	-0.1100	1.3700	4
H	3.2990	-0.8490	2.7380	4
H	2.5160	-1.6230	-1.3800	5
H	3.1580	-1.1950	-2.7490	5
H	-1.1050	2.2250	0.0990	6
H	-0.1270	1.2560	0.8400	6
H	-1.5160	-2.2910	-0.0830	7
H	-0.4660	-1.4140	-0.8360	7
H	-0.2530	-0.9380	1.2650	8
H	0.8080	-0.3280	2.2100	8
H	2.3320	4.0300	0.4080	9
H	1.3030	2.9310	-0.0020	9
H	-3.0700	0.8820	1.4520	10
H	-2.0640	0.0230	2.2570	10
H	-3.5760	2.8470	-0.2110	11
H	-3.0530	1.4890	-0.8150	11
H	-4.1110	-2.4230	0.2200	12
H	-3.3230	-1.2070	0.8360	12
H	3.3960	0.3880	-0.7380	13
H	3.2260	1.7300	0.0390	13