Supplementary Information for

Intermolecular Interaction in Water Hexamer

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Table S1. MP2/aug-cc-pV5Z-h//MP2/aug-cc-pVTZ pair interaction energies and many-body effects (MBE) in the prism structure (kcal/mol).

Pairs	R_{OO} (Å)	ΔE_{ele}	ΔE_{ex}	ΔE_{rep}	ΔE_{pol}	ΔE_{HF}	ΔE_{disp}	ΔE_{MP2}
1,2	2.785	-9.09	-14.74	+26.96	-3.29	-0.15	-2.06	-2.22
1,3	2.909	-6.48	-6.53	+11.54	-1.30	-2.77	-1.11	-3.89
1,4	3.863	-1.29	-0.27	+0.43	-0.06	-1.19	-0.18	-1.37
1,5	2.651	-15.05	-22.77	+42.83	-6.51	-1.51	-2.58	-4.09
1,6	3.945	-1.51	-0.14	+0.23	-0.06	-1.48	-0.14	-1.62
2,3	2.926	-5.05	-6.69	+11.92	-1.53	-1.35	-1.40	-2.76
2,4	3.936	+0.03	-0.25	+0.40	-0.07	+0.11	-0.32	-0.21
2,5	3.904	-1.41	-0.16	+0.26	-0.06	-1.37	-0.17	-1.54
2,6	2.907	-8.06	-8.57	+15.43	-2.19	-3.39	-1.36	-4.75
3,4	2.734	-12.14	-16.43	+30.47	-4.50	-2.61	-2.11	-4.72
3,5	4.027	-1.32	-0.06	+0.09	-0.05	-1.33	-0.10	-1.44
3,6	4.190	-0.03	-0.03	+0.04	-0.03	-0.05	-0.13	-0.18
4,5	2.860	-7.96	-8.85	+15.91	-2.03	-2.93	-1.37	-4.30
4,6	2.931	-3.69	-6.07	+10.71	-1.14	-0.18	-1.34	-1.52
5,6	2.764	-8.97	-11.73	+21.52	-3.12	-2.30	-1.94	-4.24
Sum	49.332	-82.03	-103.30	+188.74	-25.94	-22.52	-16.31	-38.84
Prism		-82.03	-103.30	+187.94	-34.79	-32.17	-16.28	-48.45
MBE		0.00	0.00	-0.80	-8.85	-9.65	+0.03	-9.62

Table S2. Coordinates (Å) of the prism structure optimized with MP2/aug-cc-pVTZ.

O	8.0	−2.1675526522	−2.0544029015	−0.4337647119
H	1.0	−1.3531471666	−2.5389321875	−0.6352882840
H	1.0	−1.8715507614	−1.1308550588	−0.5712015155
O	8.0	−0.6716977019	0.2944490104	−0.4731366656
H	1.0	0.0613027114	−0.3301277055	−0.5823914443
H	1.0	−0.6662754913	0.4977657773	0.4757800816
O	8.0	0.7338021938	−2.2712610461	−0.4178562959
H	1.0	1.5224027002	−2.7112002511	−0.7469640553
H	1.0	0.7912691510	−2.3178568450	0.5623860615
O	8.0	0.5477615506	−2.2081713860	2.3095474506
H	1.0	0.5487271572	−1.2696791005	2.5435981222
H	1.0	−0.3848259533	−2.4450162628	2.4407198618
O	8.0	−2.3039695896	−2.0206189589	2.2137143494
H	1.0	−2.3596274689	−2.0978839796	1.2226652906
H	1.0	−3.1107672987	−2.4106894763	2.5610245710
O	8.0	−0.8889898251	0.3442982323	2.4253171742
H	1.0	−1.1868458820	1.0730525498	2.9769993607
H	1.0	−1.5792840937	−0.3439096032	2.4908364462

Table S3. MP2/aug-cc-pV5Z-h//MP2/aug-cc-pVTZ pair interaction energies and many-body effects (MBE) in the cage structure (kcal/mol).

Pairs	R_{OO} (Å)	ΔE_{ele}	ΔE_{ex}	ΔE_{rep}	ΔE_{pol}	ΔE_{HF}	ΔE_{disp}	ΔE_{MP2}
1,2	2.898	-7.47	-7.98	+14.32	-1.96	-3.10	-1.32	-4.42
1,3	3.541	-1.32	-0.23	+0.37	-0.09	-1.27	-0.34	-1.62
1,4	2.911	-6.45	-8.07	+14.49	-1.99	-2.02	-1.39	-3.41
1,5	2.715	-11.84	-16.27	+30.19	-4.45	-2.37	-2.13	-4.50
1,6	4.167	-0.11	-0.05	+0.08	-0.04	-0.13	-0.12	-0.25
2,3	2.661	-14.49	-21.92	+41.13	-6.18	-1.46	-2.56	-4.02
2,4	3.415	-0.88	-1.32	+2.18	-0.15	-0.18	-0.56	-0.73
2,5	3.930	-1.22	-0.11	+0.18	-0.05	-1.21	-0.20	-1.40
2,6	2.776	-9.00	-12.74	+23.34	-3.17	-1.57	-1.97	-3.54
3,4	2.939	-6.54	-7.20	+12.85	-1.66	-2.55	-1.29	-3.84
3,5	2.746	-10.69	-14.15	+26.09	-3.81	-2.56	-1.94	-4.50
3,6	3.890	-1.44	-0.13	+0.21	-0.06	-1.42	-0.13	-1.55
4,5	3.885	0.03	-0.32	+0.51	-0.09	0.14	-0.36	-0.22
4,6	2.755	-11.27	-14.95	+27.60	-3.93	-2.55	-2.04	-4.59
5,6	5.686	-0.02	0.00	+0.00	0.00	-0.02	-0.03	-0.05
Sum	50.915	-82.71	-105.44	+193.53	-27.64	-22.27	-16.37	-38.64
Cage		-82.71	-105.44	+192.75	-36.68	-32.08	-16.32	-48.40
MBE		0.00	0.00	-0.78	-9.03	-9.81	+0.05	-9.76

Table S4. Coordinates (Å) of the cage structure optimized with MP2/aug-cc-pVTZ

O	8.0	0.8634914674	−1.7143673074	−0.4741365632
H	1.0	1.6845114437	−1.2009609705	−0.3060416283
H	1.0	1.1483169414	−2.5867262583	−0.7599681260
O	8.0	−0.7299047016	0.4096715757	−1.6351241263
H	1.0	−0.2619799874	−0.4307057374	−1.5063721281
H	1.0	−1.6087257340	0.2486397068	−1.2415069170
O	8.0	0.5900565495	1.7399853269	0.2543910955
H	1.0	0.0684443305	1.3769428043	−0.5108717695
H	1.0	0.4969865775	2.6958048105	0.2114944514
O	8.0	−0.7016254183	−0.4962687726	1.6572398252
H	1.0	−0.1985397589	−1.0975560336	1.0848960591
H	1.0	−0.2835849417	0.3622190949	1.4890071308
O	8.0	2.7948126799	0.1131103418	0.0772101137
H	1.0	2.1478127218	0.8405977998	0.1822028538
H	1.0	3.2944188159	0.0967015736	0.8982725451
O	8.0	−2.8900746358	0.0126654709	0.0633274047
H	1.0	−2.2538075250	−0.2528040191	0.7600992895
H	1.0	−3.6453194804	−0.5733750589	0.1547136558

Table S5. MP2/aug-cc-pV5Z-h//MP2/aug-cc-pVTZ pair interaction energies and many-body effects (MBE) in the book-1 structure (kcal/mol).

Pairs	R_{OO} (Å)	ΔE_{ele}	ΔE_{ex}	ΔE_{rep}	ΔE_{pol}	ΔE_{HF}	ΔE_{disp}	ΔE_{MP2}
1,2	2.686	-13.44	-19.29	+36.02	-5.40	-2.10	-2.29	-4.40
1,3	4.733	-0.57	-0.01	+0.01	-0.02	-0.59	-0.04	-0.63
1,4	5.391	-0.28	0.00	+0.00	-0.01	-0.29	0.00	-0.29
1,5	2.686	-13.30	-19.04	+35.54	-5.33	-2.13	-2.28	-4.41
1,6	3.946	-1.46	-0.14	+0.22	-0.06	-1.44	-0.16	-1.60
2,3	2.794	-9.35	-13.74	+25.19	-3.49	-1.39	-1.95	-3.33
2,4	3.806	-0.04	-0.32	+0.51	-0.11	0.05	-0.30	-0.25
2,5	3.811	-1.62	-0.23	+0.37	-0.07	-1.55	-0.20	-1.75
2,6	2.923	-7.75	-8.01	+14.38	-2.02	-3.40	-1.34	-4.73
3,4	2.768	-10.89	-13.87	+25.55	-3.79	-3.00	-1.87	-4.86
3,5	5.530	-0.31	0.00	+0.00	0.00	-0.32	0.01	-0.31
3,6	4.146	-0.41	-0.05	+0.07	-0.04	-0.42	-0.10	-0.53
4,5	4.730	-0.73	-0.02	+0.03	-0.03	-0.75	-0.04	-0.78
4,6	2.775	-9.66	-12.98	+23.88	-3.60	-2.36	-1.92	-4.28
5,6	2.679	-13.59	-19.65	+36.75	-5.59	-2.08	-2.31	-4.39
Sum	55.404	-83.39	-107.33	+198.54	-29.56	-21.75	-14.79	-36.54
Book-1		-83.39	-107.33	+197.88	-40.49	-33.34	-14.87	-48.21
MBE		0.00	0.00	-0.65	-10.93	-11.58	-0.08	-11.66

Table S6. Coordinates (Å) of the book-1 structure optimized with MP2/aug-cc-pVTZ

O	8.0	-3.0854928721	-1.6651786858	-0.5223587729
H	1.0	-3.6726378394	-1.1888090901	-1.1150018292
H	1.0	-2.2008946391	-1.2372066061	-0.6257115954
O	8.0	-0.6998771674	-0.4340151383	-0.4516077844
H	1.0	0.1154602187	-0.9533508376	-0.5932090636
H	1.0	-0.6653670843	-0.2040337737	0.4894459499
O	8.0	1.6374497796	-1.9639476207	-0.4413087505
H	1.0	2.4747756100	-1.6005680962	-0.7416387876
H	1.0	1.7069733476	-1.9961029553	0.5335898309
O	8.0	1.4910606540	-1.8501248193	2.3201609357
H	1.0	0.6560810041	-1.3703165109	2.4847559173
H	1.0	1.4477416092	-2.6352295046	2.8722734488
O	8.0	-3.2284040445	-1.5812479943	2.1583065588
H	1.0	-3.2981584470	-1.6447171613	1.1756776037
H	1.0	-3.4116788404	-2.4664105170	2.4841084972
O	8.0	-0.8552193355	-0.3761124026	2.4669460700
H	1.0	-0.9637845423	0.3850065090	3.0441713573
H	1.0	-1.7334789770	-0.8299294511	2.4508624649

Table S7. MP2/aug-cc-pV5Z-h//MP2/aug-cc-pVTZ pair interaction energies and many-body effects (MBE) in the book-2 structure (kcal/mol).

Pairs	R_{OO} (Å)	ΔE_{ele}	ΔE_{ex}	ΔE_{rep}	ΔE_{pol}	ΔE_{HF}	ΔE_{disp}	ΔE_{MP2}
1,2	2.686	-13.37	-19.18	+35.81	-5.39	-2.13	-2.29	-4.42
1,3	3.852	-1.69	-0.20	+0.33	-0.07	-1.64	-0.17	-1.81
1,4	5.354	-0.41	0.00	+0.00	-0.01	-0.41	0.00	-0.41
1,5	4.418	-1.16	-0.03	+0.04	-0.04	-1.18	0.00	-1.18
1,6	2.682	-12.56	-18.77	+35.05	-5.30	-1.58	-2.34	-3.92
2,3	2.697	-12.67	-19.12	+35.65	-5.27	-1.41	-2.35	-3.76
2,4	4.499	-1.09	-0.02	+0.04	-0.03	-1.11	0.01	-1.11
2,5	5.088	-0.42	0.00	+0.01	-0.01	-0.42	-0.01	-0.43
2,6	3.915	-1.60	-0.13	+0.21	-0.06	-1.59	-0.14	-1.73
3,4	2.792	-9.32	-13.66	+25.05	-3.51	-1.43	-1.97	-3.40
3,5	3.831	-0.08	-0.30	+0.49	-0.10	0.01	-0.29	-0.29
3,6	2.924	-7.62	-7.78	+13.95	-1.95	-3.40	-1.30	-4.69
4,5	2.760	-11.16	-14.40	+26.57	-3.94	-2.93	-1.91	-4.85
4,6	4.118	-0.35	-0.05	+0.08	-0.04	-0.37	-0.12	-0.48
5,6	2.779	-9.65	-13.25	+24.37	-3.64	-2.17	-1.98	-4.14
Sum	54.395	-83.15	-106.90	+197.65	-29.35	-21.75	-14.85	-36.61
Book-2		-83.15	-106.90	+197.00	-39.92	-32.97	-14.95	-47.92
MBE		0.00	0.00	-0.65	-10.57	-11.21	-0.10	-11.31

Table S8. Coordinates (Å) of the book-2 structure optimized with MP2/aug-cc-pVTZ

O	8.0	2.3404263846	1.2435327972	-0.3808182726
H	1.0	3.2460853978	1.4487071872	-0.1338685555
H	1.0	2.3329775291	0.2724628071	-0.5603995763
O	8.0	2.0865529964	-1.4176255203	-0.6401238838
H	1.0	1.8963060648	-1.8459744814	-1.4789253779
H	1.0	1.2754180771	-1.5449980042	-0.0899353423
O	8.0	-0.0912751488	-1.4305674639	0.9502922663
H	1.0	-0.0670728065	-0.5112540349	1.2563412503
H	1.0	-0.9323644564	-1.4857830160	0.4563117730
O	8.0	-2.4075455233	-1.2212001589	-0.5941203907
H	1.0	-3.2836665686	-1.4571719637	-0.2778523865
H	1.0	-2.4025973339	-0.2433048369	-0.6345994625
O	8.0	-2.0677533948	1.5157273078	-0.4952150854
H	1.0	-1.8771240735	2.0241446678	-1.2882623513
H	1.0	-1.2743400231	1.6122738782	0.0670054790
O	8.0	0.1606927504	1.4744527545	1.1646161561
H	1.0	0.2701179405	2.0604303660	1.9186248168
H	1.0	1.0169042093	1.4937728371	0.6722116224

Table S9. MP2/aug-cc-pV5Z-h//MP2/aug-cc-pVTZ pair interaction energies and many-body effects (MBE) in the cyclic-chair structure (kcal/mol).

Pairs	R_{OO} (Å)	ΔE_{ele}	ΔE_{ex}	ΔE_{rep}	ΔE_{pol}	ΔE_{HF}	ΔE_{disp}	ΔE_{MP2}
1,2	4.666	-0.84	-0.02	+0.02	-0.03	-0.86	-0.03	-0.89
1,3	2.708	-12.56	-17.62	+32.79	-4.97	-2.36	-2.10	-4.46
1,4	5.395	-0.46	0.00	+0.00	-0.01	-0.47	0.01	-0.46
1,5	4.666	-0.84	-0.02	+0.02	-0.03	-0.86	-0.03	-0.89
1,6	2.708	-12.56	-17.62	+32.79	-4.97	-2.36	-2.10	-4.46
2,3	5.392	-0.46	0.00	+0.00	-0.01	-0.47	0.01	-0.46
2,4	2.707	-12.58	-17.66	+32.87	-4.98	-2.35	-2.10	-4.45
2,5	4.663	-0.84	-0.02	+0.02	-0.03	-0.86	-0.03	-0.89
2,6	2.708	-12.57	-17.62	+32.81	-4.97	-2.36	-2.10	-4.46
3,4	4.663	-0.84	-0.02	+0.02	-0.03	-0.86	-0.03	-0.89
3,5	2.708	-12.57	-17.62	+32.80	-4.97	-2.36	-2.10	-4.46
3,6	4.662	-0.84	-0.02	+0.02	-0.03	-0.86	-0.03	-0.89
4,5	2.708	-12.58	-17.64	+32.84	-4.98	-2.36	-2.10	-4.46
4,6	4.663	-0.84	-0.02	+0.02	-0.03	-0.86	-0.03	-0.89
5,6	5.392	-0.46	0.00	+0.00	-0.01	-0.47	0.01	-0.46
Sum	60.409	-81.86	-105.87	+197.05	-30.02	-20.70	-12.75	-33.44
Chair		-81.85	-105.87	+196.43	-43.12	-34.42	-12.86	-47.28
MBE		0.00	0.00	-0.62	-13.10	-13.72	-0.11	-13.84

Table S10. Coordinates (Å) of the cyclic-chair structure optimized with MP2/aug-cc-pVTZ

O	8.0	-0.0005424934	2.6948690517	0.1415781594
H	1.0	-0.1280674529	3.2264479727	0.9315154193
H	1.0	-0.8417944116	2.1978390492	0.0299790754
O	8.0	-2.3314311473	-1.3474816621	0.1438884123
H	1.0	-1.4806911043	-1.8276797356	0.0303508837
H	1.0	-2.7255324810	-1.7225340928	0.9356431807
O	8.0	2.3308774498	1.3464156743	-0.1421691881
H	1.0	2.7255644107	1.7180093663	-0.9352596601
H	1.0	1.4819477012	1.8297991094	-0.0285785374
O	8.0	0.0004941093	-2.6924890031	-0.1449337962
H	1.0	0.8441512269	-2.1994161158	-0.0333155779
H	1.0	0.1230569006	-3.2223845635	-0.9368017155
O	8.0	2.3318438779	-1.3463725866	0.1443212425
H	1.0	2.8514219621	-1.5043002642	0.9367458638
H	1.0	2.3247620686	-0.3691396798	0.0333816062
O	8.0	-2.3311192932	1.3452273421	-0.1425919979
H	1.0	-2.8507582417	1.5024831503	-0.9350910528
H	1.0	-2.3260047923	0.3681965690	-0.0300427967

Table S11. MP2/aug-cc-pV5Z-h//MP2/aug-cc-pVTZ pair interaction energies and many-body effects (MBE) in the bag structure (kcal/mol).

Pairs	R_{OO} (Å)	ΔE_{ele}	ΔE_{ex}	ΔE_{rep}	ΔE_{pol}	ΔE_{HF}	ΔE_{disp}	ΔE_{MP2}
1,2	3.777	-1.69	-0.21	+0.33	-0.08	-1.65	-0.12	-1.77
1,3	2.655	-14.53	-22.12	+41.56	-6.41	-1.50	-2.45	-3.95
1,4	4.206	-1.22	-0.05	+0.08	-0.04	-1.24	-0.07	-1.31
1,5	2.818	-8.65	-10.50	+19.15	-2.81	-2.81	-1.70	-4.51
1,6	2.818	-9.08	-11.33	+20.70	-3.06	-2.77	-1.74	-4.50
2,3	4.066	-1.22	-0.14	+0.22	-0.05	-1.19	-0.12	-1.31
2,4	2.688	-13.46	-20.15	+37.66	-5.63	-1.57	-2.36	-3.93
2,5	2.851	-8.00	-10.56	+19.14	-2.60	-2.02	-1.65	-3.68
2,6	2.823	-8.46	-11.61	+21.15	-2.91	-1.83	-1.80	-3.63
3,4	2.676	-13.82	-20.29	+37.96	-5.72	-1.88	-2.32	-4.19
3,5	3.946	-1.25	-0.12	+0.18	-0.05	-1.24	-0.12	-1.36
3,6	4.213	-1.04	-0.03	+0.05	-0.03	-1.06	-0.08	-1.14
4,5	4.260	-0.49	-0.02	+0.03	-0.03	-0.51	-0.13	-0.64
4,6	4.112	-1.08	-0.07	+0.10	-0.04	-1.08	-0.06	-1.14
5,6	3.902	1.62	-0.21	+0.34	-0.07	1.68	-0.37	1.31
Sum	51.811	-82.38	-107.40	+198.65	-29.54	-20.65	-15.10	-35.76
Bag		-82.38	-107.40	+197.82	-40.37	-32.33	-15.14	-47.47
MBE		0.00	0.00	-0.84	-10.84	-11.68	-0.04	-11.71

Table S12. Coordinates (Å) of the bag structure optimized with MP2/aug-cc-pVTZ

O	8.0	-1.0237806610	1.6056744956	-0.4616149281
H	1.0	-0.0369228580	1.6954637530	-0.3768366596
H	1.0	-1.3306840648	2.4579446838	-0.7840190888
O	8.0	-0.0945909351	-1.9278797407	0.4941911243
H	1.0	-0.5261654934	-1.3487143224	1.1457854165
H	1.0	-0.5852817730	-1.7402789360	-0.3255772012
O	8.0	1.6169958427	1.6953820155	-0.1974021704
H	1.0	1.9550978906	2.1035479736	0.6049103827
H	1.0	1.9435966478	0.7625327762	-0.1567930988
O	8.0	2.3374567197	-0.8688616882	0.0568820395
H	1.0	2.7769669270	-1.3702958458	-0.6347140298
H	1.0	1.4832464708	-1.3394248515	0.2247711958
O	8.0	-1.3266682854	0.1881460818	1.9554945044
H	1.0	-2.1889270248	0.2005808693	2.3791529828
H	1.0	-1.3998060114	0.7899068371	1.1938485254
O	8.0	-1.3291420145	-0.8520927532	-1.8049168730
H	1.0	-1.3266477928	0.0619636988	-1.4663878437
H	1.0	-2.2129685601	-0.9966701436	-2.1527065672

Table S13. MP2/aug-cc-pV5Z-h//MP2/aug-cc-pVTZ pair interaction energies and many-body effects (MBE) in the cyclic-boat-1 structure (kcal/mol).

Pairs	R_{OO} (Å)	ΔE_{ele}	ΔE_{ex}	ΔE_{rep}	ΔE_{pol}	ΔE_{HF}	ΔE_{disp}	ΔE_{MP2}
1,2	2.711	-12.52	-17.58	+32.73	-4.96	-2.34	-2.11	-4.45
1,3	4.557	-0.92	-0.02	+0.03	-0.03	-0.94	-0.03	-0.97
1,4	2.714	-11.53	-16.75	+31.13	-4.72	-1.87	-2.16	-4.03
1,5	5.226	-0.47	0.00	+0.00	-0.01	-0.47	0.00	-0.47
1,6	4.511	-1.03	-0.02	+0.03	-0.03	-1.05	0.00	-1.05
2,3	2.713	-12.45	-17.51	+32.57	-4.92	-2.32	-2.10	-4.41
2,4	4.636	-0.92	-0.02	+0.03	-0.03	-0.93	-0.01	-0.94
2,5	4.526	-1.02	-0.02	+0.03	-0.03	-1.04	0.00	-1.05
2,6	5.310	-0.44	0.00	+0.00	-0.01	-0.45	0.01	-0.44
3,4	5.079	-0.39	0.00	+0.01	-0.01	-0.39	-0.02	-0.41
3,5	2.714	-11.53	-16.74	+31.12	-4.72	-1.87	-2.16	-4.03
3,6	4.633	-0.92	-0.02	+0.03	-0.03	-0.93	-0.01	-0.95
4,5	4.559	-0.92	-0.02	+0.03	-0.03	-0.94	-0.03	-0.97
4,6	2.714	-12.45	-17.52	+32.59	-4.92	-2.31	-2.10	-4.41
5,6	2.711	-12.52	-17.58	+32.72	-4.96	-2.34	-2.11	-4.45
Sum	59.314	-80.03	-103.80	+193.04	-29.40	-20.19	-12.83	-33.02
Boat-1		-80.03	-103.80	+192.40	-41.91	-33.34	-12.96	-46.30
MBE		0.00	0.00	-0.64	-12.51	-13.15	-0.13	-13.28

Table S14. Coordinates (Å) of the cyclic-boat-1 structure optimized with MP2/aug-cc-pVTZ

O	8.0	−0.9571470293	−2.1163862508	−0.5097688977
H	1.0	−1.1365470085	−2.8878661184	−1.0527737817
H	1.0	0.0223654232	−2.0733484870	−0.4313264184
O	8.0	1.7411065688	−1.9523740288	−0.3071884771
H	1.0	2.0998035503	−1.0372031993	−0.3392949519
H	1.0	2.1662966769	−2.3576701983	0.4532040041
O	8.0	2.7156250622	0.5786511314	−0.3904946911
H	1.0	2.2067028076	1.2445685592	0.1225823907
H	1.0	2.8510755864	0.9727316261	−1.2558953157
O	8.0	−2.3420229922	0.2110043850	−0.6798489605
H	1.0	−2.4055092906	0.4542090138	−1.6068875797
H	1.0	−1.8500849338	−0.6395598247	−0.6664706724
O	8.0	1.2791521270	2.3181117914	1.1176464996
H	1.0	1.4635456083	3.2585724038	1.1788464556
H	1.0	0.2984024012	2.2445770088	1.1042990346
O	8.0	−1.4211120556	2.0931586767	1.0445234954
H	1.0	−1.7620505485	1.4146932189	0.4194822603
H	1.0	−1.8904342427	1.9302717378	1.8669505474

Table S15. MP2/aug-cc-pV5Z-h//MP2/aug-cc-pVTZ pair interaction energies and many-body effects (MBE) in the cyclic-boat-2 structure (kcal/mol).

Pairs	R_{OO} (Å)	ΔE_{ele}	ΔE_{ex}	ΔE_{rep}	ΔE_{pol}	ΔE_{HF}	ΔE_{disp}	ΔE_{MP2}
1,2	2.714	-11.99	-16.71	+31.05	-4.72	-2.36	-2.03	-4.40
1,3	4.640	-0.86	-0.02	+0.02	-0.03	-0.88	-0.02	-0.90
1,4	2.713	-12.66	-17.86	+33.23	-5.01	-2.29	-2.13	-4.42
1,5	5.464	-0.23	0.00	+0.00	0.00	-0.24	-0.03	-0.27
1,6	4.530	-0.96	-0.02	+0.03	-0.03	-0.97	-0.03	-1.01
2,3	2.717	-12.05	-16.98	+31.56	-4.78	-2.25	-2.05	-4.30
2,4	4.468	-0.87	-0.02	+0.04	-0.03	-0.89	-0.06	-0.95
2,5	4.537	-0.95	-0.02	+0.03	-0.03	-0.97	-0.03	-1.00
2,6	5.093	-0.27	0.00	+0.00	-0.01	-0.28	-0.03	-0.31
3,4	4.936	-0.42	-0.01	+0.01	-0.01	-0.42	-0.01	-0.44
3,5	2.713	-12.63	-17.83	+33.18	-5.00	-2.28	-2.13	-4.41
3,6	4.468	-0.87	-0.02	+0.04	-0.03	-0.89	-0.06	-0.95
4,5	4.640	-0.86	-0.02	+0.02	-0.03	-0.88	-0.02	-0.90
4,6	2.717	-12.02	-16.94	+31.48	-4.77	-2.25	-2.05	-4.29
5,6	2.714	-11.99	-16.70	+31.05	-4.72	-2.36	-2.03	-4.39
Sum	59.064	-79.63	-103.14	+191.76	-29.20	-20.21	-12.72	-32.93
Boat-2		-79.63	-103.14	+191.12	-41.71	-33.35	-12.82	-46.17
MBE		0.00	0.00	-0.63	-12.51	-13.15	-0.09	-13.24

Table S16. Coordinates (Å) of the cyclic-boat-2 structure optimized with MP2/aug-cc-pVTZ

O	8.0	−1.0299768771	−2.2072066655	−0.5425401570
H	1.0	−1.3108760089	−2.7479715772	0.2004591379
H	1.0	−0.0553787323	−2.1289497648	−0.4471278927
O	8.0	1.6497383624	−1.8952125788	−0.2490000092
H	1.0	2.0204105416	−0.9896372938	−0.3408922402
H	1.0	2.3184613857	−2.4844209575	−0.6061245142
O	8.0	2.6415803040	0.6272772021	−0.4348565957
H	1.0	2.1845900675	1.2762787258	0.1468076517
H	1.0	2.7376375508	1.0758948327	−1.2788135994
O	8.0	−2.2663452447	0.1998152386	−0.7330568144
H	1.0	−2.3197784069	0.3863555211	−1.6738266877
H	1.0	−1.8267906951	−0.6785592053	−0.6718357600
O	8.0	1.3511854760	2.4091719327	1.1533084497
H	1.0	1.5843649457	2.3759429807	2.0849215750
H	1.0	0.3749035823	2.3019792308	1.1306878978
O	8.0	−1.3331925451	2.0210724411	1.0546496514
H	1.0	−1.6809834877	1.3835100500	0.3925418610
H	1.0	−1.9935080456	2.7156013984	1.1140978138