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水团簇$(H_2O)_n$中多体作用强度与水分子间距的关系

杨 微 李晓蕾 王长生*

(辽宁师范大学化学化工学院, 辽宁 大连 116029)

Dependence of the Many-Body Interaction Strength in Water Clusters $(H_2O)_n$ on the Water–Water Distance

YANG Wei LI Xiao-Lei WANG Chang-Sheng*

(*School of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, Liaoning Province, P. R. China*)

*Corresponding author. Email: chwangcs@lnnu.edu.cn; Tel: +86-411-82159391.

Table S1 The Cartesian coordinates for the water clusters shown in Fig.1

$8W_1$: The optimal structure is obtained at the MP2/6-31+G(d,p) level

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	0.000000	2.099007	1.371731
1	0	0.000000	2.990801	1.738180
1	0	0.000000	2.189889	0.384356
8	0	-2.099007	0.000000	-1.371731
1	0	-2.990801	0.000000	-1.738180
1	0	-2.189889	0.000000	-0.384356
8	0	0.000000	-2.099007	1.371731
1	0	0.000000	-2.189889	0.384356
1	0	0.000000	-2.990801	1.738180
8	0	0.000000	1.951548	-1.317280
1	0	-0.773519	1.406215	-1.547514
1	0	0.773519	1.406215	-1.547514
8	0	-1.951548	0.000000	1.317280
1	0	-1.406215	-0.773519	1.547514
1	0	-1.406215	0.773519	1.547514
8	0	1.951548	0.000000	1.317280
1	0	1.406215	0.773519	1.547514
1	0	1.406215	-0.773519	1.547514
8	0	2.099007	0.000000	-1.371731
1	0	2.189889	0.000000	-0.384356
1	0	2.990801	0.000000	-1.738180
8	0	0.000000	-1.951548	-1.317280
1	0	0.773519	-1.406215	-1.547514
1	0	-0.773519	-1.406215	-1.547514

E= -610.742051 a.u.; IE_{tot}=-304.6 kJ·mol^{-1}; IE^t_{2b}=-240.5 kJ·mol^{-1}; IE^t_{3b}=-61.9 kJ·mol^{-1}; IE^t_{4b}=-2.3 kJ·mol^{-1}

$8W_2$: The optimal structure is obtained at the MP2/6-31+G(d,p) level

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	1.526868	1.329030	1.491413
1	0	2.172422	1.676290	2.117734
1	0	1.560047	0.340146	1.557715
8	0	-1.329030	1.526868	-1.491413
1	0	-1.676290	2.172422	-2.117734

1	0	-0.340146	1.560047	-1.557715
8	0	1.329030	-1.526868	-1.491413
1	0	0.340146	-1.560047	-1.557715
1	0	1.676290	-2.172422	-2.117734
8	0	-1.347879	1.347879	1.373642
1	0	-1.497349	1.586578	0.441077
1	0	-0.410496	1.554973	1.538637
8	0	1.347879	1.347879	-1.373642
1	0	1.554973	0.410496	-1.538637
1	0	1.586578	1.497349	-0.441077
8	0	1.347879	-1.347879	1.373642
1	0	1.497349	-1.586578	0.441077
1	0	0.410496	-1.554973	1.538637
8	0	-1.526868	-1.329030	1.491413
1	0	-2.172422	-1.676290	2.117734
1	0	-1.560047	-0.340146	1.557715
8	0	-1.347879	-1.347879	-1.373642
1	0	-1.586578	-1.497349	-0.441077
1	0	-1.554973	-0.410496	-1.538637

E= -610.742007 a.u.; IE_{tot}=-304.5 kJ ṁol^{-1}; IE^{t}_{2b}=-238.1 kJ ṁol^{-1}; IE^{t}_{3b}=-63.8 kJ ṁol^{-1}; IE^{t}_{4b}=-3.7 kJ ṁol^{-1}

10W: The optimal structure is taken from reference [7]

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-0.970508	2.454333	1.174186
1	0	-1.568370	1.714856	1.263156
1	0	-1.359460	3.185743	1.625015
8	0	-2.589474	0.126309	1.242786
1	0	-2.029439	-0.644042	1.382401
1	0	-3.391970	-0.031627	1.712724
8	0	-0.976306	-2.084793	1.458043
1	0	-0.090628	-1.882667	1.739297
1	0	-0.895362	-2.416343	0.571000
8	0	1.771821	-1.241396	1.874400
1	0	2.362696	-1.484556	2.568138
1	0	1.782134	-0.282461	1.818318
8	0	1.786945	1.491923	1.465729
1	0	2.075640	1.573251	0.563815
1	0	0.919894	1.878968	1.494549
8	0	2.238912	1.201241	-1.399808

1	0	2.205641	0.241922	-1.365884
1	0	2.980307	1.433102	-1.934626
8	0	2.098577	-1.536534	-1.037393
1	0	2.137813	-1.626191	-0.092869
1	0	1.259246	-1.901969	-1.294794
8	0	-0.646663	-2.419052	-1.422376
1	0	-1.171330	-1.635449	-1.613198
1	0	-0.945363	-3.099155	-2.003539
8	0	-2.174729	-0.156082	-1.715171
1	0	-2.542769	-0.011651	-0.853493
1	0	-1.658909	0.624935	-1.903934
8	0	-0.514939	2.161705	-1.764842
1	0	-0.657647	2.477254	-0.882378
1	0	0.398793	1.904851	-1.798119

E= -763.421596 a.u.; IE_{tot}=-355.6 kJ·mol^{-1}; IE^{t}_{2b}=-293.1 kJ·mol^{-1}; IE^{t}_{3b}=-58.6 kJ·mol^{-1}; IE^{t}_{4b}=-2.4 kJ·mol^{-1}

16W: The optimal structure is taken from reference [24]

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-0.001129	1.354614	1.411949
1	0	0.126913	0.390038	1.542379
1	0	0.864979	1.770430	1.582482
8	0	-4.125476	-0.028856	1.581829
1	0	-4.814213	0.077733	2.244157
1	0	-3.599307	0.814450	1.594024
8	0	2.572880	2.430317	1.343267
1	0	2.867234	3.288600	1.661980
1	0	2.563274	2.489457	0.349112
8	0	4.127842	0.029896	-1.579877
1	0	3.600724	-0.812781	-1.591804
1	0	4.815995	-0.077460	-2.242705
8	0	-2.852467	2.205111	-1.514910
1	0	-3.378470	1.362952	-1.518139
1	0	-3.299273	2.802486	-2.121389
8	0	-2.468873	-2.297615	1.300312
1	0	-1.556695	-2.050648	1.536477
1	0	-3.019992	-1.535560	1.555467
8	0	2.467114	2.296838	-1.300824
1	0	1.555524	2.048838	-1.538250
1	0	3.019654	1.535701	-1.555504

8	0	2.853334	-2.203244	1.517310
1	0	3.380054	-1.361488	1.520671
1	0	3.298745	-2.800785	2.124668
8	0	2.666349	-2.176385	-1.364682
1	0	1.719586	-1.990674	-1.508718
1	0	2.730811	-2.403826	-0.422219
8	0	-4.188729	-0.080832	-1.257369
1	0	-3.701092	-0.901655	-1.447598
1	0	-4.363513	-0.128522	-0.300630
8	0	0.198582	-1.381795	1.339401
1	0	0.170568	-1.426979	0.358276
1	0	1.070945	-1.753573	1.571816
8	0	-2.665578	2.178303	1.366685
1	0	-1.719060	1.990447	1.509654
1	0	-2.730360	2.406267	0.424341
8	0	4.189396	0.081728	1.260044
1	0	3.701297	0.902632	1.448738
1	0	4.366571	0.129362	0.303811
8	0	-0.000014	-1.357459	-1.415833
1	0	-0.866447	-1.773320	-1.585036
1	0	-0.127848	-0.392943	-1.547080
8	0	-2.574423	-2.429796	-1.343989
1	0	-2.564119	-2.489277	-0.349852
1	0	-2.866906	-3.288688	-1.662735
8	0	-0.199231	1.379559	-1.343271
1	0	-1.071482	1.752288	-1.574662
1	0	-0.170708	1.423429	-0.362090

E= -1221.511060 a.u.; IE_{tot}=-679.4 kJ·mol^{-1}; IE^{t}_{2b}=-511.4 kJ·mol^{-1}; IE^{t}_{3b}=-161.5 kJ·mol^{-1}; IE^{t}_{4b}=-6.5 kJ·mol^{-1}

$20W_1$: The structure is taken from reference [7]

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-1.274516	2.469324	5.410419
1	0	-1.664991	2.370767	4.550689
1	0	-1.213127	1.592584	5.770821
8	0	1.356559	3.281838	5.029161
1	0	0.431951	3.093544	5.206055
1	0	1.574593	4.069537	5.500016
8	0	1.252872	2.419417	2.274808
1	0	1.443736	2.956084	3.035651
1	0	1.601043	1.553629	2.474796

8	0	1.953197	-0.291677	2.877626
1	0	2.250199	-0.692742	2.069645
1	0	1.068489	-0.617560	3.022953
8	0	-1.526197	1.762085	2.597307
1	0	-0.643110	2.082333	2.431069
1	0	-1.952489	1.718575	1.749799
8	0	-0.815693	-0.913775	3.331433
1	0	-1.164628	-0.050701	3.121317
1	0	-0.873530	-0.992032	4.276873
8	0	-0.486264	-0.284169	6.130735
1	0	0.446203	-0.068932	6.054385
1	0	-0.603149	-0.723361	6.957265
8	0	2.138721	0.507311	5.671267
1	0	2.096114	1.448669	5.551418
1	0	2.396741	0.149139	4.830760
8	0	0.935400	1.741152	-0.504385
1	0	1.204781	2.277025	0.232284
1	0	-0.000142	1.592554	-0.391873
8	0	1.804696	-0.947798	0.077636
1	0	1.632499	-0.038306	-0.152915
1	0	2.065079	-1.376508	-0.729102
8	0	-1.809971	0.929660	-0.144791
1	0	-2.200633	0.909136	-1.010454
1	0	-1.637767	0.020335	0.086415
8	0	-0.930203	-1.723266	0.571623
1	0	0.005287	-1.574832	0.458462
1	0	-1.069168	-1.809946	1.507353
8	0	-1.960171	0.282891	-2.945499
1	0	-1.074251	0.604477	-3.095592
1	0	-2.346757	0.180429	-3.807691
8	0	0.811797	0.929636	-3.264600
1	0	1.053554	1.498707	-2.543766
1	0	1.164011	0.069499	-3.049791
8	0	-1.238646	-2.400098	-2.210355
1	0	-1.589207	-1.534313	-2.404158
1	0	-1.351392	-2.524664	-1.275654
8	0	1.523127	-1.788634	-2.660720
1	0	0.638002	-2.107508	-2.500500
1	0	1.776513	-2.144507	-3.504804
8	0	-2.294768	-0.569974	-5.684369
1	0	-2.071621	-1.487202	-5.509594
1	0	-2.982071	-0.569595	-6.330369
8	0	-1.410643	-3.121947	-5.025753

1	0	-1.471845	-3.205084	-4.082004
1	0	-0.482452	-3.122232	-5.227742
8	0	1.424343	-2.427485	-5.475558
1	0	1.193432	-1.537229	-5.750815
1	0	2.010521	-2.776359	-6.127014
8	0	0.546359	0.145512	-6.056003
1	0	0.740179	0.685407	-5.299525
1	0	-0.400593	0.081154	-6.094528

E= -1526.219609 a.u.; IE_{tot}=-786.4 kJ mol^{-1}; IE^{t}_{2b}=-659.5 kJ mol^{-1}; IE^{t}_{3b}=-126.1 kJ mol^{-1}; IE^{t}_{4b}=0.4 kJ mol^{-1}

$20W_2$: The structure is taken from reference [25]

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	1.903760	0.194334	-3.262859
1	0	0.958386	-0.047261	-3.450990
1	0	1.897803	1.103057	-2.901014
8	0	-0.674236	-0.504383	-3.667829
1	0	-0.888800	-1.365646	-3.251357
1	0	-1.323947	0.135643	-3.320789
8	0	3.119996	-1.523155	-1.799856
1	0	3.752318	-1.976627	-2.371863
1	0	2.638928	-0.835656	-2.386296
8	0	1.896977	2.752776	-2.037206
1	0	2.407805	3.436196	-2.488758
1	0	2.333716	2.602456	-1.147095
8	0	-2.509936	1.444418	-2.602845
1	0	-3.068853	1.063841	-1.873366
1	0	-3.116413	1.785327	-3.272203
8	0	-1.280815	-2.909450	-2.335818
1	0	-1.949827	-2.700397	-1.613667
1	0	-1.657587	-3.625620	-2.861844
8	0	-1.959221	-0.254373	3.306019
1	0	-1.942724	-1.155183	2.926099
1	0	-1.028224	-0.035347	3.534893
8	0	2.542130	-1.472604	2.643543
1	0	3.091247	-1.130280	1.901025
1	0	3.148059	-1.868015	3.282692
8	0	1.143269	2.943897	2.344019
1	0	0.291690	3.227800	1.921175
1	0	1.402674	3.649172	2.950168
8	0	0.702664	0.459264	3.754508

1	0	0.873613	1.300242	3.292192
1	0	1.340799	-0.184195	3.394949
8	0	-0.780846	3.377129	-1.505958
1	0	-1.359039	2.707114	-1.927890
1	0	0.144720	3.164165	-1.753448
8	0	-2.997989	-2.327823	-0.437709
1	0	-2.648008	-2.510084	0.463029
1	0	-3.305858	-1.398848	-0.442213
8	0	-3.047927	1.508654	1.622240
1	0	-2.652700	0.868040	2.279724
1	0	-2.398119	2.224705	1.491137
8	0	0.636834	-3.415004	1.656634
1	0	0.843666	-3.493508	0.691366
1	0	1.265570	-2.762169	2.015487
8	0	2.984132	2.291293	0.323334
1	0	3.274152	1.364889	0.438143
1	0	2.379466	2.504338	1.065006
8	0	-3.871748	0.381635	-0.526226
1	0	-3.544184	0.835060	0.331500
1	0	-4.836483	0.412221	-0.496829
8	0	1.152443	-3.495148	-1.021511
1	0	0.327504	-3.321727	-1.520630
1	0	1.797478	-2.822021	-1.308848
8	0	-1.881548	-2.823567	2.064974
1	0	-2.271028	-3.538626	2.583259
1	0	-0.912904	-3.065291	1.924409
8	0	3.923826	-0.407121	0.484392
1	0	4.888958	-0.374548	0.495050
1	0	3.663663	-0.847210	-0.375913
8	0	-1.156851	3.612409	1.061419
1	0	-1.011273	3.534687	0.063809
1	0	-1.565557	4.473856	1.213782

E= -1450.547791 a.u.; IE_{tot}=-856.6 kJ mol^{-1}; IE^{t}_{2b}=-613.7 kJ mol^{-1}; IE^{t}_{3b}=-220.4 kJ mol^{-1}; IE^{t}_{4b}=21.8 kJ mol^{-1}

22W: The optimal structure is obtained at the MP2/6-31+G(d,p) level

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	0.265387	-0.923119	-1.484945
1	0	1.124357	-1.288882	-1.764676
1	0	0.358496	0.053031	-1.544203
8	0	0.571174	1.827194	-1.211145

1	0	-0.191693	2.392947	-1.436239
1	0	0.616406	1.837937	-0.229276
8	0	-1.860803	3.281675	-1.361674
1	0	-2.573816	2.621444	-1.512045
1	0	-2.059524	4.033049	-1.933078
8	0	-3.637783	1.194860	-1.432153
1	0	-4.585635	1.041808	-1.612648
1	0	-3.199288	0.323066	-1.563432
8	0	-2.495527	-1.307464	-1.371907
1	0	-2.469059	-1.419068	-0.396091
1	0	-1.562653	-1.352286	-1.656627
8	0	-6.292851	0.260573	-1.347887
1	0	-6.373442	0.241880	-0.357769
1	0	-7.137334	0.574255	-1.692339
8	0	-5.128635	-2.389953	-1.377271
1	0	-5.618939	-1.573225	-1.577640
1	0	-4.209295	-2.204538	-1.639224
8	0	-1.670424	3.133902	1.617994
1	0	-1.663243	3.434158	0.695136
1	0	-0.793907	2.736851	1.767500
8	0	0.727258	1.585137	1.555724
1	0	0.498752	0.634317	1.644101
1	0	1.663386	1.655695	1.816705
8	0	0.159929	-1.140843	1.328889
1	0	-0.743372	-1.402559	1.592456
1	0	0.153694	-1.170171	0.348907
8	0	-2.622990	-1.400560	1.417174
1	0	-3.381958	-1.980234	1.614903
1	0	-2.946100	-0.482769	1.570998
8	0	-3.590793	1.169435	1.403055
1	0	-3.615412	1.269725	0.429797
1	0	-2.979862	1.883642	1.693493
8	0	-6.190220	0.062697	1.327447
1	0	-5.976687	-0.864263	1.534929
1	0	-5.414176	0.575740	1.619553
8	0	-5.172955	-2.644064	1.314134
1	0	-5.554123	-3.467259	1.641395
1	0	-5.202263	-2.685305	0.324737
8	0	3.351024	1.309198	-1.353493
1	0	2.507491	1.745914	-1.570100
1	0	3.190475	0.352150	-1.502452
8	0	3.524193	1.217899	1.422765
1	0	4.459318	1.267266	1.693436

1	0	3.527349	1.375136	0.453241
8	0	2.955861	-1.513437	1.356156
1	0	2.029482	-1.667034	1.616876
1	0	3.110137	-0.556156	1.509890
8	0	3.027947	-1.462454	-1.421908
1	0	3.889221	-1.801182	-1.728377
1	0	3.019433	-1.617571	-0.451496
8	0	6.168735	0.832767	-1.345282
1	0	5.317582	1.273463	-1.510993
1	0	6.352645	0.971000	-0.398823
8	0	5.829542	-1.828854	-1.661091
1	0	6.439222	-2.240263	-2.284870
1	0	6.038946	-0.860307	-1.650267
8	0	5.773761	-1.948035	1.227497
1	0	4.834293	-2.096337	1.432409
1	0	5.863994	-2.133679	0.275843
8	0	6.309835	0.682698	1.533450
1	0	6.200441	-0.302131	1.523317
1	0	7.043338	0.876722	2.128813

E= -1679.586433 a.u.; IE_{tot}=-954.3 kJ·mol^{-1}; IE^{t}_{2b}=-747.5 kJ·mol^{-1}; IE^{t}_{3b}=-202.7 kJ·mol^{-1}; IE^{t}_{4b}=-2.6 kJ·mol^{-1}

24W: The structure is taken from reference [7]

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	2.69131602	0.29269762	2.91320770
1	0	3.30910334	0.29435558	2.15611911
1	0	2.27598694	-0.59402183	2.92517697
8	0	4.50736599	0.48523594	0.73602383
1	0	5.37703576	0.77091530	1.04447690
1	0	4.17101877	1.24903656	0.16532361
8	0	3.62668887	2.44119132	-0.72790271
1	0	3.14770895	2.17478061	-1.53761250
1	0	2.99481304	3.01765030	-0.23341462
8	0	1.88939794	3.96546328	0.72403554
1	0	1.05407035	4.17390249	0.26661447
1	0	1.61923181	3.48030342	1.52866576
8	0	1.18259274	2.46615523	3.03055610
1	0	1.45567188	2.88573327	3.85661673
1	0	1.72113217	1.62680771	2.98668051
8	0	4.16712125	-1.77894211	-0.72352219

1	0	5.01995106	-2.12545106	-1.01517961
1	0	4.38289826	-0.97916015	-0.18383457
8	0	2.48982796	-3.61905812	0.71547150
1	0	2.20509549	-3.14400575	1.52113403
1	0	3.08734235	-2.99878461	0.25858843
8	0	1.54569854	-2.26218983	3.02530200
1	0	0.54950668	-2.30922708	2.98159957
1	0	1.77293224	-2.71020661	3.85031890
8	0	2.21343966	1.61586387	-3.04459583
1	0	2.56882526	1.98411779	-3.86371247
1	0	1.29206133	1.99466264	-2.97988222
8	0	2.43180510	-1.17245310	-2.89434737
1	0	2.33442267	-0.19926883	-2.94274859
1	0	3.02946432	-1.34040848	-2.14053047
8	0	-0.54143672	4.49930342	-0.71678501
1	0	-0.66863312	5.41094878	-1.00856689
1	0	-1.34229463	4.28496991	-0.17815467
8	0	-0.19691001	2.69617411	-2.88969669
1	0	-0.99128245	2.12571974	-2.94001871
1	0	-0.35084604	3.29659653	-2.13511817
8	0	0.29074428	-2.71940934	-3.04983191
1	0	0.43137718	-3.20995330	-3.86985518
1	0	1.07974635	-2.11119461	-2.98454989
8	0	0.30049444	-4.36042097	-0.73619756
1	0	0.30862410	-3.81096223	-1.54495429
1	0	1.11580638	-4.10186557	-0.24170432
8	0	-2.67479582	3.65947840	0.73815290
1	0	-3.16772333	2.98745993	0.16574867
1	0	-3.35703132	4.26996835	1.04625248
8	0	-1.60257669	2.18022292	2.91450006
1	0	-1.91212540	2.71547443	2.15783814
1	0	-0.62703257	2.26424026	2.92792287
8	0	-2.50248581	1.11390225	-3.04628244
1	0	-2.37005320	0.12641156	-2.98320003
1	0	-2.99784159	1.23917991	-3.86584380
8	0	-2.23277023	-1.51386096	-2.89599837
1	0	-2.67678841	-1.94911892	-2.14299502
1	0	-1.34139446	-1.91620943	-2.94584707
8	0	-3.92680647	1.92123658	-0.72999504
1	0	-4.10989651	1.08475177	-0.23718844
1	0	-3.45545608	1.64134513	-1.53963945
8	0	-3.62481762	-2.71846822	-0.72750968
1	0	-3.03958562	-3.30752587	-0.19088103

1	0	-4.35195381	-3.28227675	-1.02050047
8	0	-1.83350638	-4.14771994	0.72872542
1	0	-1.00384925	-4.23727273	0.15787417
1	0	-2.02057747	-5.04425073	1.03587199
8	0	-1.09100492	-2.48273142	2.90856802
1	0	-1.65145193	-1.67985859	2.92287753
1	0	-1.39908154	-3.01703774	2.15066698
8	0	-4.37793457	-0.34866313	0.71708918
1	0	-3.82415823	-0.34092711	1.52272386
1	0	-4.13961922	-1.17552115	0.25880176
8	0	-2.73050835	-0.21334627	3.02698540
1	0	-2.27281622	0.67278643	2.98490227
1	0	-3.23182536	-0.18758864	3.85218761

IE^{t}_{2b}=-738.9 kJ mol^{-1}; IE^{t}_{3b}=-257.3 kJ mol^{-1}; IE^{t}_{4b}=-28.8 kJ mol^{-1}