Supplementary Information for

Effect of confinement on the water rotation via quantum tunneling

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Fig. S1. Modeling and calculation for TS of water dimer in different conditions. Two TS structures related to "antigeared" and "geared" rotations types are denoted by TR1 and TR2. First, find out two TS structures for isolated water dimer. Second, put the TS structures in five calibers of CNTs and locate the former along the axis of CNTs, then continue TS optimization to get the exact geometrical structures under confinement. According to this procedure, 12 TS structures (2 rotation types * 6 conditions) are obtained.

Fig. S2. Calculated energy barrier with and without dispersion correction. The red (blue) dashed line cross the hollow square (circle) points represent the antigeared and greared rotation processes without considering the dispersion correction.

Fig. S3. The structures related to the points with low potential energy in the trajectory of QMMD for (a) (5, 5) CNT; (b) (6, 6) CNT; (c) (7, 7) CNT; (d) (8, 8) CNT; (e) (9, 9) CNT.

Fig. S4. The distances between the two O atoms of the confined water dimer and CNTs. The red and blue solid lines represent the distances related the two atoms, the dashed lines corresponding the same color solid lines are the related average values. The five confining conditions are shown in parts (a), (b), (c), (d), (e). The radii of (5, 5), (6, 6), (7, 7), (8, 8), (9, 9) CNTs are 3.41, 4.09, 4.75, 5.43, 6.09 Å, respectively.

Fig. S5. The change of the H-bond length of the confined water dimer as a function of time for (a) (5, 5) CNT; (b) (6, 6) CNT; (c) (7, 7) CNT; (d) (8, 8) CNT; (e) (9, 9) CNT. The range in which the H-bond is present can be considered to be 1.5 ~ 2.5 Å. The average of H-bond length in each confining condition is also given.

Fig. S6. The distance between the two O atoms of the confined water dimer for (a) (5, 5) CNT; (b) (6, 6) CNT; (c) (7, 7) CNT; (d) (8, 8) CNT; (e) (9, 9) CNT.

Fig. S7. Reaction paths of two rotation types in different conditions. (a) There are 12 reaction paths in total in one graph, TR1 and TR2 represent the antigeared and geared rotation types. (b) Divided graphs for two rotation types of water dimer in six conditions (one isolated and five confining conditions) to compare, which can be more clearly to estimate the difficulty between TR1 and TR2 in the same condition. The reactant energy is set as reference zero point for corresponding energy barrier. As the variant of IRC described before, the reaction paths herein are without mass weighting.

Fig. S8. Tunneling probability for two rotation types in respective conditions. The tunneling probability vary along the provided energy. Showing in six graphs according to six conditions is convenient to clearly compare and estimate the difficulty between two rotation types via quantum tunneling.

Fig. S9. The ratio along the temperature in the conditions of providing (a) 0.01 eV, (b) 0.07 eV, (c) 0.15 eV, (d) 0.30 eV to confined water dimer, respectively. The solid (dashed) lines through solid (hollow) points represent the ratio for antigeared (geared) rotation TR1 (TR2).

Table S1. The H-bond length and the O-O distance of optimized water dimer in different confining conditions obtained by the DFT-PBE0 calculation with and without dispersion correction. The unit is "Å".

Table S2. The distances between O atoms of the confined water dimer and the wall of CNTs. The unit is "Å".

Table S3. The differences of the energy barriers between the conditions with or without dispersion correction. TR1 and TR2 (TR1' and TR2') are the energy barriers of two rotation processes with (without) dispersion correction. The unit is "eV".

Table S4. Coordinates of two TS structures of the water dimer corresponding to two rotation types in different conditions.

Table S5. Reduced mass, imaginary frequency of TS and displacement of related rotation path for every rotation type in each condition.

Table S6. Progressions and coefficients of Fourier Function fitted for reaction paths for two rotation types in different conditions.

Table S7. The probability of two tunneling rotation types in different conditions. The provided energy is assigned to the vibrational mode along the reaction path. It should be noted that the data vacancies come from the different restriction on the range of x value of V(x) in tunneling probability formula.

Table S8. The frequencies of the vibrational modes of the corresponding rotation types along the reaction path for optimized water dimer.

Table S9. Expectation of tunneling rotation per second (s^{-1}).

Table S10. The temperature related to $Log_{10}(Ratio) = 0$.

Table S11. The coordinates and energies of the sampled structures of confined water dimer in (5, 5) CNT. The first structure which is highlighted with underline was used in the paper.

Table S12. The coordinates and energies of the sampled structures of confined water dimer in (6, 6) CNT. The first structure which is highlighted with underline was used in the paper.

Table S13. The coordinates and energies of the sampled structures of confined water dimer in (7, 7) CNT. The first structure which is highlighted with underline was used in the paper.

Table S14. The coordinates and energies of the sampled structures of confined water dimer in (8, 8) CNT. The first structure which is highlighted with underline was used in the paper.

Table S15. The coordinates and energies of the sampled structures of confined water dimer in (9, 9) CNT. The first structure which is highlighted with underline was used in the paper.

References

Models and Methods

First, we constructed and optimized a couple of water molecules linked with each other by H-bond, that was $(H_2O)_2$ cluster, or usually named water dimer. According to the previous report about tunneling rotation (TR) types in the water hexamer by J. O. Richardson et al, from the geometrical structure of the reactant or produce (start or end structure of the rotation process of the water dimer), we initially guessed and adjusted its structural configuration to derive two types of transition state (TS) structures, then refined them by TS optimization, got the exact two TS structures corresponding to two rotation types. Consequently, the calculation of intrinsic reaction coordinate (IRC) confirmation was employed to trace the reaction path on the potential energy surface (PES). As what is mentioned in the paper, the confinement is modeled by CNT. To construct different degrees of confinement, a series of CNTs in deferent calibers of (5, 5), (6, 6), (7, 7), (8, 8), (9, 9) were used. All CNTs were geometrical optimized with their symmetries before placing water dimer in them. The diameters (symmetries) for optimized CNT in (5, 5), (6, 6), (7, 7), (8, 8), (9, 9) are 6.83 Å (D5h), 8.19 Å (D6h), 9.50 Å (D7h), 10.87 Å (D8h), 12.19 Å (D9h). It should be mentioned that, in all calculations except for the CNT pre-optimization, all atoms of the CNTs are fixed to maintain the stable confining conditions. Before we modeled the confined water dimer in CNTs, we found two TS structures for isolated water dimer at first, then traced the reaction paths for the two rotation types. To conveniently and quickly find the TS structures in CNTs, we put the two TS structures of isolated water dimer in each CNT to get a series of initial CNT-confined water dimer combinations. And the TS optimization and IRC calculation were adopted again to refine the confined TS structures and trace corresponding reaction paths. The whole procedure of modeling and calculation is sketched in Fig. S1. The TS geometrical structures for the antigeard and geared rotation types in isolated and different confining conditions are given in Cartesian coordinates in Table S4. Some related parameters for TS and IRC are listed in Table S5.

Supplementary Text

Hybrid PBE0 Functional with Dispersion Correction

It is well known that using hybrid PBE0 functional with dispersion correction, the potential energy surface of water system obtained are more reliable and are closer to the reality.[1] Except for (5, 5) CNT, the H-bond length and the O-O distance decrease when we consider dispersion interaction (Table S1). The optimized structure of isolated water dimer is Cs symmetry no matter with or without the D3 dispersion correction, and the change of the H-bond length is 0.003 Å (1.909 Å for PBE0; 1.906 Å for PBE0-D3). The change of the H-bond length in such level are similar in the confining conditions. The distances between O atoms of the confined water dimer and the wall of CNTs are list in Table S2. The results show that in the same condition, compared with PBE0, PBE0-D3 causes the water dimer to be closer to the wall, which indicates the dispersion effects (mainly coming from the van der Waals interaction) plays an important role for attracting. Therefore, the effect of dispersion correction not only changed the structure of the water dimer, but also changed the location of it in CNTs. Moreover, with the dispersion correction, the energy barriers changed by 0.009 ~ 0.023 eV for confining conditions and 0.003 eV for isolated condition (Table S3 and Fig. S2). And the energy barriers in (7, 7) CNT confinement is highest no matter for the antigeared rotation or geared rotation. But without the dispersion correction, the energy barriers in (5, 5) CNT confinement is highest. It indicates the qualitatively difference between the results obtained by PBE0 and PBE0-D3. Compared with the increase of energy barrier for (6, 6), (7, 7), (8, 8), (9, 9) CNTs, the energy barrier is reduced for (5, 5) CNT, which belong to its tight confinement and cannot be simply affect by dispersion correction.

QMMD to verify the Equilibrium Structures

In order to verify the reliability of the equilibrium structures of the confined water dimer confirmed by geometrical guesses and optimizations (Tables S11-S15), we additionally performed all-atom QMMD for the (5, 5), (6, 6), (7, 7), (8, 8), (9, 9) CNT confining conditions. NVT simulation in DMol[3] Code was carried out, and was under the temperature of 300 K, 1fs per step, and total simulation time was 5 ps. The used exchange-correlation functional is PBE and the thermostat is massive generalized Gaussian moments (GGM). The trajectories and structures calculated from QMMD are shown in Fig. S3. It is clear that the water deviated from the axis and closer to the inner wall of CNTs with the increase of the size of CNTs. As shown in Fig. S4, for (5, 5) CNT, the distance between O atoms and the inner wall of CNT (3.18 Å) is very close to the radius of CNT (3.41 Å), which means the water dimer is very close to the axis of CNT. For (6, 6) CNT, the water dimer is slightly deviated from the axis (3.37 ~3.43 Å vs 4.09 Å). For larger CNTs, the water dimer is more deviated from the axis and closer to the wall. The statistics of the H-bond length (Fig. S5), the O-O distances (Fig. S6) were also performed. We choose the minimum from the distances distance between O atom and H atom greater than 1.5 Å, and calculated the average value of H-bond lengths in the range of 1.5 to 2.5 Å during the dynamics simulation. As shown in the figures mentioned above, we can also find: 1) The two water molecules interact with H-bond in the most of the time of the simulation; 2) The average values of the O-O distances are very similar in different conditions. 3). Except for the structures in which the water dimer deviated from the middle position of the length of the CNTs and was very close to the nozzle of CNTs during the simulation, the low-energy structural points are always near those we found by previous DFT optimization, which confirms the reliability of the latter.

Variant of IRC to calculate Tunneling Probability

Because the shape of energy barrier along IRC is the reaction path on PES,[2-6] it can perfectly describe the rotation process of the water dimer, besides, it is useful to calculate tunneling probability, we traced reaction paths of rotation process which are shown together in Fig. S7. It should be noted that, in general, the IRC is usually mass weighted, but we eliminate the mass weighting from general IRC results in this work for the calculation of tunneling probability in the following step.

Fitting Reaction Path with Fourier Function

In this work, the Fourier Function was employed to fit each reaction path of rotation process of the water dimer in different conditions. The Function is expressed as follow:

$$V(x) = a_0 + a_1 Cos(\omega x) + b_1 Sin(\omega x) + a_2 Cos(2\omega x) + b_2 Sin(2\omega x) + a_3 Cos(3\omega x) + b_3 Sin(3\omega x) + \cdots . \quad (1)$$

Each curve of reaction path shown in Fig. S7 was fitted by appropriate progression for Fourier Function to balance the precision and calculational cost. The progressions and coefficients in different conditions are listed in Table S6.

Quantum Tunneling Probability

As what is introduced in the paper, the water dimer is able to achieve rotation process immediately via quantum tunneling. The tunneling probability can be used to estimate the difficulty of the TR occurrence.[7] We employed an approach to calculate the probability of TR for each reaction path, which extend the probability expression of the quantum tunneling of particle translation to the rotation process of the water dimer and treat water dimer's TR as particle's quantum tunneling translation. These two

events can all be looked as the movement of one point on the PES, which can be expressed as the same exponential function by WKB approximation.[8, 9]

$$P = Exp\left[-\frac{2}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}\,dx\right]. \quad (2)$$

P is the probability what we calculated and the formula only make sense on the condition of $P \ll 1$. The boundary condition, *a* and *b*, demarcate the displacement of the particle in the tunneling process. Herein we defined it as the displacement without mass weighting in the IRC for the rotation process (the second column of Table S5). The provided energy *E* assigned to the vibrational mode along the reaction path of rotation process. The variable *m* is substituted with the reduced mass of TS (the forth column of Table S5). And the energy barrier function *V*(*x*) is substituted with the expression obtained by fitting the reaction path. We uniformed physical quantities in atom unit to calculate the tunneling probability, that's why we preferentially employed Hartree or milli-Hartree for energy and Bohr for distance in calculation, and atom mass unit (a.m.u, NOT the unit of mass in AU) was used for the reduced mass of water dimer. Figure S8 and Table S7 show the quantum tunneling probability related to the both rotation types in each condition.

Part of Zero-point Energy assigned to the Vibrational Mode for Rotation

In order to set the provided energy to make the water dimer rotate, E_{vib} assigned from the zero-point energy on the vibrational mode along the rotation process is calculated. The formula is as follow:

$$E_{vib} = h\nu/2\ . \quad (3)$$

h is Planck constant, values 6.62606896×10^{-34} J•s. *ν* is the frequency of the vibrational mode for rotation (values in Table S8). The energy E_{vib} is around 10^{-2} eV, therefore, we set the provided energy from 0.01 eV to make the dimer rotate and then calculate the tunneling probability and so on. Table S9 lists the expectations of tunneling rotation per second calculated by using the frequencies of the related vibrational modes.

Influence of Temperature on Tunneling Rotation

The influence can be expressed as follows:

$$P_{thermal} = exp\left(-\frac{\Delta E}{kT}\right), \quad (4)$$

where

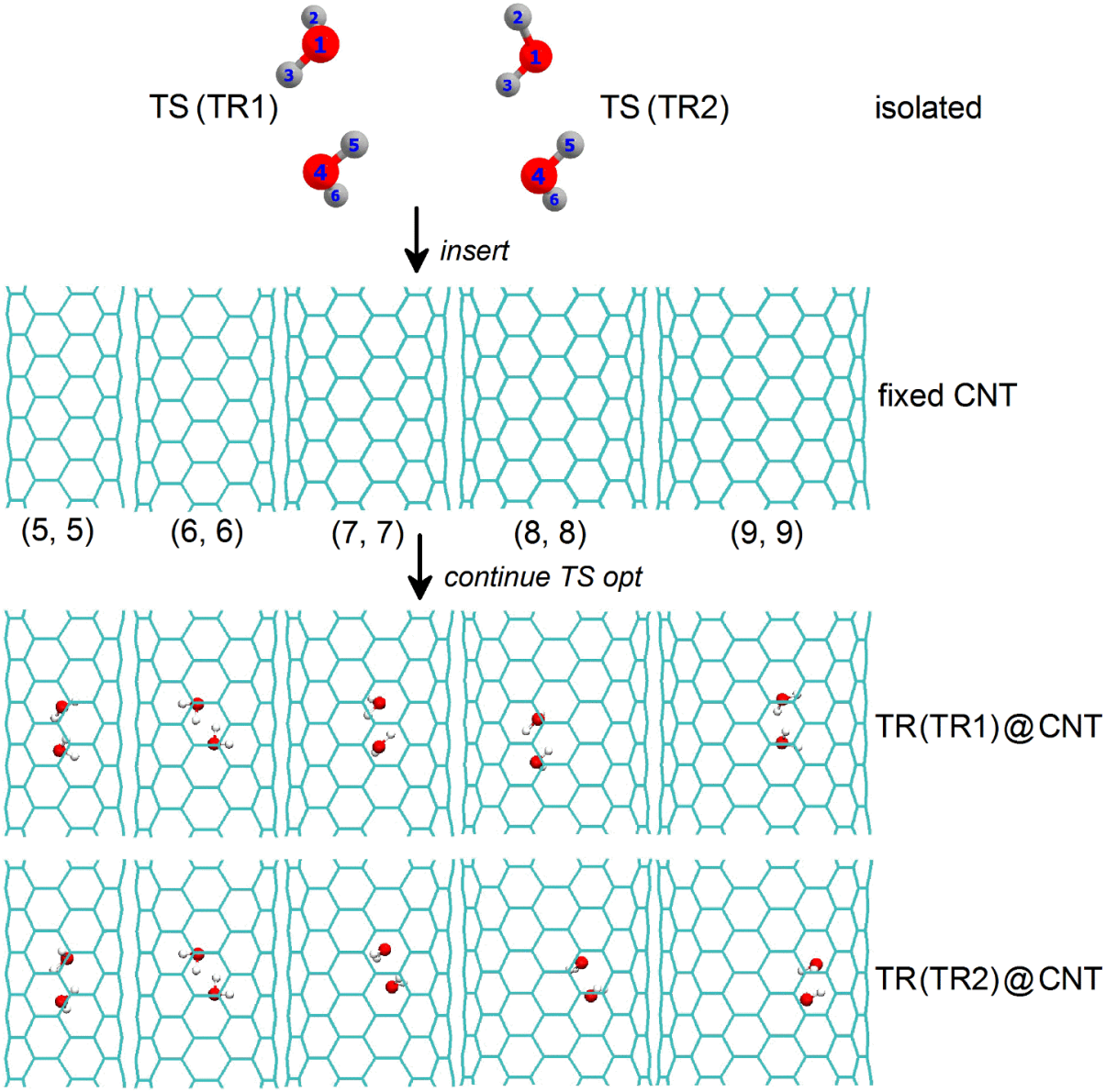
$$\Delta E = E_b - E_p\ . \quad (5)$$

Here, E_b is the potential energy barrier of rotation, E_p is the provided energy to the vibrational mode of water dimer along the rotation reaction path and $E_p < E_b$. $P_{thermal}$ presents the probability of water dimer having energy E_b to rotate freely. *k* is Boltzmann constant, which is 1.38×10^{-23} J/K. *T* presents temperature.

To compare the thermodynamic rotation probability and the quantum tunneling probability, the ratios of the tunneling probability $P_{tunneling}$ and the probability $P_{thermal}$ are calculated, in a certain temperature and energy (10, 25, 50, 100, 150, 200, 250, 300 K; 0.01, 0.07, 0.15 and 0.30 eV). The formula is as follow and the results are depicted in Fig. S9. Besides, the temperatures related to

$Log_{10}(Ratio) = 0$ (The probabilities of thermodynamic rotation and quantum tunneling are in the same order, meaning both effects are roughly equivalent) are listed in Table S10.

$$Ratio = P_{tunneling}/P_{thermal} \ . \tag{6}$$



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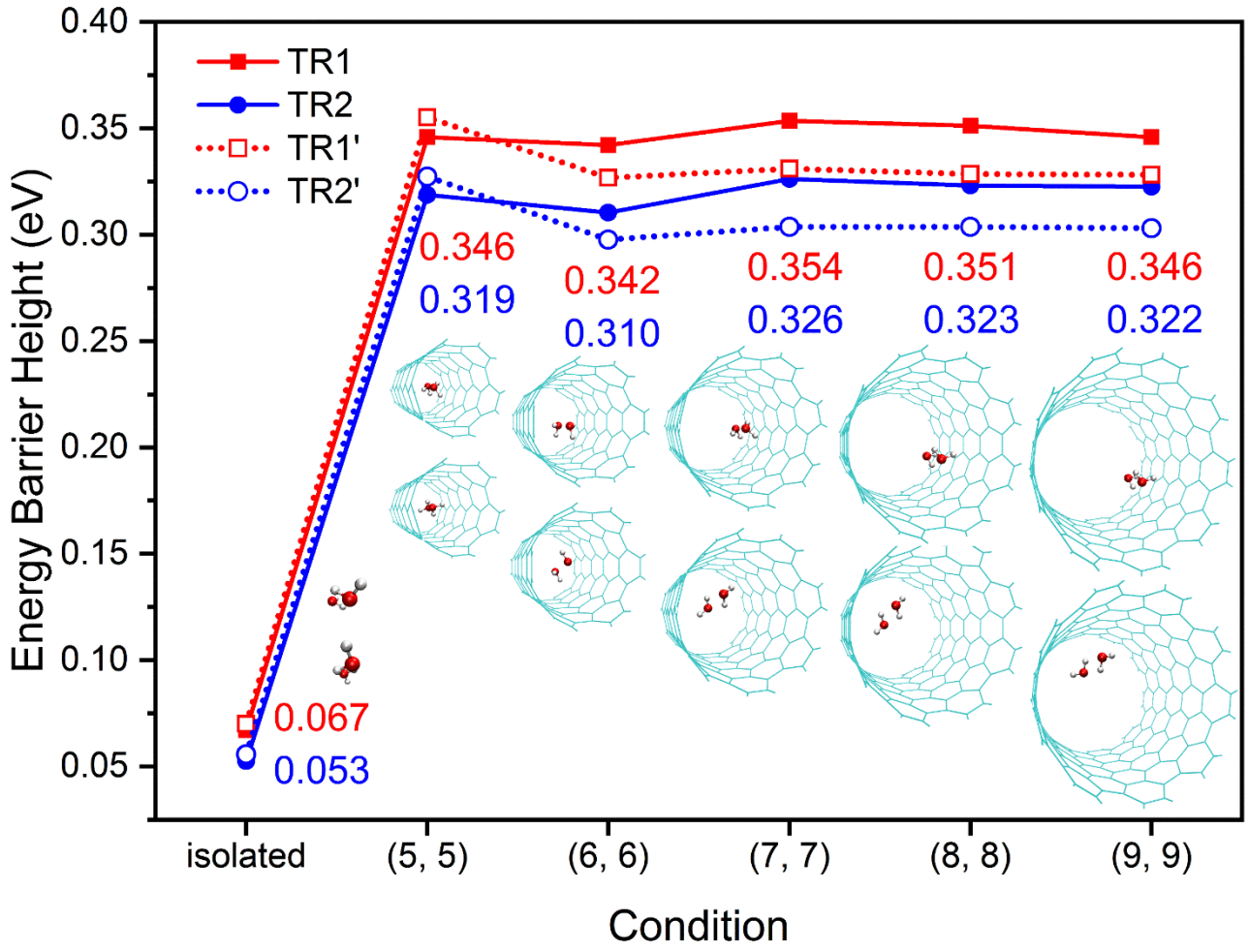


Fig. S2. Calculated energy barrier with and without dispersion correction. The red (blue) dashed line cross the hollow square (circle) points represent the antigeared and greared rotation processes without considering the dispersion correction.

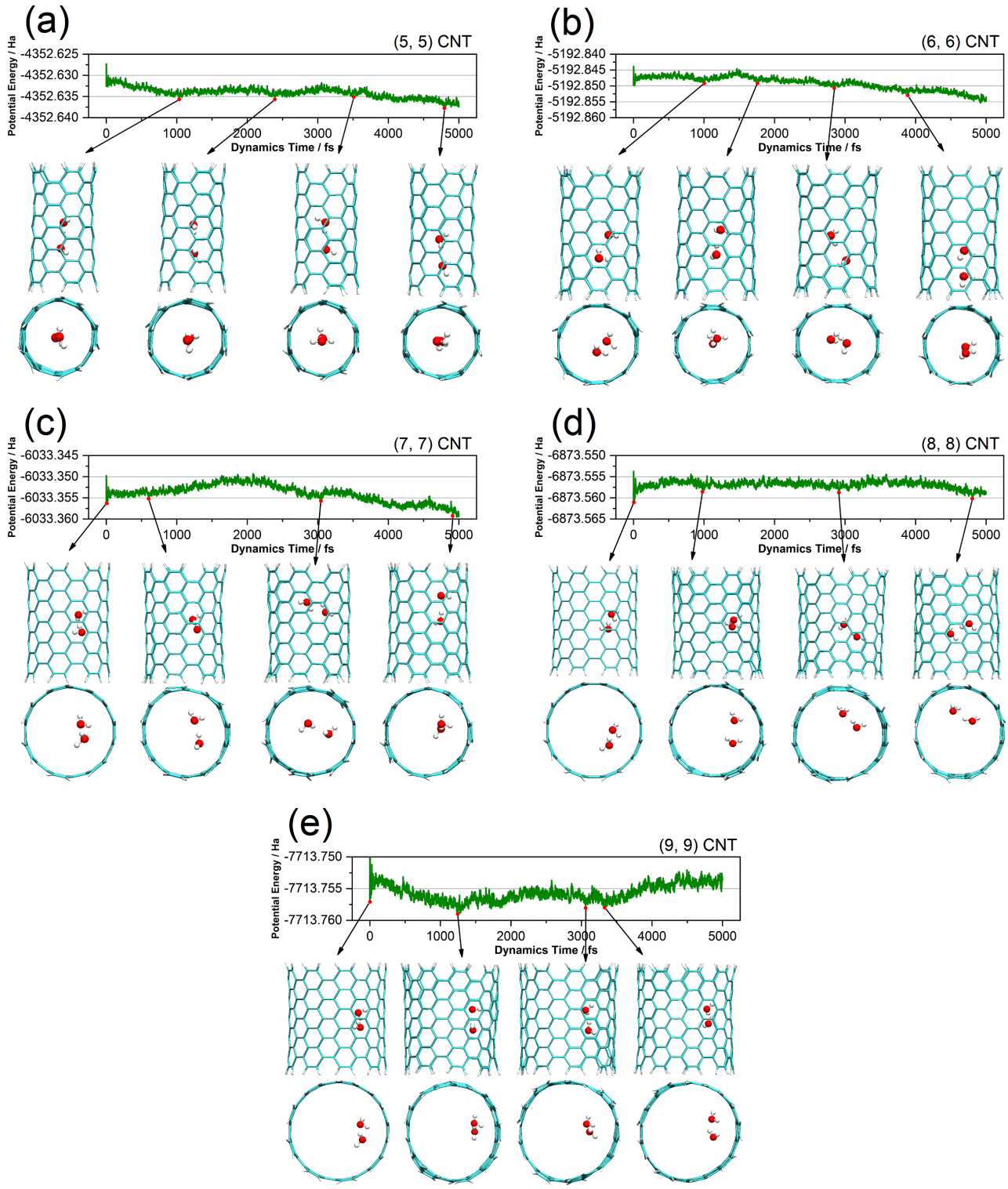
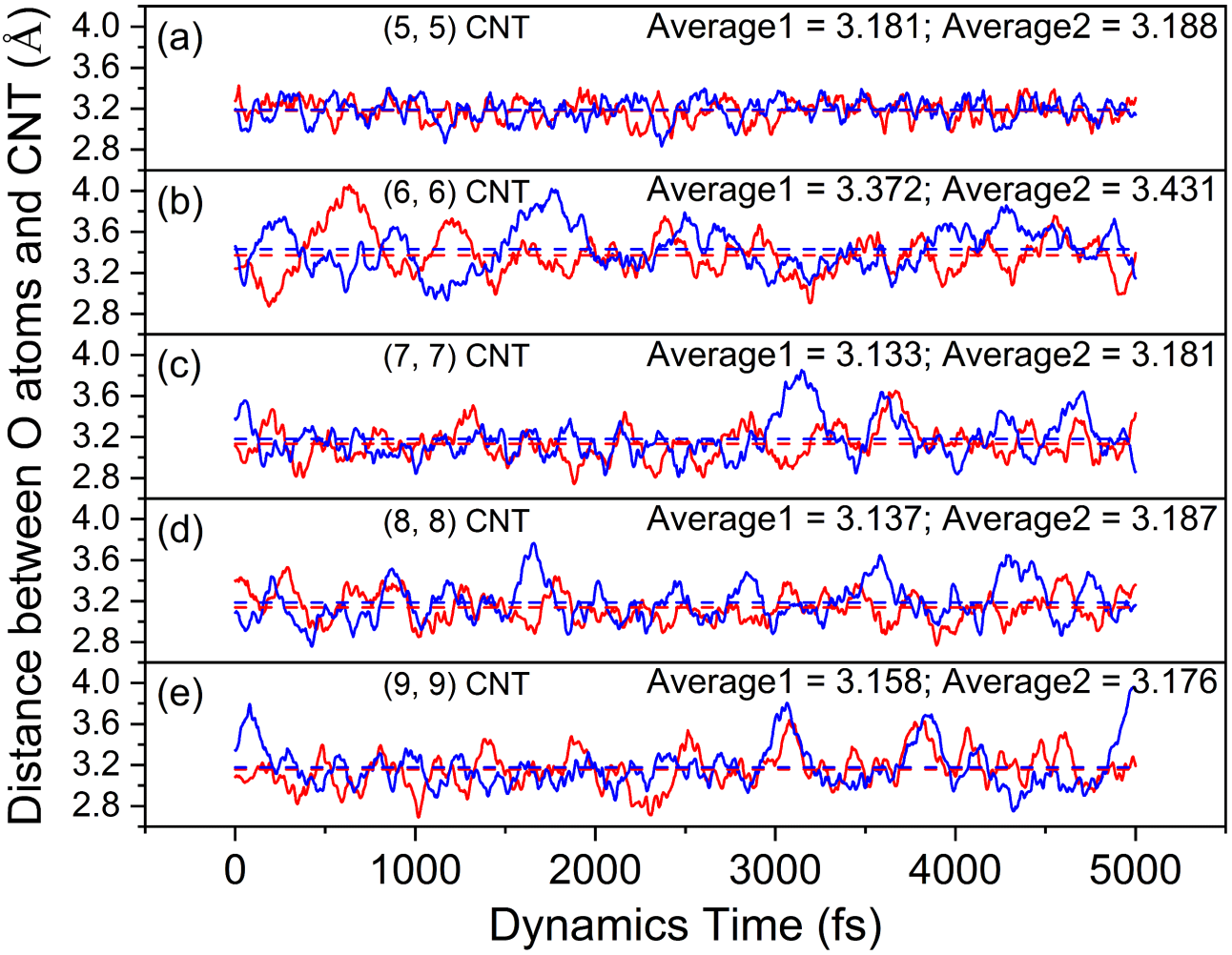


Fig. S3. The structures related to the points with low potential energy in the trajectory of QMMD for (a) (5, 5) CNT; (b) (6, 6) CNT; (c) (7, 7) CNT; (d) (8, 8) CNT; (e) (9, 9) CNT.



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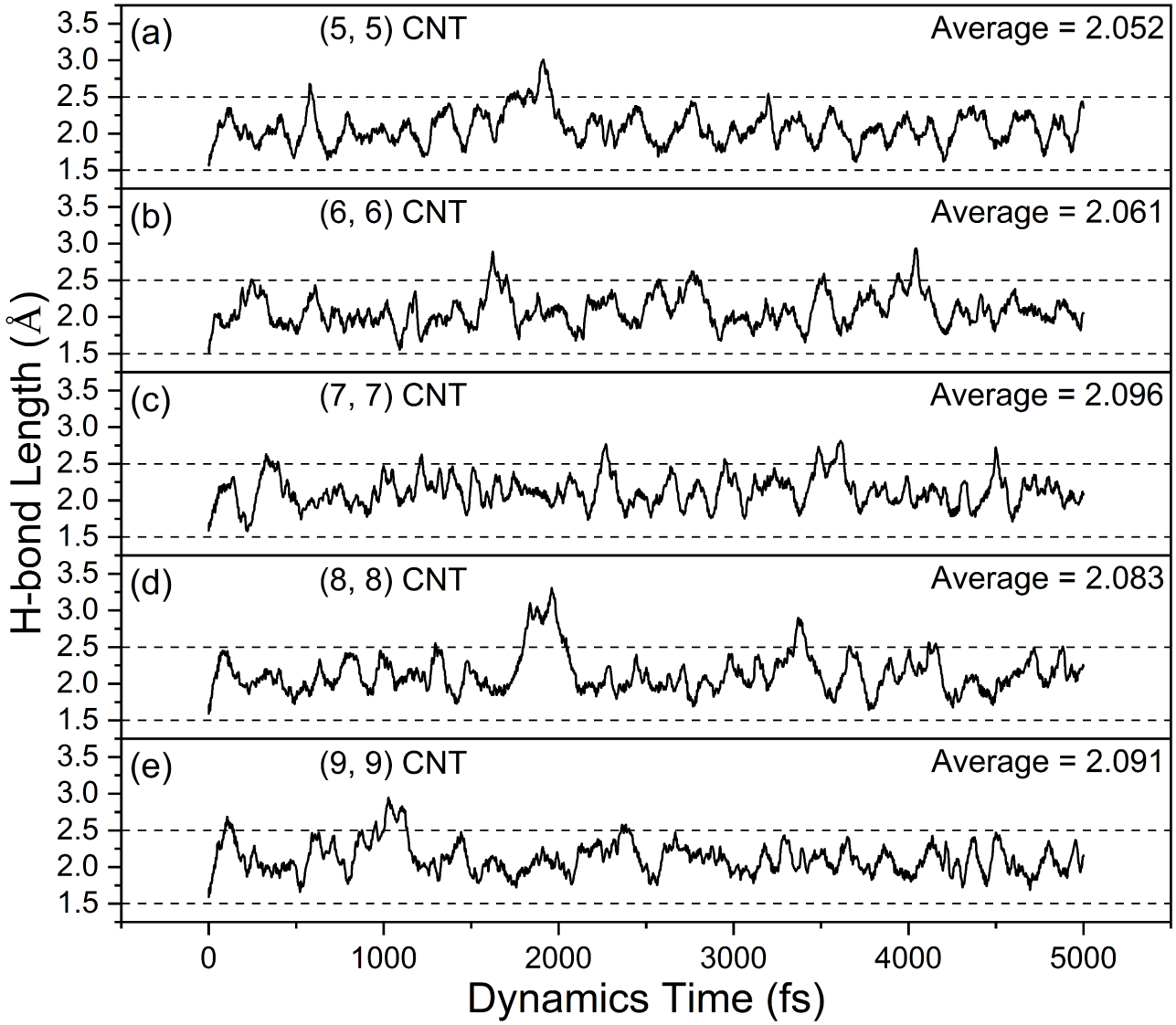


Fig. S5. The change of the H-bond length of the confined water dimer as a function of time for (a) (5, 5) CNT; (b) (6, 6) CNT; (c) (7, 7) CNT; (d) (8, 8) CNT; (e) (9, 9) CNT. The range in which the H-bond is present can be considered to be 1.5 ~ 2.5 Å. The average of H-bond length in each confining condition is also given.

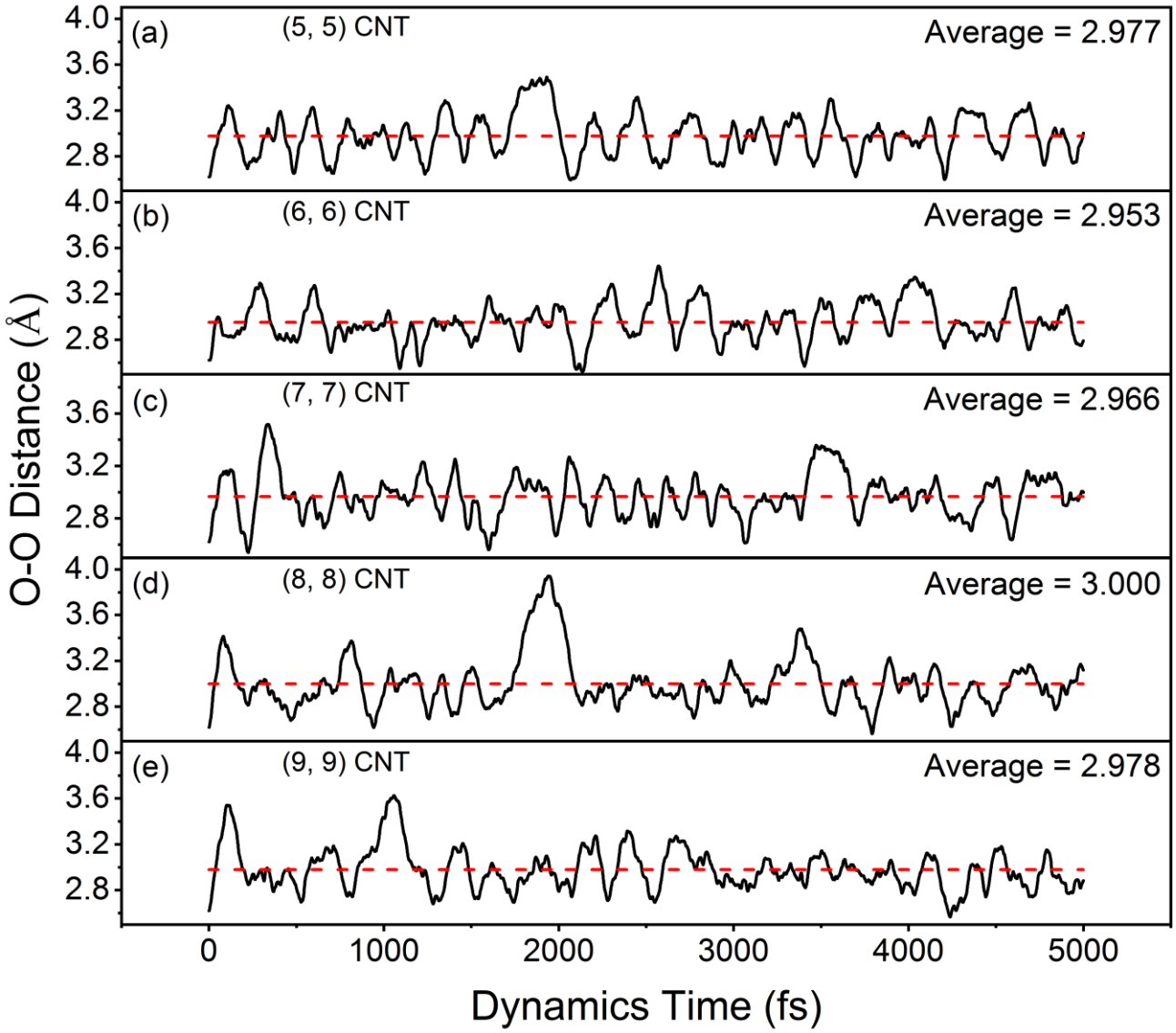


Fig. S6. The distance between the two O atoms of the confined water dimer for (a) (5, 5) CNT; (b) (6, 6) CNT; (c) (7, 7) CNT; (d) (8, 8) CNT; (e) (9, 9) CNT.

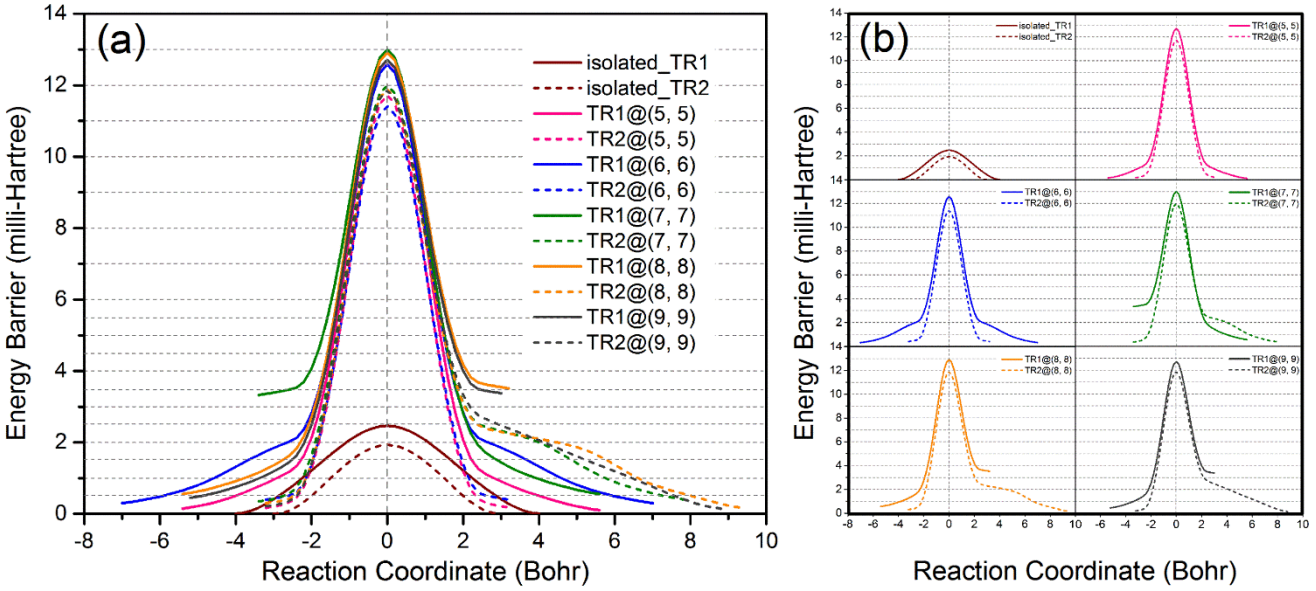
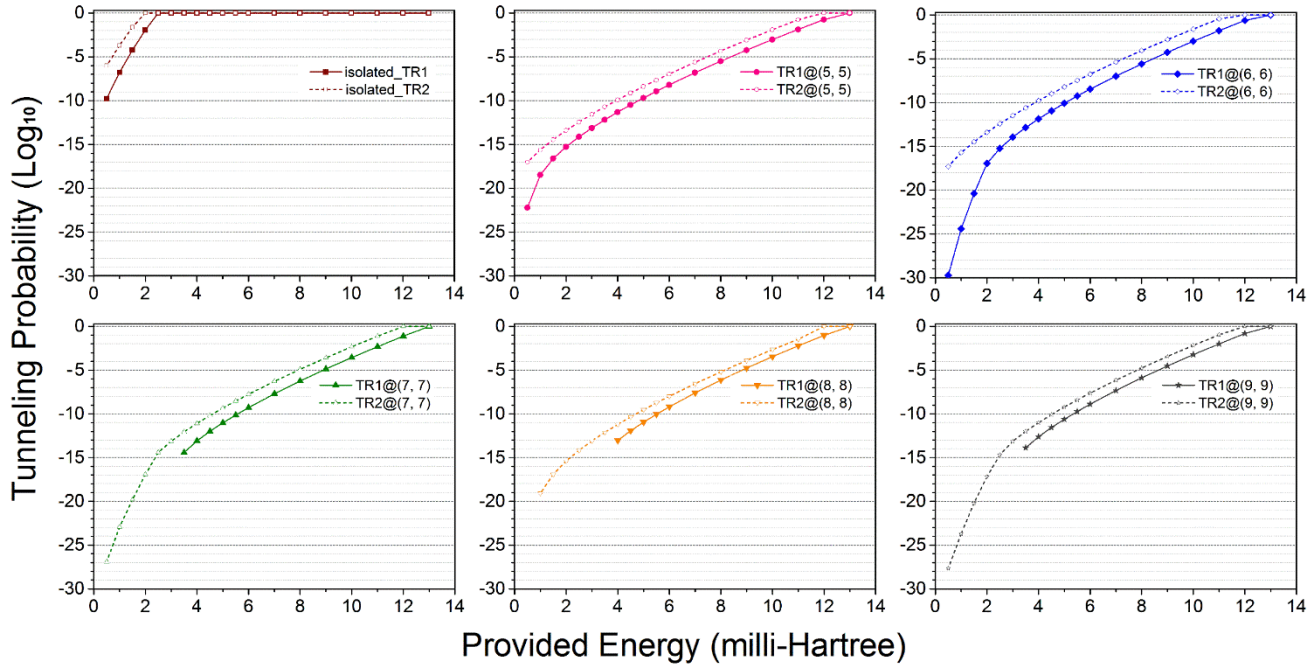


Fig. S7. Reaction paths of two rotation types in different conditions. (a) There are 12 reaction paths in total in one graph, TR1 and TR2 represent the antigeared and geared rotation types. (b) Divided graphs for two rotation types of water dimer in six conditions (one isolated and five confining conditions) to compare, which can be more clearly to estimate the difficulty between TR1 and TR2 in the same condition. The reactant energy is set as reference zero point for corresponding energy barrier. As the variant of IRC described before, the reaction paths herein are without mass weighting.



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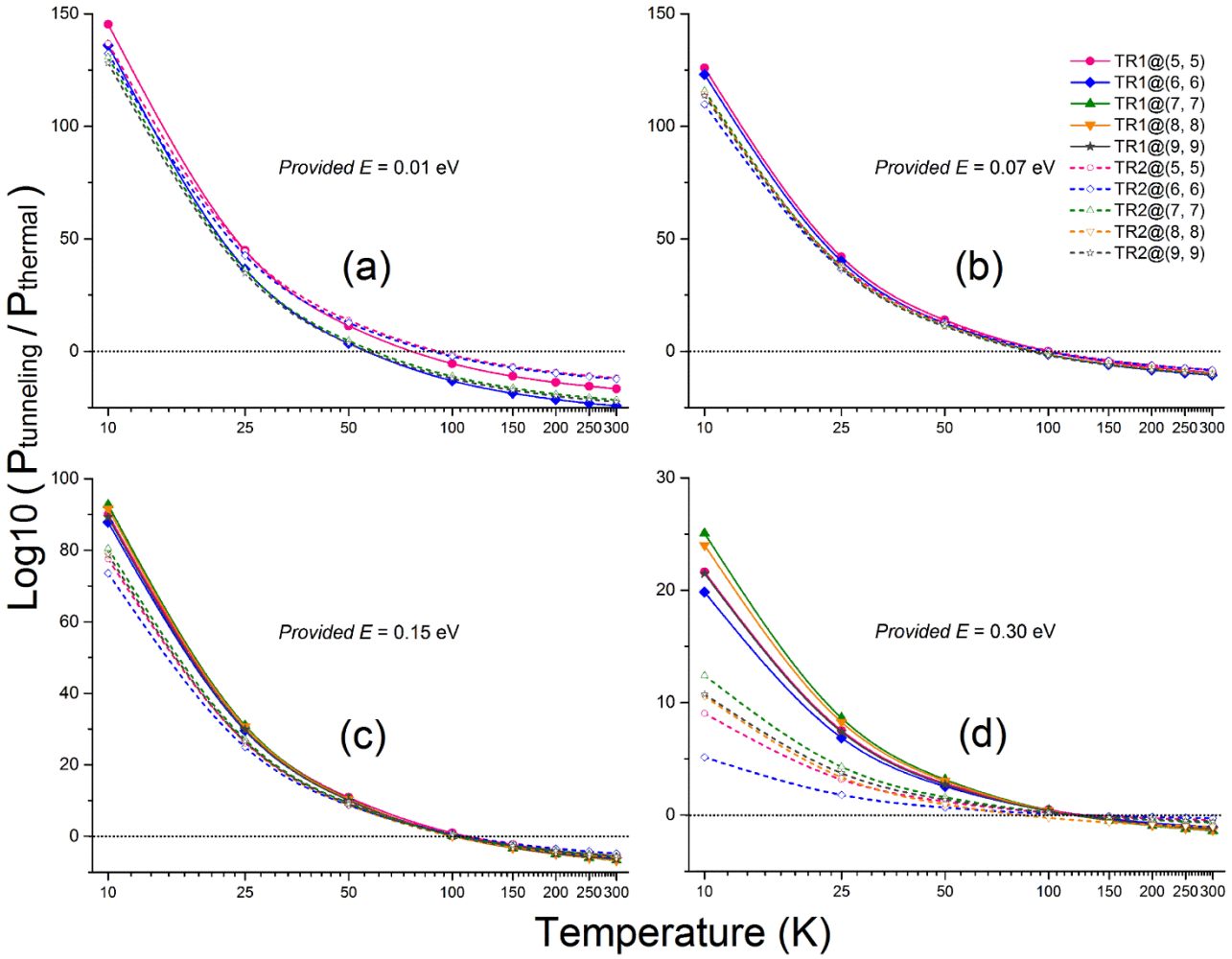

Fig. S9. The ratio along the temperature in the conditions of providing (a) 0.01 eV, (b) 0.07 eV, (c) 0.15 eV, (d) 0.30 eV to confined water dimer, respectively. The solid (dashed) lines through solid (hollow) points represent the ratio for antigeared (geared) rotation TR1 (TR2).

Table S1. The H-bond length and the O-O distance of optimized water dimer in different confining conditions obtained by the DFT-PBE0 calculation with and without dispersion correction. The unit is "Å".

Length	Method	isolated	(5, 5)	(6, 6)	(7, 7)	(8, 8)	(9, 9)
H-bond	PBE0	1.909	1.586	1.591	1.591	1.593	1.591
	PBE0-D3	1.906	1.588	1.588	1.588	1.589	1.589
O-O distance	PBE0	2.873	2.618	2.623	2.631	2.625	2.624
	PBE0-D3	2.870	2.620	2.621	2.621	2.622	2.621

Table S2. The distances between O atoms of the confined water dimer and the wall of CNTs. The unit is "Å".

Method	CNT	Distance(O_1, Wall)	Distance(O_2, Wall)
PBE0	(5, 5)	3.115	3.148
	(6, 6)	3.571	3.894
	(7, 7)	3.507	4.103
	(8, 8)	3.468	3.712
	(9, 9)	3.517	4.837
PBE0-D3	(5, 5)	3.103	3.141
	(6, 6)	3.205	3.691
	(7, 7)	3.339	2.774
	(8, 8)	3.315	3.688
	(9, 9)	3.282	3.218

Table S3. The differences of the energy barriers between the conditions with or without dispersion correction. TR1 and TR2 (TR1' and TR2') are the energy barriers of two rotation processes with (without) dispersion correction. The unit is "eV".

	isolated	(5, 5)	(6, 6)	(7, 7)	(8, 8)	(9, 9)
TR1	0.0671	0.3459	0.3422	0.3536	0.3513	0.3459
TR2	0.0525	0.3188	0.3104	0.3262	0.3232	0.3226
TR1'	0.0700	0.3552	0.3268	0.3311	0.3286	0.3282
TR2'	0.0557	0.3273	0.2977	0.3037	0.3037	0.3031

Table S4. Coordinates of two TS structures of the water dimer corresponding to two rotation types in different conditions.

TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
isolated $(H_2O)_2$ TS (TR1)	1	O	-1.505	0.240	-0.263
	2	H	-2.282	-0.018	0.233
	3	H	-0.913	0.652	0.374
	4	O	1.265	0.265	-0.109
	5	H	0.671	-0.230	-0.682
	6	H	2.015	-0.310	0.048
TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
isolated $(H_2O)_2$ TS (TR2)	1	O	-1.488	0.156	-0.175
	2	H	-2.121	0.776	0.190
	3	H	-0.932	-0.112	0.564
	4	O	1.279	-0.030	0.115
	5	H	0.722	0.237	-0.624
	6	H	1.911	-0.650	-0.250
TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(5, 5) CNT TS (TR1)	1	O	-0.219	0.105	0.951
	2	H	0.357	-0.668	1.275
	3	H	0.448	0.519	0.300
	4	O	0.015	0.251	-1.594
	5	H	-0.668	-0.134	-0.940
	6	H	0.404	-0.625	-1.931
	7	C	1.476	3.192	6.119
	8	C	1.392	3.118	1.223
	9	C	0.704	3.331	2.463
	10	C	1.386	3.128	3.698
	11	C	-0.717	3.379	4.918
	12	C	0.717	3.379	4.918
	13	C	-1.476	3.192	6.119
	14	C	1.386	3.128	-3.698
	15	C	0.704	3.331	-2.462
	16	C	1.392	3.121	-1.225
	17	C	-0.716	3.356	0.000
	18	C	0.715	3.356	0.000
	19	C	-1.392	3.121	1.225
	20	C	-0.704	3.331	2.462
	21	C	-2.547	2.285	3.698
	22	C	-1.386	3.128	3.698
	23	C	-2.992	1.726	4.918
	24	C	-2.580	2.390	6.119
	25	C	1.476	3.192	-6.119
	26	C	-0.717	3.379	-4.918
	27	C	0.717	3.379	-4.918
	28	C	-1.386	3.128	-3.698
	29	C	-0.704	3.331	-2.462
	30	C	-2.538	2.288	-1.225
	31	C	-1.392	3.121	-1.225
	32	C	-2.970	1.718	0.000
	33	C	-2.538	2.288	1.225
	34	C	-3.386	0.360	2.462
	35	C	-2.951	1.699	2.462
	36	C	-3.403	-0.352	3.698
	37	C	-3.435	0.362	4.918
	38	C	-3.070	-1.715	6.119
	39	C	-3.492	-0.417	6.119
	40	C	-2.580	2.390	-6.119
	41	C	-1.476	3.192	-6.119

42	C	-2.992	1.726	-4.918
43	C	-2.547	2.285	-3.698
44	C	-3.386	0.359	-2.463
45	C	-2.951	1.699	-2.462
46	C	-3.396	-0.359	-1.224
47	C	-3.413	0.356	0.000
48	C	-2.961	-1.707	1.225
49	C	-3.399	-0.359	1.225
50	C	-2.528	-2.281	2.462
51	C	-2.960	-1.716	3.698
52	C	-1.406	-3.155	4.918
53	C	-2.566	-2.312	4.918
54	C	-0.682	-3.450	6.119
55	C	-3.492	-0.417	-6.119
56	C	-3.435	0.362	-4.918
57	C	-2.960	-1.716	-3.698
58	C	-3.403	-0.352	-3.698
59	C	-2.528	-2.280	-2.463
60	C	-2.961	-1.706	-1.223
61	C	-1.393	-3.136	0.000
62	C	-2.552	-2.295	0.000
63	C	-0.708	-3.343	1.225
64	C	-1.388	-3.109	2.462
65	C	0.717	-3.345	3.698
66	C	-0.717	-3.345	3.698
67	C	1.406	-3.155	4.918
68	C	0.682	-3.450	6.119
69	C	-3.070	-1.715	-6.119
70	C	-1.406	-3.155	-4.918
71	C	-2.566	-2.312	-4.918
72	C	-0.717	-3.345	-3.698
73	C	-1.389	-3.109	-2.462
74	C	0.708	-3.343	-1.225
75	C	-0.708	-3.343	-1.225
76	C	1.393	-3.136	0.000
77	C	0.708	-3.343	1.225
78	C	2.528	-2.281	2.462
79	C	1.388	-3.109	2.462
80	C	2.960	-1.716	3.698
81	C	2.566	-2.312	4.918
82	C	3.492	-0.417	6.119
83	C	3.070	-1.715	6.119
84	C	0.682	-3.450	-6.119
85	C	-0.682	-3.450	-6.119
86	C	1.406	-3.155	-4.918
87	C	0.717	-3.345	-3.698
88	C	2.528	-2.281	-2.462
89	C	1.388	-3.109	-2.462
90	C	2.961	-1.707	-1.225
91	C	2.552	-2.294	0.000
92	C	3.399	-0.359	1.225
93	C	2.961	-1.707	1.225
94	C	3.386	0.360	2.462
95	C	3.403	-0.352	3.698
96	C	2.992	1.726	4.918
97	C	3.435	0.362	4.918
98	C	2.580	2.390	6.119
99	C	3.070	-1.715	-6.119
100	C	2.566	-2.312	-4.918

	101	C	3.403	-0.352	-3.698
	102	C	2.960	-1.716	-3.698
	103	C	3.386	0.360	-2.462
	104	C	3.399	-0.359	-1.225
	105	C	2.971	1.717	0.001
	106	C	3.413	0.356	0.000
	107	C	2.536	2.290	1.224
	108	C	2.951	1.700	2.463
	109	C	2.546	2.285	3.698
	110	C	3.492	-0.417	-6.119
	111	C	2.992	1.726	-4.918
	112	C	3.435	0.362	-4.918
	113	C	2.547	2.285	-3.698
	114	C	2.951	1.699	-2.462
	115	C	2.538	2.288	-1.225
	116	C	2.580	2.390	-6.119
	117	H	1.101	3.575	7.062
	118	H	-1.101	3.575	7.062
	119	H	-3.060	2.152	7.062
	120	H	1.101	3.575	-7.062
	121	H	-2.992	-2.246	7.062
	122	H	-3.740	0.058	7.062
	123	H	-3.060	2.152	-7.062
	124	H	-1.101	3.575	-7.062
	125	H	-1.211	-3.539	7.062
	126	H	-3.740	0.058	-7.062
	127	H	1.211	-3.539	7.062
	128	H	-2.992	-2.246	-7.062
	129	H	3.740	0.058	7.062
	130	H	2.992	-2.246	7.062
	131	H	1.211	-3.539	-7.062
	132	H	-1.211	-3.539	-7.062
	133	H	3.060	2.152	7.062
	134	H	2.992	-2.246	-7.062
	135	H	3.740	0.058	-7.062
	136	H	3.060	2.152	-7.062
TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(5, 5) CNT TS (TR2)	1	O	-0.247	0.024	0.870
	2	H	0.636	0.304	1.287
	3	H	0.121	-0.657	0.203
	4	O	0.245	-0.024	-1.626
	5	H	-0.134	0.650	-0.960
	6	H	-0.630	-0.299	-2.063
	7	C	1.476	3.192	6.119
	8	C	1.388	3.121	1.225
	9	C	0.706	3.331	2.461
	10	C	1.386	3.128	3.697
	11	C	-0.717	3.379	4.918
	12	C	0.717	3.379	4.918
	13	C	-1.476	3.192	6.119
	14	C	1.386	3.128	-3.698
	15	C	0.704	3.331	-2.462
	16	C	1.392	3.121	-1.225
	17	C	-0.716	3.356	0.000
	18	C	0.718	3.355	-0.001
	19	C	-1.392	3.121	1.224
	20	C	-0.705	3.331	2.464
	21	C	-2.547	2.285	3.698
	22	C	-1.386	3.128	3.698

23	C	-2.992	1.726	4.918
24	C	-2.580	2.390	6.119
25	C	1.476	3.192	-6.119
26	C	-0.717	3.379	-4.918
27	C	0.717	3.379	-4.918
28	C	-1.386	3.128	-3.698
29	C	-0.704	3.331	-2.462
30	C	-2.538	2.288	-1.225
31	C	-1.392	3.121	-1.225
32	C	-2.970	1.718	0.000
33	C	-2.538	2.288	1.225
34	C	-3.386	0.360	2.462
35	C	-2.951	1.699	2.462
36	C	-3.403	-0.352	3.698
37	C	-3.435	0.362	4.918
38	C	-3.070	-1.715	6.119
39	C	-3.492	-0.417	6.119
40	C	-2.580	2.390	-6.119
41	C	-1.476	3.192	-6.119
42	C	-2.992	1.726	-4.918
43	C	-2.547	2.285	-3.698
44	C	-3.386	0.360	-2.462
45	C	-2.951	1.699	-2.462
46	C	-3.399	-0.359	-1.225
47	C	-3.413	0.356	0.000
48	C	-2.961	-1.707	1.225
49	C	-3.399	-0.359	1.225
50	C	-2.528	-2.281	2.462
51	C	-2.960	-1.716	3.698
52	C	-1.406	-3.155	4.918
53	C	-2.566	-2.312	4.918
54	C	-0.682	-3.450	6.119
55	C	-3.492	-0.417	-6.119
56	C	-3.435	0.362	-4.918
57	C	-2.960	-1.716	-3.698
58	C	-3.403	-0.352	-3.698
59	C	-2.528	-2.281	-2.463
60	C	-2.961	-1.707	-1.225
61	C	-1.393	-3.136	0.000
62	C	-2.552	-2.294	0.000
63	C	-0.708	-3.343	1.225
64	C	-1.388	-3.109	2.462
65	C	0.717	-3.345	3.698
66	C	-0.717	-3.345	3.698
67	C	1.406	-3.155	4.918
68	C	0.682	-3.450	6.119
69	C	-3.070	-1.715	-6.119
70	C	-1.406	-3.155	-4.918
71	C	-2.566	-2.312	-4.918
72	C	-0.717	-3.346	-3.698
73	C	-1.388	-3.108	-2.462
74	C	0.708	-3.343	-1.225
75	C	-0.708	-3.343	-1.225
76	C	1.393	-3.136	0.000
77	C	0.708	-3.343	1.225
78	C	2.528	-2.281	2.462
79	C	1.388	-3.109	2.462
80	C	2.960	-1.716	3.698
81	C	2.566	-2.312	4.918

	82	C	3.492	-0.417	6.119
	83	C	3.070	-1.715	6.119
	84	C	0.682	-3.450	-6.119
	85	C	-0.682	-3.450	-6.119
	86	C	1.406	-3.155	-4.918
	87	C	0.717	-3.345	-3.698
	88	C	2.528	-2.281	-2.462
	89	C	1.388	-3.109	-2.462
	90	C	2.961	-1.707	-1.225
	91	C	2.552	-2.294	0.000
	92	C	3.399	-0.359	1.225
	93	C	2.961	-1.707	1.225
	94	C	3.386	0.360	2.462
	95	C	3.403	-0.352	3.698
	96	C	2.992	1.726	4.918
	97	C	3.435	0.362	4.918
	98	C	2.580	2.390	6.119
	99	C	3.070	-1.715	-6.119
	100	C	2.566	-2.312	-4.918
	101	C	3.403	-0.352	-3.698
	102	C	2.960	-1.716	-3.698
	103	C	3.386	0.360	-2.462
	104	C	3.399	-0.359	-1.225
	105	C	2.970	1.718	0.000
	106	C	3.413	0.356	0.000
	107	C	2.539	2.289	1.225
	108	C	2.951	1.699	2.462
	109	C	2.547	2.285	3.698
	110	C	3.492	-0.417	-6.119
	111	C	2.992	1.726	-4.918
	112	C	3.435	0.362	-4.918
	113	C	2.547	2.285	-3.698
	114	C	2.951	1.699	-2.462
	115	C	2.538	2.288	-1.225
	116	C	2.580	2.390	-6.119
	117	H	1.101	3.575	7.062
	118	H	-1.101	3.575	7.062
	119	H	-3.060	2.152	7.062
	120	H	1.101	3.575	-7.062
	121	H	-2.992	-2.246	7.062
	122	H	-3.740	0.058	7.062
	123	H	-3.060	2.152	-7.062
	124	H	-1.101	3.575	-7.062
	125	H	-1.211	-3.539	7.062
	126	H	-3.740	0.058	-7.062
	127	H	1.211	-3.539	7.062
	128	H	-2.992	-2.246	-7.062
	129	H	3.740	0.058	7.062
	130	H	2.992	-2.246	7.062
	131	H	1.211	-3.539	-7.062
	132	H	-1.211	-3.539	-7.062
	133	H	3.060	2.152	7.062
	134	H	2.992	-2.246	-7.062
	135	H	3.740	0.058	-7.062
	136	H	3.060	2.152	-7.062

TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(6, 6) CNT TS (TR1)	1	O	0.134	-0.385	1.268
	2	H	0.291	-1.357	1.523
	3	H	0.765	-0.345	0.464

4	O	-0.138	-0.384	-1.272
5	H	-0.769	-0.348	-0.468
6	H	-0.291	-1.357	-1.528
7	C	1.484	3.937	6.118
8	C	1.399	3.839	1.226
9	C	0.704	4.013	2.463
10	C	1.394	3.845	3.698
11	C	-0.717	4.072	4.920
12	C	0.717	4.072	4.920
13	C	-1.484	3.937	6.118
14	C	1.394	3.845	-3.698
15	C	0.704	4.013	-2.462
16	C	1.399	3.839	-1.226
17	C	-0.713	4.035	0.000
18	C	0.714	4.035	0.000
19	C	-1.399	3.839	1.226
20	C	-0.704	4.013	2.462
21	C	-2.633	3.130	3.698
22	C	-1.394	3.845	3.698
23	C	-3.168	2.657	4.920
24	C	-2.667	3.254	6.118
25	C	1.484	3.937	-6.118
26	C	-0.717	4.072	-4.920
27	C	0.717	4.072	-4.920
28	C	-1.394	3.845	-3.698
29	C	-0.704	4.013	-2.462
30	C	-2.625	3.131	-1.226
31	C	-1.399	3.839	-1.226
32	C	-3.137	2.635	0.000
33	C	-2.625	3.131	1.226
34	C	-3.828	1.397	2.462
35	C	-3.124	2.616	2.462
36	C	-4.027	0.715	3.698
37	C	-3.885	1.415	4.920
38	C	-4.151	-0.683	6.118
39	C	-4.151	0.683	6.118
40	C	-2.667	3.254	-6.118
41	C	-1.484	3.937	-6.118
42	C	-3.168	2.657	-4.920
43	C	-2.633	3.130	-3.698
44	C	-3.828	1.397	-2.463
45	C	-3.124	2.616	-2.462
46	C	-4.024	0.708	-1.226
47	C	-3.851	1.399	0.000
48	C	-4.024	-0.708	1.226
49	C	-4.024	0.708	1.226
50	C	-3.828	-1.397	2.462
51	C	-4.027	-0.715	3.698
52	C	-3.168	-2.657	4.920
53	C	-3.885	-1.415	4.920
54	C	-2.667	-3.254	6.118
55	C	-4.151	0.683	-6.118
56	C	-3.885	1.415	-4.920
57	C	-4.027	-0.715	-3.698
58	C	-4.027	0.715	-3.698
59	C	-3.828	-1.397	-2.462
60	C	-4.024	-0.708	-1.226
61	C	-3.137	-2.635	0.000
62	C	-3.851	-1.399	0.000

63	C	-2.625	-3.131	1.226
64	C	-3.124	-2.616	2.462
65	C	-1.394	-3.845	3.698
66	C	-2.633	-3.130	3.698
67	C	-0.717	-4.072	4.920
68	C	-1.484	-3.937	6.118
69	C	-4.151	-0.683	-6.118
70	C	-3.168	-2.657	-4.920
71	C	-3.885	-1.415	-4.920
72	C	-2.633	-3.130	-3.698
73	C	-3.124	-2.616	-2.462
74	C	-1.399	-3.839	-1.226
75	C	-2.625	-3.131	-1.226
76	C	-0.713	-4.035	0.000
77	C	-1.399	-3.839	1.226
78	C	0.704	-4.013	2.462
79	C	-0.704	-4.013	2.462
80	C	1.394	-3.845	3.698
81	C	0.717	-4.072	4.920
82	C	2.667	-3.254	6.118
83	C	1.484	-3.937	6.118
84	C	-1.484	-3.937	-6.118
85	C	-2.667	-3.254	-6.118
86	C	-0.717	-4.072	-4.920
87	C	-1.394	-3.845	-3.698
88	C	0.704	-4.013	-2.462
89	C	-0.704	-4.013	-2.462
90	C	1.399	-3.839	-1.226
91	C	0.713	-4.035	0.000
92	C	2.625	-3.131	1.226
93	C	1.399	-3.839	1.226
94	C	3.124	-2.616	2.462
95	C	2.633	-3.130	3.698
96	C	3.885	-1.415	4.920
97	C	3.168	-2.657	4.920
98	C	4.151	-0.683	6.118
99	C	1.484	-3.937	-6.118
100	C	0.717	-4.072	-4.920
101	C	2.633	-3.130	-3.698
102	C	1.394	-3.845	-3.698
103	C	3.124	-2.616	-2.462
104	C	2.625	-3.131	-1.226
105	C	3.851	-1.399	0.000
106	C	3.137	-2.635	0.000
107	C	4.024	-0.708	1.226
108	C	3.828	-1.397	2.462
109	C	4.027	0.715	3.698
110	C	4.027	-0.715	3.698
111	C	3.885	1.415	4.920
112	C	4.151	0.683	6.118
113	C	2.667	-3.254	-6.118
114	C	3.885	-1.415	-4.920
115	C	3.168	-2.657	-4.920
116	C	4.027	-0.715	-3.698
117	C	3.828	-1.397	-2.462
118	C	4.024	0.708	-1.226
119	C	4.024	-0.708	-1.226
120	C	3.851	1.399	0.000
121	C	4.024	0.708	1.226

	122	C	3.124	2.616	2.462
	123	C	3.828	1.397	2.462
	124	C	2.633	3.130	3.698
	125	C	3.168	2.657	4.920
	126	C	2.667	3.254	6.118
	127	C	4.151	0.683	-6.118
	128	C	4.151	-0.683	-6.118
	129	C	3.885	1.415	-4.920
	130	C	4.027	0.715	-3.698
	131	C	3.124	2.616	-2.462
	132	C	3.828	1.397	-2.462
	133	C	2.625	3.131	-1.226
	134	C	3.137	2.635	0.000
	135	C	2.625	3.131	1.226
	136	C	2.667	3.254	-6.118
	137	C	3.168	2.657	-4.920
	138	C	2.633	3.130	-3.698
	139	H	1.073	4.274	7.064
	140	H	-1.073	4.274	7.064
	141	H	-3.165	3.066	7.064
	142	H	1.073	4.274	-7.064
	143	H	-4.237	-1.208	7.064
	144	H	-4.237	1.208	7.064
	145	H	-3.165	3.066	-7.064
	146	H	-1.073	4.274	-7.064
	147	H	-3.165	-3.066	7.064
	148	H	-4.237	1.208	-7.064
	149	H	-1.073	-4.274	7.064
	150	H	-4.237	-1.208	-7.064
	151	H	3.165	-3.066	7.064
	152	H	1.073	-4.274	7.064
	153	H	-1.073	-4.274	-7.064
	154	H	-3.165	-3.066	-7.064
	155	H	4.237	-1.208	7.064
	156	H	1.073	-4.274	-7.064
	157	H	4.237	1.208	7.064
	158	H	3.165	-3.066	-7.064
	159	H	3.165	3.066	7.064
	160	H	4.237	1.208	-7.064
	161	H	4.237	-1.208	-7.064
	162	H	3.165	3.066	-7.064
TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(6, 6) CNT TS (TR2)	1	O	0.241	0.478	1.149
	2	H	-0.296	1.341	1.169
	3	H	0.635	0.581	0.210
	4	O	-0.241	-0.478	-1.153
	5	H	-0.635	-0.581	-0.215
	6	H	0.297	-1.341	-1.174
	7	C	1.484	3.937	6.118
	8	C	1.400	3.838	1.227
	9	C	0.703	4.014	2.462
	10	C	1.394	3.845	3.698
	11	C	-0.717	4.072	4.920
	12	C	0.717	4.072	4.920
	13	C	-1.484	3.937	6.118
	14	C	1.394	3.845	-3.698
	15	C	0.704	4.013	-2.462
	16	C	1.399	3.839	-1.226
	17	C	-0.713	4.034	0.000

18	C	0.713	4.035	0.000
19	C	-1.400	3.839	1.226
20	C	-0.703	4.012	2.462
21	C	-2.633	3.130	3.698
22	C	-1.394	3.846	3.698
23	C	-3.168	2.657	4.920
24	C	-2.667	3.254	6.118
25	C	1.484	3.937	-6.118
26	C	-0.717	4.072	-4.920
27	C	0.717	4.072	-4.920
28	C	-1.394	3.845	-3.698
29	C	-0.704	4.013	-2.462
30	C	-2.625	3.131	-1.226
31	C	-1.399	3.839	-1.226
32	C	-3.137	2.635	0.000
33	C	-2.625	3.132	1.226
34	C	-3.828	1.397	2.462
35	C	-3.124	2.616	2.462
36	C	-4.027	0.715	3.698
37	C	-3.885	1.415	4.920
38	C	-4.151	-0.683	6.118
39	C	-4.151	0.683	6.118
40	C	-2.667	3.254	-6.118
41	C	-1.484	3.937	-6.118
42	C	-3.168	2.657	-4.920
43	C	-2.633	3.130	-3.698
44	C	-3.828	1.397	-2.462
45	C	-3.124	2.616	-2.462
46	C	-4.024	0.708	-1.226
47	C	-3.851	1.399	0.000
48	C	-4.024	-0.708	1.226
49	C	-4.024	0.708	1.226
50	C	-3.828	-1.397	2.462
51	C	-4.027	-0.715	3.698
52	C	-3.168	-2.657	4.920
53	C	-3.885	-1.415	4.920
54	C	-2.667	-3.254	6.118
55	C	-4.151	0.683	-6.118
56	C	-3.885	1.415	-4.920
57	C	-4.027	-0.715	-3.698
58	C	-4.027	0.715	-3.698
59	C	-3.828	-1.397	-2.462
60	C	-4.024	-0.708	-1.226
61	C	-3.137	-2.635	0.000
62	C	-3.851	-1.399	0.000
63	C	-2.625	-3.131	1.226
64	C	-3.124	-2.616	2.462
65	C	-1.394	-3.845	3.698
66	C	-2.633	-3.130	3.698
67	C	-0.717	-4.072	4.920
68	C	-1.484	-3.937	6.118
69	C	-4.151	-0.683	-6.118
70	C	-3.168	-2.657	-4.920
71	C	-3.885	-1.415	-4.920
72	C	-2.633	-3.130	-3.698
73	C	-3.124	-2.616	-2.462
74	C	-1.399	-3.839	-1.226
75	C	-2.625	-3.132	-1.226
76	C	-0.713	-4.034	0.000

77	C	-1.400	-3.840	1.226
78	C	0.704	-4.013	2.462
79	C	-0.704	-4.013	2.462
80	C	1.394	-3.845	3.698
81	C	0.717	-4.072	4.920
82	C	2.667	-3.254	6.118
83	C	1.484	-3.937	6.118
84	C	-1.484	-3.937	-6.118
85	C	-2.667	-3.254	-6.118
86	C	-0.717	-4.072	-4.920
87	C	-1.394	-3.845	-3.698
88	C	0.704	-4.013	-2.462
89	C	-0.704	-4.013	-2.462
90	C	1.399	-3.839	-1.226
91	C	0.713	-4.035	0.000
92	C	2.625	-3.131	1.226
93	C	1.399	-3.839	1.226
94	C	3.124	-2.616	2.462
95	C	2.633	-3.130	3.698
96	C	3.885	-1.415	4.920
97	C	3.168	-2.657	4.920
98	C	4.151	-0.683	6.118
99	C	1.484	-3.937	-6.118
100	C	0.717	-4.072	-4.920
101	C	2.633	-3.130	-3.698
102	C	1.394	-3.845	-3.698
103	C	3.124	-2.616	-2.462
104	C	2.625	-3.131	-1.226
105	C	3.851	-1.399	0.000
106	C	3.137	-2.635	0.000
107	C	4.024	-0.708	1.226
108	C	3.828	-1.397	2.462
109	C	4.027	0.715	3.698
110	C	4.027	-0.715	3.698
111	C	3.885	1.415	4.920
112	C	4.151	0.683	6.118
113	C	2.667	-3.254	-6.118
114	C	3.885	-1.415	-4.920
115	C	3.168	-2.657	-4.920
116	C	4.027	-0.715	-3.698
117	C	3.828	-1.397	-2.462
118	C	4.024	0.708	-1.226
119	C	4.024	-0.708	-1.226
120	C	3.851	1.399	0.000
121	C	4.024	0.708	1.226
122	C	3.124	2.616	2.462
123	C	3.828	1.397	2.462
124	C	2.633	3.130	3.698
125	C	3.168	2.657	4.920
126	C	2.667	3.254	6.118
127	C	4.151	0.683	-6.118
128	C	4.151	-0.683	-6.118
129	C	3.885	1.415	-4.920
130	C	4.027	0.715	-3.698
131	C	3.124	2.616	-2.462
132	C	3.828	1.397	-2.462
133	C	2.625	3.131	-1.226
134	C	3.137	2.635	0.000
135	C	2.625	3.131	1.226

	136	C	2.667	3.254	-6.118
	137	C	3.168	2.657	-4.920
	138	C	2.633	3.130	-3.698
	139	H	1.073	4.274	7.064
	140	H	-1.073	4.274	7.064
	141	H	-3.165	3.066	7.064
	142	H	1.073	4.274	-7.064
	143	H	-4.237	-1.208	7.064
	144	H	-4.237	1.208	7.064
	145	H	-3.165	3.066	-7.064
	146	H	-1.073	4.274	-7.064
	147	H	-3.165	-3.066	7.064
	148	H	-4.237	1.208	-7.064
	149	H	-1.073	-4.274	7.064
	150	H	-4.237	-1.208	-7.064
	151	H	3.165	-3.066	7.064
	152	H	1.073	-4.274	7.064
	153	H	-1.073	-4.274	-7.064
	154	H	-3.165	-3.066	-7.064
	155	H	4.237	-1.208	7.064
	156	H	1.073	-4.274	-7.064
	157	H	4.237	1.208	7.064
	158	H	3.165	-3.066	-7.064
	159	H	3.165	3.066	7.064
	160	H	4.237	1.208	-7.064
	161	H	4.237	-1.208	-7.064
	162	H	3.165	3.066	-7.064
TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(7, 7) CNT TS (TR1)	1	O	1.290	0.029	1.366
	2	H	2.040	-0.582	1.682
	3	H	1.810	0.531	0.643
	4	O	1.423	0.006	-1.184
	5	H	0.838	-0.458	-0.487
	6	H	2.014	-0.786	-1.425
	7	C	0.626	-4.856	6.117
	8	C	0.651	-4.711	1.227
	9	C	1.348	-4.551	2.462
	10	C	0.658	-4.718	3.699
	11	C	2.666	-4.012	4.921
	12	C	1.365	-4.619	4.921
	13	C	3.322	-3.597	6.117
	14	C	0.658	-4.718	-3.699
	15	C	1.348	-4.551	-2.462
	16	C	0.651	-4.711	-1.227
	17	C	2.639	-3.968	0.000
	18	C	1.348	-4.570	0.000
	19	C	3.194	-3.524	1.227
	20	C	2.624	-3.955	2.462
	21	C	4.099	-2.427	3.699
	22	C	3.195	-3.533	3.699
	23	C	4.462	-1.813	4.921
	24	C	4.187	-2.539	6.117
	25	C	0.626	-4.856	-6.117
	26	C	2.666	-4.012	-4.921
	27	C	1.365	-4.619	-4.921
	28	C	3.195	-3.533	-3.699
	29	C	2.624	-3.955	-2.462
	30	C	4.089	-2.428	-1.227
	31	C	3.194	-3.524	-1.227

32	C	4.414	-1.795	0.000
33	C	4.089	-2.428	1.227
34	C	4.728	-0.415	2.462
35	C	4.399	-1.783	2.462
36	C	4.755	0.295	3.699
37	C	4.798	-0.417	4.921
38	C	4.595	1.691	6.117
39	C	4.884	0.354	6.117
40	C	4.187	-2.539	-6.117
41	C	3.322	-3.597	-6.117
42	C	4.462	-1.813	-4.921
43	C	4.099	-2.427	-3.699
44	C	4.728	-0.415	-2.462
45	C	4.399	-1.783	-2.462
46	C	4.747	0.300	-1.227
47	C	4.747	-0.411	0.000
48	C	4.448	1.683	1.227
49	C	4.747	0.300	1.227
50	C	4.137	2.327	2.462
51	C	4.453	1.692	3.699
52	C	3.318	3.491	4.921
53	C	4.200	2.358	4.921
54	C	2.768	4.039	6.117
55	C	4.884	0.354	-6.117
56	C	4.798	-0.417	-4.921
57	C	4.453	1.692	-3.699
58	C	4.755	0.295	-3.699
59	C	4.137	2.327	-2.462
60	C	4.448	1.683	-1.227
61	C	3.281	3.456	0.000
62	C	4.156	2.332	0.000
63	C	2.725	3.898	1.227
64	C	3.272	3.438	2.462
65	C	1.454	4.536	3.699
66	C	2.734	3.901	3.699
67	C	0.775	4.754	4.921
68	C	1.543	4.647	6.117
69	C	4.595	1.691	-6.117
70	C	3.318	3.491	-4.921
71	C	4.200	2.358	-4.921
72	C	2.734	3.901	-3.699
73	C	3.272	3.438	-2.462
74	C	1.458	4.527	-1.227
75	C	2.725	3.898	-1.227
76	C	0.768	4.703	0.000
77	C	1.458	4.527	1.227
78	C	-0.648	4.702	2.462
79	C	0.760	4.685	2.462
80	C	-1.345	4.570	3.699
81	C	-0.661	4.771	4.921
82	C	-2.671	4.104	6.117
83	C	-1.432	4.682	6.117
84	C	1.543	4.647	-6.117
85	C	2.768	4.039	-6.117
86	C	0.775	4.754	-4.921
87	C	1.454	4.536	-3.699
88	C	-0.648	4.702	-2.462
89	C	0.760	4.685	-2.462
90	C	-1.349	4.561	-1.227

91	C	-0.656	4.720	0.000
92	C	-2.631	3.962	1.227
93	C	-1.349	4.561	1.227
94	C	-3.189	3.515	2.462
95	C	-2.640	3.965	3.699
96	C	-4.142	2.458	4.921
97	C	-3.234	3.570	4.921
98	C	-4.554	1.800	6.117
99	C	-1.432	4.682	-6.117
100	C	-0.661	4.771	-4.921
101	C	-2.640	3.965	-3.699
102	C	-1.345	4.570	-3.699
103	C	-3.189	3.515	-2.462
104	C	-2.631	3.962	-1.227
105	C	-4.099	2.430	0.000
106	C	-3.198	3.533	0.000
107	C	-4.407	1.789	1.227
108	C	-4.080	2.425	2.462
109	C	-4.746	0.408	3.699
110	C	-4.412	1.797	3.699
111	C	-4.807	-0.303	4.921
112	C	-4.874	0.471	6.117
113	C	-2.671	4.104	-6.117
114	C	-4.142	2.458	-4.921
115	C	-3.234	3.570	-4.921
116	C	-4.412	1.797	-3.699
117	C	-4.080	2.425	-2.462
118	C	-4.738	0.414	-1.227
119	C	-4.407	1.789	-1.227
120	C	-4.756	-0.298	0.000
121	C	-4.738	0.414	1.227
122	C	-4.440	-1.678	2.462
123	C	-4.737	-0.302	2.462
124	C	-4.156	-2.329	3.699
125	C	-4.504	-1.706	4.921
126	C	-3.407	-3.517	6.117
127	C	-4.246	-2.438	6.117
128	C	-4.874	0.471	-6.117
129	C	-4.554	1.800	-6.117
130	C	-4.807	-0.303	-4.921
131	C	-4.746	0.408	-3.699
132	C	-4.440	-1.678	-2.462
133	C	-4.737	-0.302	-2.462
134	C	-4.146	-2.330	-1.227
135	C	-4.456	-1.690	0.000
136	C	-3.277	-3.446	1.227
137	C	-4.146	-2.330	1.227
138	C	-2.717	-3.892	2.462
139	C	-3.278	-3.456	3.699
140	C	-1.474	-4.585	4.921
141	C	-2.760	-3.947	4.921
142	C	-0.741	-4.840	6.117
143	C	-4.246	-2.438	-6.117
144	C	-4.504	-1.706	-4.921
145	C	-3.278	-3.456	-3.699
146	C	-4.156	-2.329	-3.699
147	C	-2.717	-3.892	-2.462
148	C	-3.277	-3.446	-1.227
149	C	-1.457	-4.537	0.000

	150	C	-2.733	-3.904	0.000
	151	C	-0.763	-4.695	1.227
	152	C	-1.457	-4.517	2.462
	153	C	-0.770	-4.701	3.699
	154	C	-3.407	-3.517	-6.117
	155	C	-1.474	-4.585	-4.921
	156	C	-2.760	-3.947	-4.921
	157	C	-0.770	-4.701	-3.699
	158	C	-1.457	-4.517	-2.462
	159	C	-0.763	-4.695	-1.227
	160	C	-0.741	-4.840	-6.117
	161	H	1.147	-4.948	7.064
	162	H	3.058	-4.056	7.064
	163	H	4.583	-2.189	7.064
	164	H	1.147	-4.948	-7.064
	165	H	4.569	2.219	7.064
	166	H	5.077	-0.138	7.064
	167	H	4.583	-2.189	-7.064
	168	H	3.058	-4.056	-7.064
	169	H	3.273	3.884	7.064
	170	H	5.077	-0.138	-7.064
	171	H	1.114	4.955	7.064
	172	H	4.569	2.219	-7.064
	173	H	-3.180	3.960	7.064
	174	H	-0.995	4.981	7.064
	175	H	1.114	4.955	-7.064
	176	H	3.273	3.884	-7.064
	177	H	-4.515	2.327	7.064
	178	H	-0.995	4.981	-7.064
	179	H	-5.079	-0.017	7.064
	180	H	-3.180	3.960	-7.064
	181	H	-3.154	-3.981	7.064
	182	H	-4.634	-2.079	7.064
	183	H	-5.079	-0.017	-7.064
	184	H	-4.515	2.327	-7.064
	185	H	-1.264	-4.919	7.064
	186	H	-4.634	-2.079	-7.064
	187	H	-3.154	-3.981	-7.064
	188	H	-1.264	-4.919	-7.064

TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(7, 7) CNT TS (TR2)	1	O	-0.563	1.479	1.365
	2	H	0.238	2.047	1.098
	3	H	-0.297	0.620	0.879
	4	O	-1.261	0.353	-0.801
	5	H	-1.504	1.199	-0.281
	6	H	-2.070	-0.207	-0.544
	7	C	0.626	-4.856	6.117
	8	C	0.651	-4.711	1.227
	9	C	1.348	-4.551	2.462
	10	C	0.658	-4.718	3.699
	11	C	2.666	-4.012	4.921
	12	C	1.365	-4.619	4.921
	13	C	3.322	-3.597	6.117
	14	C	0.658	-4.718	-3.699
	15	C	1.348	-4.551	-2.462
	16	C	0.651	-4.711	-1.227
	17	C	2.639	-3.968	0.000
	18	C	1.348	-4.570	0.000
	19	C	3.194	-3.524	1.227

20	C	2.624	-3.955	2.462
21	C	4.099	-2.427	3.699
22	C	3.195	-3.533	3.699
23	C	4.462	-1.813	4.921
24	C	4.187	-2.539	6.117
25	C	0.626	-4.856	-6.117
26	C	2.666	-4.012	-4.921
27	C	1.365	-4.619	-4.921
28	C	3.195	-3.533	-3.699
29	C	2.624	-3.955	-2.462
30	C	4.089	-2.428	-1.227
31	C	3.194	-3.524	-1.227
32	C	4.414	-1.795	0.000
33	C	4.089	-2.428	1.227
34	C	4.728	-0.415	2.462
35	C	4.399	-1.783	2.462
36	C	4.755	0.295	3.699
37	C	4.798	-0.417	4.921
38	C	4.595	1.691	6.117
39	C	4.884	0.354	6.117
40	C	4.187	-2.539	-6.117
41	C	3.322	-3.597	-6.117
42	C	4.462	-1.813	-4.921
43	C	4.099	-2.427	-3.699
44	C	4.728	-0.415	-2.462
45	C	4.399	-1.783	-2.462
46	C	4.747	0.300	-1.227
47	C	4.747	-0.411	0.000
48	C	4.448	1.683	1.227
49	C	4.747	0.300	1.227
50	C	4.136	2.327	2.462
51	C	4.453	1.692	3.699
52	C	3.318	3.492	4.921
53	C	4.200	2.358	4.921
54	C	2.768	4.039	6.117
55	C	4.884	0.354	-6.117
56	C	4.798	-0.417	-4.921
57	C	4.453	1.692	-3.699
58	C	4.755	0.295	-3.699
59	C	4.137	2.327	-2.462
60	C	4.448	1.683	-1.227
61	C	3.281	3.456	0.000
62	C	4.156	2.332	0.000
63	C	2.725	3.897	1.227
64	C	3.273	3.438	2.462
65	C	1.454	4.536	3.699
66	C	2.734	3.901	3.699
67	C	0.775	4.754	4.921
68	C	1.543	4.647	6.117
69	C	4.595	1.691	-6.117
70	C	3.318	3.491	-4.921
71	C	4.200	2.358	-4.921
72	C	2.734	3.901	-3.699
73	C	3.272	3.438	-2.462
74	C	1.457	4.527	-1.227
75	C	2.724	3.898	-1.227
76	C	0.769	4.702	0.000
77	C	1.456	4.528	1.228
78	C	-0.648	4.702	2.463

79	C	0.760	4.685	2.462
80	C	-1.346	4.570	3.698
81	C	-0.661	4.771	4.921
82	C	-2.671	4.104	6.117
83	C	-1.432	4.682	6.117
84	C	1.543	4.647	-6.117
85	C	2.768	4.039	-6.117
86	C	0.775	4.754	-4.921
87	C	1.454	4.536	-3.699
88	C	-0.648	4.702	-2.462
89	C	0.760	4.685	-2.462
90	C	-1.349	4.561	-1.227
91	C	-0.656	4.720	0.000
92	C	-2.631	3.962	1.227
93	C	-1.349	4.561	1.227
94	C	-3.189	3.515	2.462
95	C	-2.640	3.965	3.699
96	C	-4.142	2.458	4.921
97	C	-3.234	3.570	4.921
98	C	-4.554	1.800	6.117
99	C	-1.432	4.682	-6.117
100	C	-0.661	4.771	-4.921
101	C	-2.640	3.965	-3.699
102	C	-1.345	4.570	-3.699
103	C	-3.189	3.515	-2.462
104	C	-2.631	3.962	-1.227
105	C	-4.099	2.430	0.000
106	C	-3.198	3.533	0.000
107	C	-4.407	1.789	1.227
108	C	-4.080	2.425	2.462
109	C	-4.746	0.408	3.699
110	C	-4.412	1.797	3.699
111	C	-4.807	-0.303	4.921
112	C	-4.874	0.471	6.117
113	C	-2.671	4.104	-6.117
114	C	-4.142	2.458	-4.921
115	C	-3.234	3.570	-4.921
116	C	-4.412	1.797	-3.699
117	C	-4.080	2.425	-2.462
118	C	-4.738	0.414	-1.227
119	C	-4.407	1.789	-1.227
120	C	-4.756	-0.298	0.000
121	C	-4.738	0.414	1.227
122	C	-4.440	-1.678	2.462
123	C	-4.737	-0.302	2.462
124	C	-4.156	-2.329	3.699
125	C	-4.504	-1.706	4.921
126	C	-3.407	-3.517	6.117
127	C	-4.246	-2.438	6.117
128	C	-4.874	0.471	-6.117
129	C	-4.554	1.800	-6.117
130	C	-4.807	-0.303	-4.921
131	C	-4.746	0.408	-3.699
132	C	-4.440	-1.678	-2.462
133	C	-4.737	-0.302	-2.462
134	C	-4.146	-2.330	-1.227
135	C	-4.456	-1.690	0.000
136	C	-3.277	-3.446	1.227
137	C	-4.146	-2.330	1.227

	138	C	-2.717	-3.892	2.462
	139	C	-3.278	-3.456	3.699
	140	C	-1.474	-4.585	4.921
	141	C	-2.760	-3.947	4.921
	142	C	-0.741	-4.840	6.117
	143	C	-4.246	-2.438	-6.117
	144	C	-4.504	-1.706	-4.921
	145	C	-3.278	-3.456	-3.699
	146	C	-4.156	-2.329	-3.699
	147	C	-2.717	-3.892	-2.462
	148	C	-3.277	-3.446	-1.227
	149	C	-1.457	-4.537	0.000
	150	C	-2.733	-3.904	0.000
	151	C	-0.763	-4.695	1.227
	152	C	-1.457	-4.517	2.462
	153	C	-0.770	-4.701	3.699
	154	C	-3.407	-3.517	-6.117
	155	C	-1.474	-4.585	-4.921
	156	C	-2.760	-3.947	-4.921
	157	C	-0.770	-4.701	-3.699
	158	C	-1.457	-4.517	-2.462
	159	C	-0.763	-4.695	-1.227
	160	C	-0.741	-4.840	-6.117
	161	H	1.147	-4.948	7.064
	162	H	3.058	-4.056	7.064
	163	H	4.583	-2.189	7.064
	164	H	1.147	-4.948	-7.064
	165	H	4.569	2.219	7.064
	166	H	5.077	-0.138	7.064
	167	H	4.583	-2.189	-7.064
	168	H	3.058	-4.056	-7.064
	169	H	3.273	3.884	7.064
	170	H	5.077	-0.138	-7.064
	171	H	1.114	4.955	7.064
	172	H	4.569	2.219	-7.064
	173	H	-3.180	3.960	7.064
	174	H	-0.995	4.981	7.064
	175	H	1.114	4.955	-7.064
	176	H	3.273	3.884	-7.064
	177	H	-4.515	2.327	7.064
	178	H	-0.995	4.981	-7.064
	179	H	-5.079	-0.017	7.064
	180	H	-3.180	3.960	-7.064
	181	H	-3.154	-3.981	7.064
	182	H	-4.634	-2.079	7.064
	183	H	-5.079	-0.017	-7.064
	184	H	-4.515	2.327	-7.064
	185	H	-1.264	-4.919	7.064
	186	H	-4.634	-2.079	-7.064
	187	H	-3.154	-3.981	-7.064
	188	H	-1.264	-4.919	-7.064

TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(8, 8) CNT TS (TR1)	1	O	1.827	-1.154	2.341
	2	H	2.747	-0.800	2.594
	3	H	1.579	-0.433	1.661
	4	O	1.715	-1.044	-0.208
	5	H	1.887	-1.759	0.501
	6	H	2.676	-0.917	-0.516
	7	C	-1.490	-5.383	6.116

8	C	-1.406	-5.242	1.228
9	C	-0.704	-5.374	2.462
10	C	-1.404	-5.256	3.699
11	C	0.718	-5.453	4.921
12	C	-0.718	-5.453	4.921
13	C	1.490	-5.383	6.116
14	C	-1.404	-5.256	-3.699
15	C	-0.704	-5.374	-2.462
16	C	-1.406	-5.242	-1.228
17	C	0.711	-5.388	0.000
18	C	-0.711	-5.388	0.000
19	C	1.406	-5.242	1.228
20	C	0.704	-5.374	2.462
21	C	2.723	-4.709	3.699
22	C	1.404	-5.256	3.699
23	C	3.348	-4.364	4.921
24	C	2.753	-4.860	6.116
25	C	-1.490	-5.383	-6.116
26	C	0.718	-5.453	-4.921
27	C	-0.718	-5.453	-4.921
28	C	1.404	-5.256	-3.699
29	C	0.704	-5.374	-2.462
30	C	2.712	-4.701	-1.228
31	C	1.406	-5.242	-1.228
32	C	3.307	-4.313	0.000
33	C	2.712	-4.701	1.228
34	C	4.298	-3.302	2.462
35	C	3.302	-4.298	2.462
36	C	4.709	-2.723	3.699
37	C	4.364	-3.348	4.921
38	C	5.383	-1.490	6.116
39	C	4.860	-2.753	6.116
40	C	2.753	-4.860	-6.116
41	C	1.490	-5.383	-6.116
42	C	3.348	-4.364	-4.921
43	C	2.723	-4.709	-3.699
44	C	4.298	-3.302	-2.462
45	C	3.302	-4.298	-2.462
46	C	4.701	-2.712	-1.228
47	C	4.313	-3.307	0.000
48	C	5.242	-1.406	1.228
49	C	4.701	-2.712	1.228
50	C	5.374	-0.704	2.462
51	C	5.256	-1.404	3.699
52	C	5.453	0.718	4.921
53	C	5.453	-0.718	4.921
54	C	5.383	1.490	6.116
55	C	4.860	-2.753	-6.116
56	C	4.364	-3.348	-4.921
57	C	5.256	-1.404	-3.699
58	C	4.709	-2.723	-3.699
59	C	5.374	-0.704	-2.462
60	C	5.242	-1.406	-1.228
61	C	5.388	0.711	0.000
62	C	5.388	-0.711	0.000
63	C	5.242	1.406	1.228
64	C	5.374	0.704	2.462
65	C	4.709	2.723	3.699
66	C	5.256	1.404	3.699

67	C	4.364	3.348	4.921
68	C	4.860	2.753	6.116
69	C	5.383	-1.490	-6.116
70	C	5.453	0.718	-4.921
71	C	5.453	-0.718	-4.921
72	C	5.256	1.404	-3.699
73	C	5.374	0.704	-2.462
74	C	4.701	2.712	-1.228
75	C	5.242	1.406	-1.228
76	C	4.313	3.307	0.000
77	C	4.701	2.712	1.228
78	C	3.302	4.298	2.462
79	C	4.298	3.302	2.462
80	C	2.723	4.709	3.699
81	C	3.348	4.364	4.921
82	C	1.490	5.383	6.116
83	C	2.753	4.860	6.116
84	C	4.860	2.753	-6.116
85	C	5.383	1.490	-6.116
86	C	4.364	3.348	-4.921
87	C	4.709	2.723	-3.699
88	C	3.302	4.298	-2.462
89	C	4.298	3.302	-2.462
90	C	2.712	4.701	-1.228
91	C	3.307	4.313	0.000
92	C	1.406	5.242	1.228
93	C	2.712	4.701	1.228
94	C	0.704	5.374	2.462
95	C	1.404	5.256	3.699
96	C	-0.718	5.453	4.921
97	C	0.718	5.453	4.921
98	C	-1.490	5.383	6.116
99	C	2.753	4.860	-6.116
100	C	3.348	4.364	-4.921
101	C	1.404	5.256	-3.699
102	C	2.723	4.709	-3.699
103	C	0.704	5.374	-2.462
104	C	1.406	5.242	-1.228
105	C	-0.711	5.388	0.000
106	C	0.711	5.388	0.000
107	C	-1.406	5.242	1.228
108	C	-0.704	5.374	2.462
109	C	-2.723	4.709	3.699
110	C	-1.404	5.256	3.699
111	C	-3.348	4.364	4.921
112	C	-2.753	4.860	6.116
113	C	1.490	5.383	-6.116
114	C	-0.718	5.453	-4.921
115	C	0.718	5.453	-4.921
116	C	-1.404	5.256	-3.699
117	C	-0.704	5.374	-2.462
118	C	-2.712	4.701	-1.228
119	C	-1.406	5.242	-1.228
120	C	-3.307	4.313	0.000
121	C	-2.712	4.701	1.228
122	C	-4.298	3.302	2.462
123	C	-3.302	4.298	2.462
124	C	-4.709	2.723	3.699
125	C	-4.364	3.348	4.921

126	C	-5.383	1.490	6.116
127	C	-4.860	2.753	6.116
128	C	-2.753	4.860	-6.116
129	C	-1.490	5.383	-6.116
130	C	-3.348	4.364	-4.921
131	C	-2.723	4.709	-3.699
132	C	-4.298	3.302	-2.462
133	C	-3.302	4.298	-2.462
134	C	-4.701	2.712	-1.228
135	C	-4.313	3.307	0.000
136	C	-5.242	1.406	1.228
137	C	-4.701	2.712	1.228
138	C	-5.374	0.704	2.462
139	C	-5.256	1.404	3.699
140	C	-5.453	-0.718	4.921
141	C	-5.453	0.718	4.921
142	C	-5.383	-1.490	6.116
143	C	-4.860	2.753	-6.116
144	C	-4.364	3.348	-4.921
145	C	-5.256	1.404	-3.699
146	C	-4.709	2.723	-3.699
147	C	-5.374	0.704	-2.462
148	C	-5.242	1.406	-1.228
149	C	-5.388	-0.711	0.000
150	C	-5.388	0.711	0.000
151	C	-5.242	-1.406	1.228
152	C	-5.374	-0.704	2.462
153	C	-4.709	-2.723	3.699
154	C	-5.256	-1.404	3.699
155	C	-4.364	-3.348	4.921
156	C	-4.860	-2.753	6.116
157	C	-5.383	1.490	-6.116
158	C	-5.453	-0.718	-4.921
159	C	-5.453	0.718	-4.921
160	C	-5.256	-1.404	-3.699
161	C	-5.374	-0.704	-2.462
162	C	-4.701	-2.712	-1.228
163	C	-5.242	-1.406	-1.228
164	C	-4.313	-3.307	0.000
165	C	-4.701	-2.712	1.228
166	C	-3.302	-4.298	2.462
167	C	-4.298	-3.302	2.462
168	C	-2.723	-4.709	3.699
169	C	-3.348	-4.364	4.921
170	C	-2.753	-4.860	6.116
171	C	-4.860	-2.753	-6.116
172	C	-5.383	-1.490	-6.116
173	C	-4.364	-3.348	-4.921
174	C	-4.709	-2.723	-3.699
175	C	-3.302	-4.298	-2.462
176	C	-4.298	-3.302	-2.462
177	C	-2.712	-4.701	-1.228
178	C	-3.307	-4.313	0.000
179	C	-2.712	-4.701	1.228
180	C	-2.753	-4.860	-6.116
181	C	-3.348	-4.364	-4.921
182	C	-2.723	-4.709	-3.699
183	H	-1.042	-5.662	7.064
184	H	1.042	-5.662	7.064

	185	H	3.267	-4.740	7.064
	186	H	-1.042	-5.662	-7.064
	187	H	5.662	-1.042	7.064
	188	H	4.740	-3.267	7.064
	189	H	3.267	-4.740	-7.064
	190	H	1.042	-5.662	-7.064
	191	H	5.662	1.042	7.064
	192	H	4.740	-3.267	-7.064
	193	H	4.740	3.267	7.064
	194	H	5.662	-1.042	-7.064
	195	H	1.042	5.662	7.064
	196	H	3.267	4.740	7.064
	197	H	4.740	3.267	-7.064
	198	H	5.662	1.042	-7.064
	199	H	-1.042	5.662	7.064
	200	H	3.267	4.740	-7.064
	201	H	-3.267	4.740	7.064
	202	H	1.042	5.662	-7.064
	203	H	-5.662	1.042	7.064
	204	H	-4.740	3.267	7.064
	205	H	-3.267	4.740	-7.064
	206	H	-1.042	5.662	-7.064
	207	H	-5.662	-1.042	7.064
	208	H	-4.740	3.267	-7.064
	209	H	-4.740	-3.267	7.064
	210	H	-5.662	1.042	-7.064
	211	H	-3.267	-4.740	7.064
	212	H	-4.740	-3.267	-7.064
	213	H	-5.662	-1.042	-7.064
	214	H	-3.267	-4.740	-7.064

TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(8, 8) CNT TS (TR2)	1	O	-1.484	1.855	0.532
	2	H	-0.792	2.486	0.134
	3	H	-1.090	0.977	0.188
	4	O	-2.022	0.284	-1.393
	5	H	-2.386	1.159	-1.009
	6	H	-2.745	-0.336	-1.037
	7	C	-1.490	-5.383	6.116
	8	C	-1.406	-5.242	1.228
	9	C	-0.704	-5.374	2.462
	10	C	-1.404	-5.256	3.699
	11	C	0.718	-5.453	4.921
	12	C	-0.718	-5.453	4.921
	13	C	1.490	-5.383	6.116
	14	C	-1.404	-5.256	-3.699
	15	C	-0.704	-5.374	-2.462
	16	C	-1.406	-5.242	-1.228
	17	C	0.711	-5.388	0.000
	18	C	-0.711	-5.388	0.000
	19	C	1.406	-5.242	1.228
	20	C	0.704	-5.374	2.462
	21	C	2.723	-4.709	3.699
	22	C	1.404	-5.256	3.699
	23	C	3.348	-4.364	4.921
	24	C	2.753	-4.860	6.116
	25	C	-1.490	-5.383	-6.116
	26	C	0.718	-5.453	-4.921
	27	C	-0.718	-5.453	-4.921
	28	C	1.404	-5.256	-3.699

29	C	0.704	-5.374	-2.462
30	C	2.712	-4.701	-1.228
31	C	1.406	-5.242	-1.228
32	C	3.307	-4.313	0.000
33	C	2.712	-4.701	1.228
34	C	4.298	-3.302	2.462
35	C	3.302	-4.298	2.462
36	C	4.709	-2.723	3.699
37	C	4.364	-3.348	4.921
38	C	5.383	-1.490	6.116
39	C	4.860	-2.753	6.116
40	C	2.753	-4.860	-6.116
41	C	1.490	-5.383	-6.116
42	C	3.348	-4.364	-4.921
43	C	2.723	-4.709	-3.699
44	C	4.298	-3.302	-2.462
45	C	3.302	-4.298	-2.462
46	C	4.701	-2.712	-1.228
47	C	4.313	-3.307	0.000
48	C	5.242	-1.406	1.228
49	C	4.701	-2.712	1.228
50	C	5.374	-0.704	2.462
51	C	5.256	-1.404	3.699
52	C	5.453	0.718	4.921
53	C	5.453	-0.718	4.921
54	C	5.383	1.490	6.116
55	C	4.860	-2.753	-6.116
56	C	4.364	-3.348	-4.921
57	C	5.256	-1.404	-3.699
58	C	4.709	-2.723	-3.699
59	C	5.374	-0.704	-2.462
60	C	5.242	-1.406	-1.228
61	C	5.388	0.711	0.000
62	C	5.388	-0.711	0.000
63	C	5.242	1.406	1.228
64	C	5.374	0.704	2.462
65	C	4.709	2.723	3.699
66	C	5.256	1.404	3.699
67	C	4.364	3.348	4.921
68	C	4.860	2.753	6.116
69	C	5.383	-1.490	-6.116
70	C	5.453	0.718	-4.921
71	C	5.453	-0.718	-4.921
72	C	5.256	1.404	-3.699
73	C	5.374	0.704	-2.462
74	C	4.701	2.712	-1.228
75	C	5.242	1.406	-1.228
76	C	4.313	3.307	0.000
77	C	4.701	2.712	1.228
78	C	3.302	4.298	2.462
79	C	4.298	3.302	2.462
80	C	2.723	4.709	3.699
81	C	3.348	4.364	4.921
82	C	1.490	5.383	6.116
83	C	2.753	4.860	6.116
84	C	4.860	2.753	-6.116
85	C	5.383	1.490	-6.116
86	C	4.364	3.348	-4.921
87	C	4.709	2.723	-3.699

88	C	3.302	4.298	-2.462
89	C	4.298	3.302	-2.462
90	C	2.712	4.701	-1.228
91	C	3.307	4.313	0.000
92	C	1.406	5.242	1.228
93	C	2.712	4.701	1.228
94	C	0.704	5.374	2.462
95	C	1.404	5.256	3.699
96	C	-0.718	5.453	4.921
97	C	0.718	5.453	4.921
98	C	-1.490	5.383	6.116
99	C	2.753	4.860	-6.116
100	C	3.348	4.364	-4.921
101	C	1.404	5.256	-3.699
102	C	2.723	4.709	-3.699
103	C	0.704	5.374	-2.462
104	C	1.406	5.242	-1.228
105	C	-0.711	5.388	0.000
106	C	0.711	5.388	0.000
107	C	-1.406	5.242	1.228
108	C	-0.704	5.374	2.462
109	C	-2.723	4.709	3.699
110	C	-1.404	5.256	3.699
111	C	-3.348	4.364	4.921
112	C	-2.753	4.860	6.116
113	C	1.490	5.383	-6.116
114	C	-0.718	5.453	-4.921
115	C	0.718	5.453	-4.921
116	C	-1.404	5.256	-3.699
117	C	-0.704	5.374	-2.462
118	C	-2.712	4.701	-1.228
119	C	-1.406	5.242	-1.228
120	C	-3.307	4.313	0.000
121	C	-2.712	4.701	1.228
122	C	-4.298	3.302	2.462
123	C	-3.302	4.298	2.462
124	C	-4.709	2.723	3.699
125	C	-4.364	3.348	4.921
126	C	-5.383	1.490	6.116
127	C	-4.860	2.753	6.116
128	C	-2.753	4.860	-6.116
129	C	-1.490	5.383	-6.116
130	C	-3.348	4.364	-4.921
131	C	-2.723	4.709	-3.699
132	C	-4.298	3.302	-2.462
133	C	-3.302	4.298	-2.462
134	C	-4.701	2.712	-1.228
135	C	-4.313	3.307	0.000
136	C	-5.242	1.406	1.228
137	C	-4.701	2.712	1.228
138	C	-5.374	0.704	2.462
139	C	-5.256	1.404	3.699
140	C	-5.453	-0.718	4.921
141	C	-5.453	0.718	4.921
142	C	-5.383	-1.490	6.116
143	C	-4.860	2.753	-6.116
144	C	-4.364	3.348	-4.921
145	C	-5.256	1.404	-3.699
146	C	-4.709	2.723	-3.699

147	C	-5.374	0.704	-2.462
148	C	-5.242	1.406	-1.228
149	C	-5.388	-0.711	0.000
150	C	-5.388	0.711	0.000
151	C	-5.242	-1.406	1.228
152	C	-5.374	-0.704	2.462
153	C	-4.709	-2.723	3.699
154	C	-5.256	-1.404	3.699
155	C	-4.364	-3.348	4.921
156	C	-4.860	-2.753	6.116
157	C	-5.383	1.490	-6.116
158	C	-5.453	-0.718	-4.921
159	C	-5.453	0.718	-4.921
160	C	-5.256	-1.404	-3.699
161	C	-5.374	-0.704	-2.462
162	C	-4.701	-2.712	-1.228
163	C	-5.242	-1.406	-1.228
164	C	-4.313	-3.307	0.000
165	C	-4.701	-2.712	1.228
166	C	-3.302	-4.298	2.462
167	C	-4.298	-3.302	2.462
168	C	-2.723	-4.709	3.699
169	C	-3.348	-4.364	4.921
170	C	-2.753	-4.860	6.116
171	C	-4.860	-2.753	-6.116
172	C	-5.383	-1.490	-6.116
173	C	-4.364	-3.348	-4.921
174	C	-4.709	-2.723	-3.699
175	C	-3.302	-4.298	-2.462
176	C	-4.298	-3.302	-2.462
177	C	-2.712	-4.701	-1.228
178	C	-3.307	-4.313	0.000
179	C	-2.712	-4.701	1.228
180	C	-2.753	-4.860	-6.116
181	C	-3.348	-4.364	-4.921
182	C	-2.723	-4.709	-3.699
183	H	-1.042	-5.662	7.064
184	H	1.042	-5.662	7.064
185	H	3.267	-4.740	7.064
186	H	-1.042	-5.662	-7.064
187	H	5.662	-1.042	7.064
188	H	4.740	-3.267	7.064
189	H	3.267	-4.740	-7.064
190	H	1.042	-5.662	-7.064
191	H	5.662	1.042	7.064
192	H	4.740	-3.267	-7.064
193	H	4.740	3.267	7.064
194	H	5.662	-1.042	-7.064
195	H	1.042	5.662	7.064
196	H	3.267	4.740	7.064
197	H	4.740	3.267	-7.064
198	H	5.662	1.042	-7.064
199	H	-1.042	5.662	7.064
200	H	3.267	4.740	-7.064
201	H	-3.267	4.740	7.064
202	H	1.042	5.662	-7.064
203	H	-5.662	1.042	7.064
204	H	-4.740	3.267	7.064
205	H	-3.267	4.740	-7.064

	206	H	-1.042	5.662	-7.064
	207	H	-5.662	-1.042	7.064
	208	H	-4.740	3.267	-7.064
	209	H	-4.740	-3.267	7.064
	210	H	-5.662	1.042	-7.064
	211	H	-3.267	-4.740	7.064
	212	H	-4.740	-3.267	-7.064
	213	H	-5.662	-1.042	-7.064
	214	H	-3.267	-4.740	-7.064
TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(9, 9) CNT TS (TR1)	1	O	2.366	-1.614	1.163
	2	H	3.295	-1.291	1.426
	3	H	2.140	-0.873	0.496
	4	O	2.281	-1.450	-1.384
	5	H	2.426	-2.183	-0.687
	6	H	3.248	-1.345	-1.682
	7	C	6.273	-0.002	6.115
	8	C	6.098	0.040	1.228
	9	C	6.047	0.752	2.462
	10	C	6.118	0.045	3.698
	11	C	5.796	2.155	4.921
	12	C	6.136	0.758	4.921
	13	C	5.567	2.893	6.115
	14	C	6.118	0.045	-3.698
	15	C	6.047	0.752	-2.462
	16	C	6.098	0.040	-1.228
	17	C	5.721	2.128	0.000
	18	C	6.058	0.748	0.000
	19	C	5.431	2.775	1.228
	20	C	5.714	2.119	2.462
	21	C	4.658	3.967	3.698
	22	C	5.450	2.779	3.698
	23	C	4.213	4.525	4.921
	24	C	4.807	4.031	6.115
	25	C	6.273	-0.002	-6.115
	26	C	5.796	2.155	-4.921
	27	C	6.136	0.758	-4.921
	28	C	5.450	2.779	-3.698
	29	C	5.714	2.119	-2.462
	30	C	4.646	3.950	-1.228
	31	C	5.431	2.775	-1.228
	32	C	4.160	4.467	0.000
	33	C	4.646	3.950	1.228
	34	C	3.015	5.296	2.462
	35	C	4.149	4.463	2.462
	36	C	2.389	5.632	3.698
	37	C	3.055	5.376	4.921
	38	C	1.092	6.178	6.115
	39	C	2.405	5.794	6.115
	40	C	4.807	4.031	-6.115
	41	C	5.567	2.893	-6.115
	42	C	4.213	4.525	-4.921
	43	C	4.658	3.967	-3.698
	44	C	3.015	5.296	-2.462
	45	C	4.149	4.463	-2.462
	46	C	2.377	5.616	-1.228
	47	C	3.015	5.308	0.000
	48	C	1.020	6.012	1.228
	49	C	2.377	5.616	1.228

50	C	0.310	6.086	2.462
51	C	1.018	6.033	3.698
52	C	-1.115	6.082	4.921
53	C	0.319	6.175	4.921
54	C	-1.882	5.984	6.115
55	C	2.405	5.794	-6.115
56	C	3.055	5.376	-4.921
57	C	1.018	6.033	-3.698
58	C	2.389	5.632	-3.698
59	C	0.310	6.086	-2.462
60	C	1.020	6.012	-1.228
61	C	-1.102	6.004	0.000
62	C	0.316	6.096	0.000
63	C	-1.789	5.830	1.228
64	C	-1.095	5.995	2.462
65	C	-3.098	5.276	3.698
66	C	-1.791	5.850	3.698
67	C	-3.725	4.935	4.921
68	C	-3.135	5.434	6.115
69	C	1.092	6.178	-6.115
70	C	-1.115	6.082	-4.921
71	C	0.319	6.175	-4.921
72	C	-1.791	5.850	-3.698
73	C	-1.095	5.995	-2.462
74	C	-3.084	5.261	-1.228
75	C	-1.789	5.830	-1.228
76	C	-3.677	4.873	0.000
77	C	-3.084	5.261	1.228
78	C	-4.692	3.888	2.462
79	C	-3.675	4.861	2.462
80	C	-5.132	3.330	3.698
81	C	-4.764	3.942	4.921
82	C	-5.894	2.148	6.115
83	C	-5.288	3.374	6.115
84	C	-3.135	5.434	-6.115
85	C	-1.882	5.984	-6.115
86	C	-3.725	4.935	-4.921
87	C	-3.098	5.276	-3.698
88	C	-4.692	3.888	-2.462
89	C	-3.675	4.861	-2.462
90	C	-5.118	3.316	-1.228
91	C	-4.703	3.891	0.000
92	C	-5.744	2.048	1.228
93	C	-5.118	3.316	1.228
94	C	-5.940	1.362	2.462
95	C	-5.764	2.050	3.698
96	C	-6.183	-0.042	4.921
97	C	-6.026	1.386	4.921
98	C	-6.220	-0.814	6.115
99	C	-5.288	3.374	-6.115
100	C	-4.764	3.942	-4.921
101	C	-5.764	2.050	-3.698
102	C	-5.132	3.330	-3.698
103	C	-5.940	1.362	-2.462
104	C	-5.744	2.048	-1.228
105	C	-6.104	-0.043	0.000
106	C	-5.948	1.369	0.000
107	C	-6.052	-0.750	1.228
108	C	-6.094	-0.037	2.462

109	C	-5.734	-2.134	3.698
110	C	-6.072	-0.748	3.698
111	C	-5.507	-2.811	4.921
112	C	-5.896	-2.143	6.115
113	C	-5.894	2.148	-6.115
114	C	-6.183	-0.042	-4.921
115	C	-6.026	1.386	-4.921
116	C	-6.072	-0.748	-3.698
117	C	-6.094	-0.037	-2.462
118	C	-5.717	-2.123	-1.228
119	C	-6.052	-0.750	-1.228
120	C	-5.437	-2.775	0.000
121	C	-5.717	-2.123	1.228
122	C	-4.644	-3.946	2.462
123	C	-5.426	-2.775	2.462
124	C	-4.171	-4.476	3.698
125	C	-4.709	-4.007	4.921
126	C	-3.139	-5.432	6.115
127	C	-4.242	-4.622	6.115
128	C	-5.896	-2.143	-6.115
129	C	-6.220	-0.814	-6.115
130	C	-5.507	-2.811	-4.921
131	C	-5.734	-2.134	-3.698
132	C	-4.644	-3.946	-2.462
133	C	-5.426	-2.775	-2.462
134	C	-4.154	-4.465	-1.228
135	C	-4.648	-3.956	0.000
136	C	-3.014	-5.301	1.228
137	C	-4.154	-4.465	1.228
138	C	-2.373	-5.613	2.462
139	C	-3.020	-5.321	3.698
140	C	-1.032	-6.096	4.921
141	C	-2.411	-5.693	4.921
142	C	-0.278	-6.267	6.115
143	C	-4.242	-4.622	-6.115
144	C	-4.709	-4.007	-4.921
145	C	-3.020	-5.321	-3.698
146	C	-4.171	-4.476	-3.698
147	C	-2.373	-5.613	-2.462
148	C	-3.014	-5.301	-1.228
149	C	-1.018	-6.019	0.000
150	C	-2.382	-5.620	0.000
151	C	-0.312	-6.090	1.228
152	C	-1.021	-6.008	2.462
153	C	1.106	-6.017	3.698
154	C	-0.318	-6.110	3.698
155	C	1.812	-5.912	4.921
156	C	1.087	-6.179	6.115
157	C	-3.139	-5.432	-6.115
158	C	-1.032	-6.096	-4.921
159	C	-2.411	-5.693	-4.921
160	C	-0.318	-6.110	-3.698
161	C	-1.021	-6.008	-2.462
162	C	1.098	-5.999	-1.228
163	C	-0.312	-6.090	-1.228
164	C	1.788	-5.836	0.000
165	C	1.098	-5.999	1.228
166	C	3.079	-5.259	2.462
167	C	1.790	-5.825	2.462

168	C	3.684	-4.885	3.698
169	C	3.128	-5.333	4.921
170	C	4.804	-4.034	6.115
171	C	3.815	-4.980	6.115
172	C	1.087	-6.179	-6.115
173	C	-0.278	-6.267	-6.115
174	C	1.812	-5.912	-4.921
175	C	1.106	-6.017	-3.698
176	C	3.079	-5.259	-2.462
177	C	1.790	-5.825	-2.462
178	C	3.675	-4.866	-1.228
179	C	3.089	-5.265	0.000
180	C	4.697	-3.889	1.228
181	C	3.675	-4.866	1.228
182	C	5.116	-3.311	2.462
183	C	4.715	-3.898	3.698
184	C	5.825	-2.075	4.921
185	C	5.188	-3.364	4.921
186	C	6.124	-1.362	6.115
187	C	3.815	-4.980	-6.115
188	C	3.128	-5.333	-4.921
189	C	4.715	-3.898	-3.698
190	C	3.684	-4.885	-3.698
191	C	5.116	-3.311	-2.462
192	C	4.697	-3.889	-1.228
193	C	5.751	-2.047	0.000
194	C	5.121	-3.321	0.000
195	C	5.943	-1.365	1.228
196	C	5.739	-2.049	2.462
197	C	5.962	-1.374	3.698
198	C	4.804	-4.034	-6.115
199	C	5.825	-2.075	-4.921
200	C	5.188	-3.364	-4.921
201	C	5.962	-1.374	-3.698
202	C	5.739	-2.049	-2.462
203	C	5.943	-1.365	-1.228
204	C	6.124	-1.362	-6.115
205	H	6.416	0.504	7.064
206	H	5.926	2.509	7.064
207	H	4.591	4.510	7.064
208	H	6.416	0.504	-7.064
209	H	0.618	6.406	7.064
210	H	2.927	5.732	7.064
211	H	4.591	4.510	-7.064
212	H	5.926	2.509	-7.064
213	H	-1.442	6.272	7.064
214	H	2.927	5.732	-7.064
215	H	-3.644	5.305	7.064
216	H	0.618	6.406	-7.064
217	H	-6.202	1.721	7.064
218	H	-5.136	3.878	7.064
219	H	-3.644	5.305	-7.064
220	H	-1.442	6.272	-7.064
221	H	-6.427	-0.331	7.064
222	H	-5.136	3.878	-7.064
223	H	-5.857	-2.668	7.064
224	H	-6.202	1.721	-7.064
225	H	-2.772	-5.808	7.064
226	H	-4.711	-4.385	7.064

	227	H	-5.857	-2.668	-7.064
	228	H	-6.427	-0.331	-7.064
	229	H	-0.790	-6.387	7.064
	230	H	-4.711	-4.385	-7.064
	231	H	1.610	-6.231	7.064
	232	H	-2.772	-5.808	-7.064
	233	H	5.239	-3.738	7.064
	234	H	3.500	-5.401	7.064
	235	H	1.610	-6.231	-7.064
	236	H	-0.790	-6.387	-7.064
	237	H	6.153	-1.887	7.064
	238	H	3.500	-5.401	-7.064
	239	H	5.239	-3.738	-7.064
	240	H	6.153	-1.887	-7.064
TS Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(9, 9) CNT TS (TR2)	1	O	-1.003	2.908	0.464
	2	H	-0.065	3.156	0.156
	3	H	-1.029	1.957	0.091
	4	O	-2.034	1.828	-1.593
	5	H	-1.981	2.759	-1.171
	6	H	-2.989	1.607	-1.322
	7	C	6.273	-0.002	6.115
	8	C	6.098	0.040	1.228
	9	C	6.047	0.752	2.462
	10	C	6.118	0.045	3.698
	11	C	5.796	2.155	4.921
	12	C	6.136	0.758	4.921
	13	C	5.567	2.893	6.115
	14	C	6.118	0.045	-3.698
	15	C	6.047	0.752	-2.462
	16	C	6.098	0.040	-1.228
	17	C	5.721	2.128	0.000
	18	C	6.058	0.748	0.000
	19	C	5.431	2.775	1.228
	20	C	5.714	2.119	2.462
	21	C	4.658	3.967	3.698
	22	C	5.450	2.779	3.698
	23	C	4.213	4.525	4.921
	24	C	4.807	4.031	6.115
	25	C	6.273	-0.002	-6.115
	26	C	5.796	2.155	-4.921
	27	C	6.136	0.758	-4.921
	28	C	5.450	2.779	-3.698
	29	C	5.714	2.119	-2.462
	30	C	4.646	3.950	-1.228
	31	C	5.431	2.775	-1.228
	32	C	4.160	4.467	0.000
	33	C	4.646	3.950	1.228
	34	C	3.015	5.296	2.462
	35	C	4.149	4.463	2.462
	36	C	2.389	5.632	3.698
	37	C	3.055	5.376	4.921
	38	C	1.092	6.178	6.115
	39	C	2.405	5.794	6.115
	40	C	4.807	4.031	-6.115
	41	C	5.567	2.893	-6.115
	42	C	4.213	4.525	-4.921
	43	C	4.658	3.967	-3.698
	44	C	3.015	5.296	-2.462

45	C	4.149	4.463	-2.462
46	C	2.377	5.616	-1.228
47	C	3.015	5.308	0.000
48	C	1.020	6.012	1.228
49	C	2.377	5.616	1.228
50	C	0.310	6.086	2.462
51	C	1.018	6.033	3.698
52	C	-1.115	6.082	4.921
53	C	0.319	6.175	4.921
54	C	-1.882	5.984	6.115
55	C	2.405	5.794	-6.115
56	C	3.055	5.376	-4.921
57	C	1.018	6.033	-3.698
58	C	2.389	5.632	-3.698
59	C	0.310	6.086	-2.462
60	C	1.020	6.012	-1.228
61	C	-1.102	6.004	0.000
62	C	0.316	6.096	0.000
63	C	-1.789	5.830	1.228
64	C	-1.095	5.995	2.462
65	C	-3.098	5.276	3.698
66	C	-1.791	5.850	3.698
67	C	-3.725	4.935	4.921
68	C	-3.135	5.434	6.115
69	C	1.092	6.178	-6.115
70	C	-1.115	6.082	-4.921
71	C	0.319	6.175	-4.921
72	C	-1.791	5.850	-3.698
73	C	-1.095	5.995	-2.462
74	C	-3.084	5.261	-1.228
75	C	-1.789	5.830	-1.228
76	C	-3.677	4.873	0.000
77	C	-3.084	5.261	1.228
78	C	-4.692	3.888	2.462
79	C	-3.675	4.861	2.462
80	C	-5.132	3.330	3.698
81	C	-4.764	3.942	4.921
82	C	-5.894	2.148	6.115
83	C	-5.288	3.374	6.115
84	C	-3.135	5.434	-6.115
85	C	-1.882	5.984	-6.115
86	C	-3.725	4.935	-4.921
87	C	-3.098	5.276	-3.698
88	C	-4.692	3.888	-2.462
89	C	-3.675	4.861	-2.462
90	C	-5.118	3.316	-1.228
91	C	-4.703	3.891	0.000
92	C	-5.744	2.048	1.228
93	C	-5.118	3.316	1.228
94	C	-5.940	1.362	2.462
95	C	-5.764	2.050	3.698
96	C	-6.183	-0.042	4.921
97	C	-6.026	1.386	4.921
98	C	-6.220	-0.814	6.115
99	C	-5.288	3.374	-6.115
100	C	-4.764	3.942	-4.921
101	C	-5.764	2.050	-3.698
102	C	-5.132	3.330	-3.698
103	C	-5.940	1.362	-2.462

104	C	-5.744	2.048	-1.228
105	C	-6.104	-0.043	0.000
106	C	-5.948	1.369	0.000
107	C	-6.052	-0.750	1.228
108	C	-6.094	-0.037	2.462
109	C	-5.734	-2.134	3.698
110	C	-6.072	-0.748	3.698
111	C	-5.507	-2.811	4.921
112	C	-5.896	-2.143	6.115
113	C	-5.894	2.148	-6.115
114	C	-6.183	-0.042	-4.921
115	C	-6.026	1.386	-4.921
116	C	-6.072	-0.748	-3.698
117	C	-6.094	-0.037	-2.462
118	C	-5.717	-2.123	-1.228
119	C	-6.052	-0.750	-1.228
120	C	-5.437	-2.775	0.000
121	C	-5.717	-2.123	1.228
122	C	-4.644	-3.946	2.462
123	C	-5.426	-2.775	2.462
124	C	-4.171	-4.476	3.698
125	C	-4.709	-4.007	4.921
126	C	-3.139	-5.432	6.115
127	C	-4.242	-4.622	6.115
128	C	-5.896	-2.143	-6.115
129	C	-6.220	-0.814	-6.115
130	C	-5.507	-2.811	-4.921
131	C	-5.734	-2.134	-3.698
132	C	-4.644	-3.946	-2.462
133	C	-5.426	-2.775	-2.462
134	C	-4.154	-4.465	-1.228
135	C	-4.648	-3.956	0.000
136	C	-3.014	-5.301	1.228
137	C	-4.154	-4.465	1.228
138	C	-2.373	-5.613	2.462
139	C	-3.020	-5.321	3.698
140	C	-1.032	-6.096	4.921
141	C	-2.411	-5.693	4.921
142	C	-0.278	-6.267	6.115
143	C	-4.242	-4.622	-6.115
144	C	-4.709	-4.007	-4.921
145	C	-3.020	-5.321	-3.698
146	C	-4.171	-4.476	-3.698
147	C	-2.373	-5.613	-2.462
148	C	-3.014	-5.301	-1.228
149	C	-1.018	-6.019	0.000
150	C	-2.382	-5.620	0.000
151	C	-0.312	-6.090	1.228
152	C	-1.021	-6.008	2.462
153	C	1.106	-6.017	3.698
154	C	-0.318	-6.110	3.698
155	C	1.812	-5.912	4.921
156	C	1.087	-6.179	6.115
157	C	-3.139	-5.432	-6.115
158	C	-1.032	-6.096	-4.921
159	C	-2.411	-5.693	-4.921
160	C	-0.318	-6.110	-3.698
161	C	-1.021	-6.008	-2.462
162	C	1.098	-5.999	-1.228

163	C	-0.312	-6.090	-1.228
164	C	1.788	-5.836	0.000
165	C	1.098	-5.999	1.228
166	C	3.079	-5.259	2.462
167	C	1.790	-5.825	2.462
168	C	3.684	-4.885	3.698
169	C	3.128	-5.333	4.921
170	C	4.804	-4.034	6.115
171	C	3.815	-4.980	6.115
172	C	1.087	-6.179	-6.115
173	C	-0.278	-6.267	-6.115
174	C	1.812	-5.912	-4.921
175	C	1.106	-6.017	-3.698
176	C	3.079	-5.259	-2.462
177	C	1.790	-5.825	-2.462
178	C	3.675	-4.866	-1.228
179	C	3.089	-5.265	0.000
180	C	4.697	-3.889	1.228
181	C	3.675	-4.866	1.228
182	C	5.116	-3.311	2.462
183	C	4.715	-3.898	3.698
184	C	5.825	-2.075	4.921
185	C	5.188	-3.364	4.921
186	C	6.124	-1.362	6.115
187	C	3.815	-4.980	-6.115
188	C	3.128	-5.333	-4.921
189	C	4.715	-3.898	-3.698
190	C	3.684	-4.885	-3.698
191	C	5.116	-3.311	-2.462
192	C	4.697	-3.889	-1.228
193	C	5.751	-2.047	0.000
194	C	5.121	-3.321	0.000
195	C	5.943	-1.365	1.228
196	C	5.739	-2.049	2.462
197	C	5.962	-1.374	3.698
198	C	4.804	-4.034	-6.115
199	C	5.825	-2.075	-4.921
200	C	5.188	-3.364	-4.921
201	C	5.962	-1.374	-3.698
202	C	5.739	-2.049	-2.462
203	C	5.943	-1.365	-1.228
204	C	6.124	-1.362	-6.115
205	H	6.416	0.504	7.064
206	H	5.926	2.509	7.064
207	H	4.591	4.510	7.064
208	H	6.416	0.504	-7.064
209	H	0.618	6.406	7.064
210	H	2.927	5.732	7.064
211	H	4.591	4.510	-7.064
212	H	5.926	2.509	-7.064
213	H	-1.442	6.272	7.064
214	H	2.927	5.732	-7.064
215	H	-3.644	5.305	7.064
216	H	0.618	6.406	-7.064
217	H	-6.202	1.721	7.064
218	H	-5.136	3.878	7.064
219	H	-3.644	5.305	-7.064
220	H	-1.442	6.272	-7.064
221	H	-6.427	-0.331	7.064

222	H	-5.136	3.878	-7.064
223	H	-5.857	-2.668	7.064
224	H	-6.202	1.721	-7.064
225	H	-2.772	-5.808	7.064
226	H	-4.711	-4.385	7.064
227	H	-5.857	-2.668	-7.064
228	H	-6.427	-0.331	-7.064
229	H	-0.790	-6.387	7.064
230	H	-4.711	-4.385	-7.064
231	H	1.610	-6.231	7.064
232	H	-2.772	-5.808	-7.064
233	H	5.239	-3.738	7.064
234	H	3.500	-5.401	7.064
235	H	1.610	-6.231	-7.064
236	H	-0.790	-6.387	-7.064
237	H	6.153	-1.887	7.064
238	H	3.500	-5.401	-7.064
239	H	5.239	-3.738	-7.064
240	H	6.153	-1.887	-7.064

Table S5. Reduced mass, imaginary frequency of TS and displacement of related rotation path for every rotation type in each condition.

	Displacement of Reaction Path to Fit (Bohr)	Mass Weighted Path (Bohr)	Red. Mass of TS (a.m.u)	Imaginary Frequency of Relevant TS (cm^{-1})
isolated TR1	-4 ~ 4	-4.066 ~ 4.066	1.0332	-153.6825
isolated TR2	-3 ~ 3	-3.051 ~ 3.051	1.0346	-172.4154
TR1@(5, 5)	-5.4 ~ 5.6	-5.556 ~ 5.761	1.0585	-561.7236
TR2@(5, 5)	-3.2 ~ 3.2	-3.297 ~3.297	1.0617	-548.8237
TR1@(6, 6)	-7 ~ 7	-7.193 ~ 7.193	1.0560	-542.4435
TR2@(6, 6)	-3.2 ~ 3.2	-3.291 ~ 3.291	1.0579	-535.2242
TR1@(7, 7)	-3.4 ~ 5.6	-3.495 ~ 5.757	1.0567	-536.9628
TR2@(7, 7)	-3.4 ~ 8.0	-3.496 ~ 8.226	1.0572	-530.7901
TR1@(8, 8)	-5.4 ~ 3.2	-5.550 ~ 3.289	1.0564	-535.3206
TR2@(8, 8)	-3.2 ~ 9.4	-3.291 ~ 9.667	1.0577	-532.1781
TR1@(9, 9)	-5.2 ~ 3.0	-5.344 ~ 3.083	1.0563	-535.4078
TR2@(9, 9)	-3.2 ~ 8.8	-3.291 ~ 9.049	1.0575	-529.1286

Table S6. Progressions and coefficients of Fourier Function fitted for reaction paths for two rotation types in different conditions.

	isolated TR1	isolated TR2	TR1@(5, 5)	TR2@(5, 5)	TR1@(6, 6)	TR2@(6, 6)
ω	0.3927	1.047	0.5712	0.9817	0.4488	0.9817
a_0	0.002515	0.0009762	0.003256	0.00444	0.003114	0.004469
a_1	-0.002275	0.0009628	0.004781	0.005694	0.004095	0.005454
a_2	0.002754	-1.623e-05	0.002702	0.001501	0.002319	0.001426
a_3	-0.0007728	--	0.001413	5.338e-05	0.001615	2.515e-05
a_4	0.0002424	--	0.0004683	--	0.0009146	2.829e-05
a_5	--	--	8.087e-05	--	0.0003967	--
a_6	--	--	--	--	8.91e-05	--
a_7	--	--	--	--	--	--
a_8	--	--	--	--	--	--
b_1	-2.974e-07	5.04e-09	-1.854e-05	-2.411e-05	4.575e-06	4.64e-07
b_2	4.496e-07	-1.026e-09	-1.168e-06	1.116e-05	-1.646e-06	-3.937e-07
b_3	-3.158e-07	--	1.618e-05	1.26e-05	-1.353e-07	1.988e-07
b_4	-8.667e-10	--	7.412e-06	--	-1.817e-07	-1.261e-07
b_5	--	--	7.908e-07	--	1.044e-07	--
b_6	--	--	--	--	-3.585e-07	--
b_7	--	--	--	--	--	--
b_8	--	--	--	--	--	--
	TR1@(7, 7)	TR2@(7, 7)	TR1@(8, 8)	TR2@(8, 8)	TR1@(9, 9)	TR2@(9, 9)
ω	0.3491	0.5512	0.3653	0.2493	0.3831	0.5236
a_0	-0.09809	0.003487	-0.08048	-1.81	-0.06969	0.003355
a_1	0.1714	0.004036	0.1411	2.231	0.1223	0.003804
a_2	-0.0891	0.002561	-0.06984	0.3253	-0.05775	0.002585
a_3	0.02603	0.001344	0.01805	-1.488	0.01305	0.001377
a_4	0.006549	0.0004488	0.007674	0.9892	0.008297	0.0005633
a_5	-0.006767	8.867e-05	-0.006028	-0.2031	-0.005484	0.0001426
a_6	0.00295	--	0.002413	-0.07159	0.00199	--
a_7	--	--	--	0.04379	--	--
a_8	--	--	--	-0.004331	--	--
b_1	0.07492	0.0008617	-0.06401	2.513	-0.05726	0.001022
b_2	-0.1039	-0.0001181	0.08794	-2.649	0.07786	-1.418e-05
b_3	0.08051	-0.0001091	-0.06659	1.017	-0.05765	-0.0001474
b_4	-0.03961	-4.167e-05	0.03148	0.2604	0.02615	-7.852e-05
b_5	0.01179	-1.362e-05	-0.008783	-0.4264	-0.006753	-3.465e-05
b_6	-0.001558	--	0.0009939	0.1548	0.0006094	--
b_7	--	--	--	-0.009553	--	--
b_8	--	--	--	-0.004759	--	--

Table S7. The probability of two tunneling rotation types in different conditions. The provided energy is assigned to the vibrational mode along the reaction path. It should be noted that the data vacancies come from the different restriction on the range of x value of $V(x)$ in tunneling probability formula.

Provided Energy		isolated TR1	isolated TR2	TR1@(5, 5)	TR2@(5, 5)	TR1@(6, 6)	TR2@(6, 6)
(eV)	(milli-Hartree)						
0.01	0.5	1.74E-10	9.66E-07	6.03E-23	9.40E-18	1.89E-30	5.10E-18
0.03	1.0	1.63E-07	1.96E-04	3.21E-19	2.46E-16	3.94E-25	1.98E-16
0.04	1.5	6.05E-05	2.31E-02	2.52E-17	3.60E-15	4.13E-21	3.31E-15
0.05	2.0	1.17E-02	1	5.46E-16	3.92E-14	1.16E-17	3.97E-14
0.07	2.5	1	1	7.38E-15	3.52E-13	6.07E-16	3.86E-13
0.08	3.0	1	1	7.62E-14	2.74E-12	1.13E-14	3.24E-12
0.10	3.5	1	1	6.54E-13	1.92E-11	1.41E-13	2.42E-11
0.11	4.0	1	1	4.90E-12	1.23E-10	1.38E-12	1.64E-10
0.12	4.5	1	1	3.29E-11	7.29E-10	1.15E-11	1.03E-09
0.14	5.0	1	1	2.03E-10	4.06E-09	8.40E-11	6.06E-09
0.15	5.5	1	1	1.16E-09	2.14E-08	5.57E-10	3.35E-08
0.16	6.0	1	1	6.23E-09	1.07E-07	3.41E-09	1.76E-07
0.19	7.0	1	1	1.53E-07	2.38E-06	1.04E-07	4.20E-06
0.22	8.0	1	1	3.17E-06	4.59E-05	2.59E-06	8.59E-05
0.24	9.0	1	1	5.70E-05	7.83E-04	5.43E-05	1.54E-03
0.27	10.0	1	1	9.08E-04	1.21E-02	9.95E-04	2.44E-02
0.30	11.0	1	1	1.31E-02	1.70E-01	1.62E-02	3.51E-01
0.33	12.0	1	1	1.72E-01	1	2.40E-01	1
0.35	13.0	1	1	1	1	1	1

Provided Energy		TR1@(7, 7)	TR2@(7, 7)	TR1@(8, 8)	TR2@(8, 8)	TR1@(9, 9)	TR2@(9, 9)
(eV)	(milli-Hartree)						
0.01	0.5	——	1.23E-27	——	——	——	2.16E-28
0.03	1.0	——	1.23E-23	——	8.11E-20	——	1.93E-24
0.04	1.5	——	1.56E-20	——	1.20E-17	——	6.11E-21
0.05	2.0	——	1.19E-17	——	4.19E-16	——	6.67E-18
0.07	2.5	——	3.84E-15	——	6.91E-15	——	2.09E-15
0.08	3.0	——	7.45E-14	——	8.08E-14	——	7.38E-14
0.10	3.5	3.76E-15	8.78E-13	——	7.64E-13	1.35E-14	1.00E-12
0.11	4.0	8.29E-14	8.15E-12	9.16E-14	6.20E-12	2.46E-13	9.96E-12
0.12	4.5	1.01E-12	6.46E-11	1.17E-12	4.48E-11	2.76E-12	8.22E-11
0.14	5.0	9.47E-12	4.56E-10	1.13E-11	2.95E-10	2.47E-11	5.96E-10
0.15	5.5	7.53E-11	2.93E-09	9.15E-11	1.79E-09	1.90E-10	3.90E-09
0.16	6.0	5.30E-10	1.75E-08	6.52E-10	1.02E-08	1.30E-09	2.36E-08
0.19	7.0	2.00E-08	5.14E-07	2.50E-08	2.80E-07	4.72E-08	7.09E-07
0.22	8.0	5.77E-07	1.24E-05	7.26E-07	6.41E-06	1.32E-06	1.73E-05
0.24	9.0	1.36E-05	2.56E-04	1.71E-05	1.27E-04	3.00E-05	3.61E-04
0.27	10.0	2.73E-04	4.62E-03	3.44E-04	2.21E-03	5.85E-04	6.58E-03
0.30	11.0	4.79E-03	7.46E-02	6.02E-03	3.46E-02	9.97E-03	1.07E-01
0.33	12.0	7.53E-02	1	9.42E-02	1	1.52E-01	1
0.35	13.0	1	1	1	1	1	1

Table S8. The frequencies of the vibrational modes of the corresponding rotation types along the reaction path for optimized water dimer.

	isolated TR1	isolated TR2	TR1 @(5, 5)	TR2 @(5, 5)	TR1 @(6, 6)	TR2 @(6, 6)
Freq. (cm^{-1})	691.49	180.46	997.20	419.99	985.79	405.68
Freq. (Hz)	**2.0730e+13**	**5.4101e+12**	**2.9895e+13**	**1.2591e+13**	**2.9553e+13**	**1.2162e+13**
E_{vib} **(eV)**	**0.043**	**0.011**	**0.062**	**0.026**	**0.061**	**0.025**
	TR1 @(7, 7)	TR2 @(7, 7)	TR1 @(8, 8)	TR2 @(8, 8)	TR1 @(9, 9)	TR2 @(9, 9)
Freq. (cm^{-1})	991.73	401.61	990.53	394.63	989.08	392.95
Freq. (Hz)	**2.9731e+13**	**1.2040e+13**	**2.9695e+13**	**1.1831e+13**	**2.9652e+13**	**1.1781e+13**
E_{vib} **(eV)**	**0.061**	**0.025**	**0.061**	**0.024**	**0.061**	**0.024**

Table S9. Expectation of tunneling rotation per second (s^{-1}).

Provide E (eV)	isolated TR1	isolated TR2	@(5, 5) TR1	@(5, 5) TR2	@(6, 6) TR1	@(6, 6) TR2
0.01	3.61E+03	5.23E+06	1.80E-09	1.18E-04	5.59E-17	6.20E-05
0.03	3.38E+06	1.06E+09	9.60E-06	3.10E-03	1.16E-11	2.41E-03
0.04	1.25E+09	1.25E+11	7.53E-04	4.53E-02	1.22E-07	4.03E-02
0.05	2.43E+11	5.41E+12	1.63E-02	4.94E-01	3.43E-04	4.83E-01
0.07	**2.07E+13**	**5.41E+12**	**2.21E-01**	**4.43E+00**	**1.79E-02**	**4.69E+00**
0.08	2.07E+13	5.41E+12	2.28E+00	3.45E+01	3.34E-01	3.94E+01
0.10	2.07E+13	5.41E+12	1.96E+01	2.42E+02	4.17E+00	2.94E+02
0.11	2.07E+13	5.41E+12	1.46E+02	1.55E+03	4.08E+01	1.99E+03
0.12	2.07E+13	5.41E+12	9.84E+02	9.18E+03	3.40E+02	1.25E+04
0.14	2.07E+13	5.41E+12	6.07E+03	5.11E+04	2.48E+03	7.37E+04
0.15	**2.07E+13**	**5.41E+12**	**3.47E+04**	**2.69E+05**	**1.65E+04**	**4.07E+05**
0.16	2.07E+13	5.41E+12	1.86E+05	1.35E+06	1.01E+05	2.14E+06
0.19	2.07E+13	5.41E+12	4.57E+06	3.00E+07	3.07E+06	5.11E+07
0.22	2.07E+13	5.41E+12	9.48E+07	5.78E+08	7.65E+07	1.04E+09
0.24	2.07E+13	5.41E+12	1.70E+09	9.86E+09	1.60E+09	1.87E+10
0.27	2.07E+13	5.41E+12	2.71E+10	1.52E+11	2.94E+10	2.97E+11
0.30	2.07E+13	5.41E+12	3.92E+11	2.14E+12	4.79E+11	4.27E+12
0.33	2.07E+13	5.41E+12	5.14E+12	1.26E+13	7.09E+12	1.22E+13
0.35	2.07E+13	5.41E+12	2.99E+13	1.26E+13	2.96E+13	1.22E+13

Provided E (eV)	@(7, 7) TR1	@(7, 7) TR2	@(8, 8) TR1	@(8, 8) TR2	@(9, 9) TR1	@(9, 9) TR2
0.01	——	1.48E-14	——	——	——	2.54E-15
0.03	——	1.48E-10	——	9.59E-07	——	2.27E-11
0.04	——	1.88E-07	——	1.42E-04	——	7.20E-08
0.05	——	1.43E-04	——	4.96E-03	——	7.86E-05
0.07	**——**	**4.62E-02**	**——**	**8.18E-02**	**——**	**2.46E-02**
0.08	——	8.97E-01	——	9.56E-01	——	8.69E-01
0.10	1.12E-01	1.06E+01	——	9.04E+00	4.00E-01	1.18E+01
0.11	2.46E+00	9.81E+01	2.72E+00	7.34E+01	7.29E+00	1.17E+02
0.12	3.00E+01	7.78E+02	3.47E+01	5.30E+02	8.18E+01	9.68E+02
0.14	2.82E+02	5.49E+03	3.36E+02	3.49E+03	7.32E+02	7.02E+03
0.15	**2.24E+03**	**3.53E+04**	**2.72E+03**	**2.12E+04**	**5.63E+03**	**4.59E+04**
0.16	1.58E+04	2.11E+05	1.94E+04	1.21E+05	3.85E+04	2.78E+05
0.19	5.95E+05	6.19E+06	7.42E+05	3.31E+06	1.40E+06	8.35E+06
0.22	1.72E+07	1.49E+08	2.16E+07	7.58E+07	3.91E+07	2.04E+08
0.24	4.04E+08	3.08E+09	5.08E+08	1.50E+09	8.90E+08	4.25E+09
0.27	8.12E+09	5.56E+10	1.02E+10	2.61E+10	1.73E+10	7.75E+10
0.30	1.42E+11	8.98E+11	1.79E+11	4.09E+11	2.96E+11	1.26E+12
0.33	2.24E+12	1.20E+13	2.80E+12	1.18E+13	4.51E+12	1.18E+13
0.35	2.97E+13	1.20E+13	2.97E+13	1.18E+13	2.97E+13	1.18E+13

Table S10. The temperature related to Log_{10}(Ratio) = 0.

Provided Energy	Path	System	Temp. (K)	Provided Energy	Path	System	Temp. (K)
0.01 eV	TR1	(5, 5)	81.25	0.15 eV	TR1	(5, 5)	109.40
		(6, 6)	59.38			(6, 6)	104.00
		(7, 7)	--			(7, 7)	104.00
		(8, 8)	--			(8, 8)	104.00
		(9, 9)	--			(9, 9)	104.00
	TR2	(5, 5)	93.75		TR2	(5, 5)	109.60
		(6, 6)	90.63			(6, 6)	107.00
		(7, 7)	62.50			(7, 7)	106.50
		(8, 8)	--			(8, 8)	100.00
		(9, 9)	59.38			(9, 9)	106.00
0.07 eV	TR1	(5, 5)	100.00	0.30 eV	TR1	(5, 5)	119.00
		(6, 6)	93.75			(6, 6)	115.63
		(7, 7)	--			(7, 7)	119.25
		(8, 8)	--			(8, 8)	112.50
		(9, 9)	--			(9, 9)	112.50
	TR2	(5, 5)	100.00		TR2	(5, 5)	126.00
		(6, 6)	102.00			(6, 6)	118.00
		(7, 7)	109.00			(7, 7)	119.00
		(8, 8)	93.75			(8, 8)	81.25
		(9, 9)	93.75			(9, 9)	119.00

Table S11. The coordinates and energies of the sampled structures of confined water dimer in (5, 5) CNT. The first structure which is highlighted with underline was used in the paper.

Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$\underline{(H_2O)_2}$@(5, 5) CNT_1	0.000000	1	O	-0.186	-0.244	0.606
		2	H	0.407	0.504	0.953
		3	H	-0.056	-0.073	-0.404
		4	O	0.110	0.142	-1.969
		5	H	-0.842	0.150	-2.318
		6	H	0.398	-0.767	-2.314
		7	C	1.478	3.188	6.127
		8	C	1.394	3.115	1.231
		9	C	0.706	3.328	2.471
		10	C	1.388	3.125	3.706
		11	C	-0.715	3.376	4.926
		12	C	0.719	3.376	4.926
		13	C	-1.474	3.188	6.127
		14	C	1.388	3.124	-3.689
		15	C	0.706	3.328	-2.454
		16	C	1.394	3.118	-1.216
		17	C	-0.714	3.352	0.008
		18	C	0.717	3.352	0.009
		19	C	-1.390	3.118	1.233
		20	C	-0.702	3.328	2.471
		21	C	-2.545	2.281	3.706
		22	C	-1.384	3.124	3.706
		23	C	-2.990	1.723	4.926
		24	C	-2.578	2.387	6.127
		25	C	1.478	3.188	-6.110
		26	C	-0.715	3.376	-4.910
		27	C	0.719	3.376	-4.910
		28	C	-1.384	3.125	-3.689
		29	C	-0.702	3.328	-2.454
		30	C	-2.536	2.285	-1.216
		31	C	-1.390	3.118	-1.216
		32	C	-2.968	1.714	0.008
		33	C	-2.536	2.285	1.233
		34	C	-3.384	0.356	2.471
		35	C	-2.949	1.696	2.471
		36	C	-3.401	-0.355	3.706
		37	C	-3.434	0.359	4.926
		38	C	-3.068	-1.718	6.127
		39	C	-3.490	-0.421	6.127
		40	C	-2.578	2.387	-6.110
		41	C	-1.474	3.188	-6.110
		42	C	-2.990	1.723	-4.910
		43	C	-2.545	2.281	-3.689
		44	C	-3.384	0.356	-2.454
		45	C	-2.949	1.696	-2.454
		46	C	-3.394	-0.362	-1.216
		47	C	-3.411	0.353	0.008
		48	C	-2.959	-1.710	1.233
		49	C	-3.397	-0.363	1.233
		50	C	-2.526	-2.285	2.471
		51	C	-2.958	-1.719	3.706
		52	C	-1.404	-3.159	4.926
		53	C	-2.564	-2.316	4.926
		54	C	-0.680	-3.453	6.127
		55	C	-3.490	-0.421	-6.110

56	C	-3.434	0.359	-4.910
57	C	-2.958	-1.719	-3.689
58	C	-3.401	-0.355	-3.689
59	C	-2.526	-2.284	-2.455
60	C	-2.959	-1.709	-1.215
61	C	-1.391	-3.139	0.008
62	C	-2.550	-2.299	0.008
63	C	-0.706	-3.347	1.233
64	C	-1.386	-3.113	2.471
65	C	0.719	-3.349	3.706
66	C	-0.715	-3.349	3.706
67	C	1.408	-3.159	4.926
68	C	0.684	-3.453	6.127
69	C	-3.068	-1.718	-6.110
70	C	-1.404	-3.159	-4.910
71	C	-2.564	-2.316	-4.910
72	C	-0.715	-3.349	-3.689
73	C	-1.387	-3.113	-2.454
74	C	0.710	-3.347	-1.216
75	C	-0.706	-3.347	-1.216
76	C	1.395	-3.139	0.008
77	C	0.710	-3.347	1.233
78	C	2.530	-2.285	2.471
79	C	1.390	-3.113	2.471
80	C	2.962	-1.719	3.706
81	C	2.568	-2.316	4.926
82	C	3.494	-0.421	6.127
83	C	3.072	-1.718	6.127
84	C	0.684	-3.453	-6.110
85	C	-0.680	-3.453	-6.110
86	C	1.408	-3.159	-4.910
87	C	0.719	-3.349	-3.689
88	C	2.530	-2.285	-2.454
89	C	1.391	-3.113	-2.454
90	C	2.963	-1.710	-1.216
91	C	2.554	-2.298	0.008
92	C	3.401	-0.363	1.233
93	C	2.963	-1.710	1.233
94	C	3.388	0.356	2.471
95	C	3.405	-0.355	3.706
96	C	2.994	1.723	4.926
97	C	3.437	0.359	4.926
98	C	2.582	2.387	6.127
99	C	3.072	-1.718	-6.110
100	C	2.568	-2.316	-4.910
101	C	3.405	-0.355	-3.689
102	C	2.962	-1.719	-3.689
103	C	3.388	0.356	-2.454
104	C	3.400	-0.363	-1.216
105	C	2.973	1.714	0.009
106	C	3.415	0.353	0.008
107	C	2.538	2.286	1.233
108	C	2.953	1.696	2.471
109	C	2.548	2.281	3.706
110	C	3.494	-0.421	-6.110
111	C	2.994	1.723	-4.910
112	C	3.437	0.359	-4.910
113	C	2.549	2.281	-3.689
114	C	2.953	1.696	-2.454

		115	C	2.540	2.285	-1.216
		116	C	2.582	2.387	-6.110
		117	H	1.103	3.572	7.071
		118	H	-1.099	3.572	7.071
		119	H	-3.058	2.148	7.071
		120	H	1.103	3.572	-7.054
		121	H	-2.990	-2.249	7.071
		122	H	-3.739	0.055	7.071
		123	H	-3.058	2.148	-7.054
		124	H	-1.099	3.572	-7.054
		125	H	-1.209	-3.543	7.071
		126	H	-3.739	0.055	-7.054
		127	H	1.213	-3.543	7.071
		128	H	-2.990	-2.249	-7.054
		129	H	3.742	0.055	7.071
		130	H	2.994	-2.249	7.071
		131	H	1.213	-3.543	-7.054
		132	H	-1.209	-3.543	-7.054
		133	H	3.062	2.148	7.071
		134	H	2.994	-2.249	-7.054
		135	H	3.742	0.055	-7.054
		136	H	3.062	2.148	-7.054
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(5, 5) CNT_2	0.000046	1	O	-0.105	-0.150	1.000
		2	H	0.851	-0.138	1.338
		3	H	-0.404	0.758	1.338
		4	O	0.182	0.251	-1.571
		5	H	0.050	0.068	-0.563
		6	H	-0.366	-0.527	-1.928
		7	C	1.478	3.188	6.127
		8	C	1.394	3.115	1.231
		9	C	0.706	3.328	2.471
		10	C	1.388	3.125	3.706
		11	C	-0.715	3.376	4.926
		12	C	0.719	3.376	4.926
		13	C	-1.474	3.188	6.127
		14	C	1.388	3.124	-3.689
		15	C	0.706	3.328	-2.454
		16	C	1.394	3.118	-1.216
		17	C	-0.714	3.352	0.008
		18	C	0.717	3.353	0.009
		19	C	-1.390	3.118	1.233
		20	C	-0.702	3.328	2.471
		21	C	-2.545	2.281	3.706
		22	C	-1.384	3.124	3.706
		23	C	-2.990	1.723	4.926
		24	C	-2.578	2.387	6.127
		25	C	1.478	3.188	-6.110
		26	C	-0.715	3.376	-4.910
		27	C	0.719	3.376	-4.910
		28	C	-1.384	3.124	-3.689
		29	C	-0.702	3.328	-2.454
		30	C	-2.536	2.285	-1.216
		31	C	-1.390	3.118	-1.216
		32	C	-2.968	1.714	0.008
		33	C	-2.536	2.285	1.233
		34	C	-3.384	0.356	2.471
		35	C	-2.949	1.696	2.471
		36	C	-3.401	-0.355	3.706

37	C	-3.434	0.359	4.926
38	C	-3.068	-1.718	6.127
39	C	-3.490	-0.421	6.127
40	C	-2.578	2.387	-6.110
41	C	-1.474	3.188	-6.110
42	C	-2.990	1.723	-4.910
43	C	-2.545	2.281	-3.689
44	C	-3.384	0.356	-2.454
45	C	-2.949	1.696	-2.454
46	C	-3.394	-0.362	-1.215
47	C	-3.411	0.353	0.008
48	C	-2.959	-1.710	1.233
49	C	-3.397	-0.363	1.233
50	C	-2.526	-2.285	2.471
51	C	-2.958	-1.719	3.706
52	C	-1.404	-3.159	4.926
53	C	-2.564	-2.316	4.926
54	C	-0.680	-3.453	6.127
55	C	-3.490	-0.421	-6.110
56	C	-3.434	0.359	-4.910
57	C	-2.958	-1.719	-3.689
58	C	-3.401	-0.355	-3.689
59	C	-2.526	-2.284	-2.455
60	C	-2.959	-1.709	-1.215
61	C	-1.391	-3.139	0.008
62	C	-2.550	-2.299	0.008
63	C	-0.706	-3.347	1.233
64	C	-1.386	-3.113	2.471
65	C	0.719	-3.349	3.706
66	C	-0.715	-3.349	3.706
67	C	1.408	-3.159	4.926
68	C	0.684	-3.453	6.127
69	C	-3.068	-1.718	-6.110
70	C	-1.404	-3.159	-4.910
71	C	-2.564	-2.316	-4.910
72	C	-0.715	-3.349	-3.689
73	C	-1.387	-3.113	-2.454
74	C	0.710	-3.347	-1.216
75	C	-0.706	-3.347	-1.216
76	C	1.395	-3.139	0.008
77	C	0.710	-3.347	1.233
78	C	2.530	-2.285	2.471
79	C	1.390	-3.113	2.471
80	C	2.962	-1.719	3.706
81	C	2.568	-2.316	4.926
82	C	3.494	-0.421	6.127
83	C	3.072	-1.718	6.127
84	C	0.684	-3.453	-6.110
85	C	-0.680	-3.453	-6.110
86	C	1.408	-3.159	-4.910
87	C	0.719	-3.349	-3.689
88	C	2.530	-2.285	-2.454
89	C	1.390	-3.113	-2.454
90	C	2.963	-1.710	-1.216
91	C	2.554	-2.298	0.008
92	C	3.400	-0.363	1.233
93	C	2.963	-1.710	1.233
94	C	3.388	0.356	2.471
95	C	3.405	-0.355	3.706

		96	C	2.994	1.723	4.926
		97	C	3.437	0.359	4.926
		98	C	2.582	2.387	6.127
		99	C	3.072	-1.718	-6.110
		100	C	2.568	-2.316	-4.910
		101	C	3.405	-0.355	-3.689
		102	C	2.962	-1.719	-3.689
		103	C	3.388	0.356	-2.454
		104	C	3.400	-0.363	-1.216
		105	C	2.973	1.714	0.009
		106	C	3.415	0.353	0.008
		107	C	2.538	2.286	1.233
		108	C	2.953	1.696	2.471
		109	C	2.548	2.281	3.706
		110	C	3.494	-0.421	-6.110
		111	C	2.994	1.723	-4.910
		112	C	3.437	0.359	-4.910
		113	C	2.549	2.281	-3.689
		114	C	2.953	1.696	-2.454
		115	C	2.540	2.285	-1.216
		116	C	2.582	2.387	-6.110
		117	H	1.103	3.572	7.071
		118	H	-1.099	3.572	7.071
		119	H	-3.058	2.148	7.071
		120	H	1.103	3.572	-7.054
		121	H	-2.990	-2.249	7.071
		122	H	-3.739	0.055	7.071
		123	H	-3.058	2.148	-7.054
		124	H	-1.099	3.572	-7.054
		125	H	-1.209	-3.543	7.071
		126	H	-3.739	0.055	-7.054
		127	H	1.213	-3.543	7.071
		128	H	-2.990	-2.249	-7.054
		129	H	3.742	0.055	7.071
		130	H	2.994	-2.249	7.071
		131	H	1.213	-3.543	-7.054
		132	H	-1.209	-3.543	-7.054
		133	H	3.062	2.148	7.071
		134	H	2.994	-2.249	-7.054
		135	H	3.742	0.055	-7.054
		136	H	3.062	2.148	-7.054
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(5, 5) CNT_3	0.000099	1	O	-0.293	0.086	0.535
		2	H	0.624	-0.179	0.883
		3	H	-0.085	0.026	-0.475
		4	O	0.175	-0.054	-2.039
		5	H	-0.164	0.835	-2.390
		6	H	-0.568	-0.653	-2.381
		7	C	1.476	3.192	6.128
		8	C	1.388	3.121	1.235
		9	C	0.706	3.331	2.471
		10	C	1.386	3.128	3.707
		11	C	-0.717	3.379	4.928
		12	C	0.717	3.379	4.928
		13	C	-1.476	3.192	6.128
		14	C	1.386	3.128	-3.688
		15	C	0.704	3.332	-2.452
		16	C	1.392	3.121	-1.215
		17	C	-0.716	3.357	0.010

18	C	0.718	3.355	0.009
19	C	-1.392	3.121	1.234
20	C	-0.704	3.331	2.474
21	C	-2.547	2.285	3.707
22	C	-1.386	3.128	3.707
23	C	-2.992	1.726	4.928
24	C	-2.580	2.390	6.128
25	C	1.476	3.192	-6.109
26	C	-0.717	3.379	-4.908
27	C	0.717	3.379	-4.908
28	C	-1.386	3.128	-3.688
29	C	-0.704	3.332	-2.453
30	C	-2.538	2.288	-1.215
31	C	-1.392	3.121	-1.215
32	C	-2.970	1.718	0.010
33	C	-2.538	2.288	1.235
34	C	-3.386	0.360	2.472
35	C	-2.951	1.699	2.472
36	C	-3.403	-0.352	3.707
37	C	-3.435	0.362	4.928
38	C	-3.070	-1.715	6.128
39	C	-3.492	-0.417	6.128
40	C	-2.580	2.390	-6.109
41	C	-1.476	3.192	-6.109
42	C	-2.992	1.726	-4.908
43	C	-2.547	2.285	-3.688
44	C	-3.386	0.360	-2.453
45	C	-2.951	1.699	-2.452
46	C	-3.399	-0.359	-1.215
47	C	-3.413	0.356	0.010
48	C	-2.961	-1.707	1.235
49	C	-3.398	-0.359	1.235
50	C	-2.528	-2.281	2.472
51	C	-2.960	-1.716	3.707
52	C	-1.406	-3.155	4.928
53	C	-2.566	-2.312	4.928
54	C	-0.682	-3.450	6.128
55	C	-3.492	-0.417	-6.109
56	C	-3.435	0.362	-4.908
57	C	-2.960	-1.716	-3.688
58	C	-3.403	-0.352	-3.688
59	C	-2.528	-2.281	-2.452
60	C	-2.961	-1.707	-1.215
61	C	-1.393	-3.136	0.010
62	C	-2.552	-2.294	0.010
63	C	-0.708	-3.343	1.235
64	C	-1.388	-3.109	2.472
65	C	0.717	-3.345	3.707
66	C	-0.717	-3.345	3.707
67	C	1.406	-3.155	4.928
68	C	0.682	-3.450	6.128
69	C	-3.070	-1.715	-6.109
70	C	-1.406	-3.155	-4.908
71	C	-2.566	-2.312	-4.908
72	C	-0.717	-3.346	-3.688
73	C	-1.388	-3.108	-2.453
74	C	0.708	-3.343	-1.215
75	C	-0.708	-3.343	-1.215
76	C	1.393	-3.136	0.010

77	C	0.708	-3.343	1.235
78	C	2.528	-2.281	2.472
79	C	1.388	-3.109	2.472
80	C	2.960	-1.716	3.707
81	C	2.566	-2.312	4.928
82	C	3.492	-0.417	6.128
83	C	3.070	-1.715	6.128
84	C	0.682	-3.450	-6.109
85	C	-0.682	-3.450	-6.109
86	C	1.406	-3.155	-4.908
87	C	0.717	-3.345	-3.688
88	C	2.528	-2.281	-2.453
89	C	1.388	-3.109	-2.453
90	C	2.961	-1.707	-1.215
91	C	2.552	-2.294	0.010
92	C	3.399	-0.359	1.235
93	C	2.961	-1.707	1.235
94	C	3.386	0.360	2.472
95	C	3.403	-0.352	3.707
96	C	2.992	1.726	4.928
97	C	3.436	0.362	4.928
98	C	2.580	2.390	6.128
99	C	3.070	-1.715	-6.109
100	C	2.566	-2.312	-4.908
101	C	3.403	-0.352	-3.688
102	C	2.960	-1.716	-3.688
103	C	3.386	0.360	-2.453
104	C	3.399	-0.359	-1.215
105	C	2.970	1.718	0.010
106	C	3.413	0.356	0.010
107	C	2.539	2.289	1.235
108	C	2.951	1.699	2.472
109	C	2.547	2.285	3.707
110	C	3.492	-0.417	-6.109
111	C	2.992	1.726	-4.908
112	C	3.436	0.362	-4.908
113	C	2.547	2.285	-3.688
114	C	2.951	1.699	-2.453
115	C	2.538	2.288	-1.215
116	C	2.580	2.390	-6.109
117	H	1.101	3.575	7.072
118	H	-1.101	3.575	7.072
119	H	-3.060	2.152	7.072
120	H	1.101	3.575	-7.052
121	H	-2.992	-2.246	7.072
122	H	-3.740	0.058	7.072
123	H	-3.060	2.152	-7.052
124	H	-1.101	3.575	-7.052
125	H	-1.211	-3.539	7.072
126	H	-3.740	0.058	-7.052
127	H	1.211	-3.539	7.072
128	H	-2.992	-2.246	-7.052
129	H	3.741	0.058	7.072
130	H	2.992	-2.246	7.072
131	H	1.211	-3.539	-7.052
132	H	-1.211	-3.539	-7.052
133	H	3.060	2.152	7.072
134	H	2.992	-2.246	-7.052
135	H	3.741	0.058	-7.052

		136	H	3.060	2.152	-7.052
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(5, 5) CNT_4	0.000147	1	O	-0.173	0.051	0.945
		2	H	0.560	0.668	1.276
		3	H	0.194	-0.830	1.290
		4	O	0.301	-0.083	-1.626
		5	H	0.084	-0.025	-0.618
		6	H	-0.618	0.162	-1.984
		7	C	1.476	3.192	6.128
		8	C	1.388	3.121	1.235
		9	C	0.706	3.331	2.471
		10	C	1.386	3.128	3.707
		11	C	-0.717	3.379	4.928
		12	C	0.717	3.379	4.928
		13	C	-1.476	3.192	6.128
		14	C	1.386	3.128	-3.688
		15	C	0.704	3.331	-2.453
		16	C	1.392	3.121	-1.215
		17	C	-0.716	3.356	0.010
		18	C	0.718	3.355	0.009
		19	C	-1.392	3.121	1.234
		20	C	-0.704	3.331	2.474
		21	C	-2.547	2.285	3.707
		22	C	-1.386	3.128	3.707
		23	C	-2.992	1.726	4.928
		24	C	-2.580	2.390	6.128
		25	C	1.476	3.192	-6.109
		26	C	-0.717	3.379	-4.908
		27	C	0.717	3.379	-4.908
		28	C	-1.386	3.128	-3.688
		29	C	-0.704	3.331	-2.453
		30	C	-2.538	2.288	-1.215
		31	C	-1.392	3.121	-1.215
		32	C	-2.970	1.718	0.010
		33	C	-2.538	2.288	1.235
		34	C	-3.386	0.360	2.472
		35	C	-2.951	1.699	2.472
		36	C	-3.403	-0.352	3.707
		37	C	-3.435	0.362	4.928
		38	C	-3.070	-1.715	6.128
		39	C	-3.492	-0.417	6.128
		40	C	-2.580	2.390	-6.109
		41	C	-1.476	3.192	-6.109
		42	C	-2.992	1.726	-4.908
		43	C	-2.547	2.285	-3.688
		44	C	-3.386	0.360	-2.453
		45	C	-2.951	1.699	-2.452
		46	C	-3.399	-0.359	-1.215
		47	C	-3.413	0.356	0.010
		48	C	-2.961	-1.707	1.235
		49	C	-3.398	-0.359	1.235
		50	C	-2.528	-2.281	2.472
		51	C	-2.960	-1.716	3.707
		52	C	-1.406	-3.155	4.928
		53	C	-2.566	-2.312	4.928
		54	C	-0.682	-3.450	6.128
		55	C	-3.492	-0.417	-6.109
		56	C	-3.435	0.362	-4.908
		57	C	-2.960	-1.716	-3.688

58	C	-3.403	-0.352	-3.688
59	C	-2.528	-2.281	-2.453
60	C	-2.961	-1.707	-1.215
61	C	-1.393	-3.136	0.010
62	C	-2.552	-2.294	0.010
63	C	-0.708	-3.343	1.235
64	C	-1.388	-3.109	2.472
65	C	0.717	-3.345	3.707
66	C	-0.717	-3.345	3.707
67	C	1.406	-3.155	4.928
68	C	0.682	-3.450	6.128
69	C	-3.070	-1.715	-6.109
70	C	-1.406	-3.155	-4.908
71	C	-2.566	-2.312	-4.908
72	C	-0.717	-3.346	-3.688
73	C	-1.388	-3.108	-2.452
74	C	0.708	-3.343	-1.215
75	C	-0.708	-3.343	-1.215
76	C	1.393	-3.136	0.010
77	C	0.708	-3.343	1.235
78	C	2.528	-2.281	2.472
79	C	1.388	-3.109	2.472
80	C	2.960	-1.716	3.707
81	C	2.566	-2.312	4.928
82	C	3.492	-0.417	6.128
83	C	3.070	-1.715	6.128
84	C	0.682	-3.450	-6.109
85	C	-0.682	-3.450	-6.109
86	C	1.406	-3.155	-4.908
87	C	0.717	-3.345	-3.688
88	C	2.528	-2.281	-2.453
89	C	1.388	-3.109	-2.453
90	C	2.961	-1.707	-1.215
91	C	2.552	-2.294	0.010
92	C	3.399	-0.359	1.235
93	C	2.961	-1.707	1.235
94	C	3.386	0.360	2.472
95	C	3.403	-0.352	3.707
96	C	2.992	1.726	4.928
97	C	3.436	0.362	4.928
98	C	2.580	2.390	6.128
99	C	3.070	-1.715	-6.109
100	C	2.566	-2.312	-4.908
101	C	3.403	-0.352	-3.688
102	C	2.960	-1.716	-3.688
103	C	3.386	0.360	-2.453
104	C	3.399	-0.359	-1.215
105	C	2.970	1.718	0.010
106	C	3.413	0.356	0.010
107	C	2.539	2.289	1.235
108	C	2.951	1.699	2.472
109	C	2.547	2.285	3.707
110	C	3.492	-0.417	-6.109
111	C	2.992	1.726	-4.908
112	C	3.436	0.362	-4.908
113	C	2.547	2.285	-3.688
114	C	2.951	1.699	-2.453
115	C	2.538	2.288	-1.215
116	C	2.580	2.390	-6.109

117	H	1.101	3.575	7.072
118	H	-1.101	3.575	7.072
119	H	-3.060	2.152	7.072
120	H	1.101	3.575	-7.052
121	H	-2.992	-2.246	7.072
122	H	-3.740	0.058	7.072
123	H	-3.060	2.152	-7.052
124	H	-1.101	3.575	-7.052
125	H	-1.211	-3.539	7.072
126	H	-3.740	0.058	-7.052
127	H	1.211	-3.539	7.072
128	H	-2.992	-2.246	-7.052
129	H	3.741	0.058	7.072
130	H	2.992	-2.246	7.072
131	H	1.211	-3.539	-7.052
132	H	-1.211	-3.539	-7.052
133	H	3.060	2.152	7.072
134	H	2.992	-2.246	-7.052
135	H	3.741	0.058	-7.052
136	H	3.060	2.152	-7.052

Table S12. The coordinates and energies of the sampled structures of confined water dimer in (6, 6) CNT. The first structure which is highlighted with underline was used in the paper.

Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$\underline{(H_2O)_2@(6, 6)\ CNT\_1}$	0.000000	1	O	0.803	-0.373	1.392
		2	H	0.913	0.639	1.411
		3	H	0.434	-0.455	0.430
		4	O	-0.143	-0.623	-1.040
		5	H	-1.066	-1.024	-0.910
		6	H	0.334	-1.450	-1.387
		7	C	1.484	3.937	6.118
		8	C	1.400	3.838	1.227
		9	C	0.703	4.014	2.462
		10	C	1.394	3.845	3.698
		11	C	-0.717	4.072	4.920
		12	C	0.717	4.072	4.920
		13	C	-1.484	3.937	6.118
		14	C	1.394	3.845	-3.698
		15	C	0.704	4.013	-2.462
		16	C	1.399	3.839	-1.226
		17	C	-0.713	4.034	0.000
		18	C	0.713	4.035	0.000
		19	C	-1.400	3.839	1.226
		20	C	-0.703	4.012	2.462
		21	C	-2.633	3.130	3.698
		22	C	-1.394	3.846	3.698
		23	C	-3.168	2.657	4.920
		24	C	-2.667	3.254	6.118
		25	C	1.484	3.937	-6.118
		26	C	-0.717	4.072	-4.920
		27	C	0.717	4.072	-4.920
		28	C	-1.394	3.845	-3.698
		29	C	-0.704	4.013	-2.462
		30	C	-2.625	3.131	-1.226
		31	C	-1.399	3.839	-1.226
		32	C	-3.137	2.635	0.000
		33	C	-2.625	3.132	1.226
		34	C	-3.828	1.397	2.462

35	C	-3.124	2.616	2.462
36	C	-4.027	0.715	3.698
37	C	-3.885	1.415	4.920
38	C	-4.151	-0.683	6.118
39	C	-4.151	0.683	6.118
40	C	-2.667	3.254	-6.118
41	C	-1.484	3.937	-6.118
42	C	-3.168	2.657	-4.920
43	C	-2.633	3.130	-3.698
44	C	-3.828	1.397	-2.462
45	C	-3.124	2.616	-2.462
46	C	-4.024	0.708	-1.226
47	C	-3.851	1.399	0.000
48	C	-4.024	-0.708	1.226
49	C	-4.024	0.708	1.226
50	C	-3.828	-1.397	2.462
51	C	-4.027	-0.715	3.698
52	C	-3.168	-2.657	4.920
53	C	-3.885	-1.415	4.920
54	C	-2.667	-3.254	6.118
55	C	-4.151	0.683	-6.118
56	C	-3.885	1.415	-4.920
57	C	-4.027	-0.715	-3.698
58	C	-4.027	0.715	-3.698
59	C	-3.828	-1.397	-2.462
60	C	-4.024	-0.708	-1.226
61	C	-3.137	-2.635	0.000
62	C	-3.851	-1.399	0.000
63	C	-2.625	-3.131	1.226
64	C	-3.124	-2.616	2.462
65	C	-1.394	-3.845	3.698
66	C	-2.633	-3.130	3.698
67	C	-0.717	-4.072	4.920
68	C	-1.484	-3.937	6.118
69	C	-4.151	-0.683	-6.118
70	C	-3.168	-2.657	-4.920
71	C	-3.885	-1.415	-4.920
72	C	-2.633	-3.130	-3.698
73	C	-3.124	-2.616	-2.462
74	C	-1.399	-3.839	-1.226
75	C	-2.625	-3.131	-1.226
76	C	-0.713	-4.034	0.000
77	C	-1.400	-3.840	1.226
78	C	0.704	-4.013	2.462
79	C	-0.704	-4.013	2.462
80	C	1.394	-3.845	3.698
81	C	0.717	-4.072	4.920
82	C	2.667	-3.254	6.118
83	C	1.484	-3.937	6.118
84	C	-1.484	-3.937	-6.118
85	C	-2.667	-3.254	-6.118
86	C	-0.717	-4.072	-4.920
87	C	-1.394	-3.845	-3.698
88	C	0.704	-4.013	-2.462
89	C	-0.704	-4.013	-2.462
90	C	1.399	-3.839	-1.226
91	C	0.714	-4.035	0.000
92	C	2.625	-3.131	1.226
93	C	1.399	-3.839	1.226

94	C	3.124	-2.616	2.462
95	C	2.633	-3.130	3.698
96	C	3.885	-1.415	4.920
97	C	3.168	-2.657	4.920
98	C	4.151	-0.683	6.118
99	C	1.484	-3.937	-6.118
100	C	0.717	-4.072	-4.920
101	C	2.633	-3.130	-3.698
102	C	1.394	-3.845	-3.698
103	C	3.124	-2.616	-2.462
104	C	2.625	-3.131	-1.226
105	C	3.851	-1.399	0.000
106	C	3.137	-2.635	0.000
107	C	4.024	-0.708	1.226
108	C	3.828	-1.397	2.462
109	C	4.027	0.715	3.698
110	C	4.027	-0.715	3.698
111	C	3.885	1.415	4.920
112	C	4.151	0.683	6.118
113	C	2.667	-3.254	-6.118
114	C	3.885	-1.415	-4.920
115	C	3.168	-2.657	-4.920
116	C	4.027	-0.715	-3.698
117	C	3.828	-1.397	-2.462
118	C	4.024	0.708	-1.226
119	C	4.024	-0.708	-1.226
120	C	3.851	1.399	0.000
121	C	4.024	0.708	1.226
122	C	3.124	2.616	2.462
123	C	3.828	1.397	2.462
124	C	2.633	3.130	3.698
125	C	3.168	2.657	4.920
126	C	2.667	3.254	6.118
127	C	4.151	0.683	-6.118
128	C	4.151	-0.683	-6.118
129	C	3.885	1.415	-4.920
130	C	4.027	0.715	-3.698
131	C	3.124	2.616	-2.462
132	C	3.828	1.397	-2.462
133	C	2.625	3.131	-1.226
134	C	3.137	2.635	0.000
135	C	2.625	3.131	1.226
136	C	2.667	3.254	-6.118
137	C	3.168	2.657	-4.920
138	C	2.633	3.130	-3.698
139	H	1.073	4.274	7.064
140	H	-1.073	4.274	7.064
141	H	-3.165	3.066	7.064
142	H	1.073	4.274	-7.064
143	H	-4.237	-1.208	7.064
144	H	-4.237	1.208	7.064
145	H	-3.165	3.066	-7.064
146	H	-1.073	4.274	-7.064
147	H	-3.165	-3.066	7.064
148	H	-4.237	1.208	-7.064
149	H	-1.073	-4.274	7.064
150	H	-4.237	-1.208	-7.064
151	H	3.165	-3.066	7.064
152	H	1.073	-4.274	7.064

		153	H	-1.073	-4.274	-7.064
		154	H	-3.165	-3.066	-7.064
		155	H	4.237	-1.208	7.064
		156	H	1.073	-4.274	-7.064
		157	H	4.237	1.208	7.064
		158	H	3.165	-3.066	-7.064
		159	H	3.165	3.066	7.064
		160	H	4.237	1.208	-7.064
		161	H	4.237	-1.208	-7.064
		162	H	3.165	3.066	-7.064
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(6, 6) CNT_2	0.000003	1	O	0.142	0.623	1.039
		2	H	-0.334	1.450	1.386
		3	H	1.066	1.023	0.910
		4	O	-0.803	0.372	-1.393
		5	H	-0.434	0.455	-0.431
		6	H	-0.913	-0.639	-1.412
		7	C	1.484	3.937	6.118
		8	C	1.401	3.838	1.227
		9	C	0.703	4.014	2.462
		10	C	1.394	3.845	3.698
		11	C	-0.717	4.072	4.920
		12	C	0.717	4.072	4.920
		13	C	-1.484	3.937	6.118
		14	C	1.394	3.845	-3.698
		15	C	0.704	4.013	-2.462
		16	C	1.399	3.839	-1.226
		17	C	-0.714	4.034	0.000
		18	C	0.713	4.035	0.000
		19	C	-1.399	3.839	1.227
		20	C	-0.703	4.012	2.462
		21	C	-2.633	3.130	3.698
		22	C	-1.394	3.846	3.698
		23	C	-3.168	2.657	4.920
		24	C	-2.667	3.254	6.118
		25	C	1.484	3.937	-6.118
		26	C	-0.717	4.072	-4.920
		27	C	0.717	4.072	-4.920
		28	C	-1.394	3.845	-3.698
		29	C	-0.704	4.013	-2.462
		30	C	-2.625	3.131	-1.226
		31	C	-1.399	3.839	-1.226
		32	C	-3.137	2.635	0.000
		33	C	-2.625	3.131	1.226
		34	C	-3.828	1.397	2.462
		35	C	-3.124	2.616	2.462
		36	C	-4.027	0.715	3.698
		37	C	-3.885	1.415	4.920
		38	C	-4.151	-0.683	6.118
		39	C	-4.151	0.683	6.118
		40	C	-2.667	3.254	-6.118
		41	C	-1.484	3.937	-6.118
		42	C	-3.168	2.657	-4.920
		43	C	-2.633	3.130	-3.698
		44	C	-3.828	1.397	-2.462
		45	C	-3.124	2.616	-2.462
		46	C	-4.024	0.708	-1.226
		47	C	-3.851	1.399	0.000
		48	C	-4.024	-0.708	1.226

49	C	-4.024	0.708	1.226
50	C	-3.828	-1.397	2.462
51	C	-4.027	-0.715	3.698
52	C	-3.168	-2.657	4.920
53	C	-3.885	-1.415	4.920
54	C	-2.667	-3.254	6.118
55	C	-4.151	0.683	-6.118
56	C	-3.885	1.415	-4.920
57	C	-4.027	-0.715	-3.698
58	C	-4.027	0.715	-3.698
59	C	-3.828	-1.397	-2.462
60	C	-4.024	-0.708	-1.226
61	C	-3.137	-2.635	0.000
62	C	-3.851	-1.399	0.000
63	C	-2.625	-3.131	1.226
64	C	-3.124	-2.616	2.462
65	C	-1.394	-3.845	3.698
66	C	-2.633	-3.130	3.698
67	C	-0.717	-4.072	4.920
68	C	-1.484	-3.937	6.118
69	C	-4.151	-0.683	-6.118
70	C	-3.168	-2.657	-4.920
71	C	-3.885	-1.415	-4.920
72	C	-2.633	-3.130	-3.698
73	C	-3.124	-2.616	-2.462
74	C	-1.399	-3.839	-1.226
75	C	-2.625	-3.132	-1.226
76	C	-0.713	-4.034	0.000
77	C	-1.400	-3.840	1.226
78	C	0.704	-4.013	2.462
79	C	-0.704	-4.013	2.462
80	C	1.394	-3.845	3.698
81	C	0.717	-4.072	4.920
82	C	2.667	-3.254	6.118
83	C	1.484	-3.937	6.118
84	C	-1.484	-3.937	-6.118
85	C	-2.667	-3.254	-6.118
86	C	-0.717	-4.072	-4.920
87	C	-1.394	-3.845	-3.698
88	C	0.704	-4.013	-2.462
89	C	-0.704	-4.013	-2.462
90	C	1.399	-3.839	-1.226
91	C	0.713	-4.035	0.000
92	C	2.625	-3.131	1.226
93	C	1.399	-3.839	1.226
94	C	3.124	-2.616	2.462
95	C	2.633	-3.130	3.698
96	C	3.885	-1.415	4.920
97	C	3.168	-2.657	4.920
98	C	4.151	-0.683	6.118
99	C	1.484	-3.937	-6.118
100	C	0.717	-4.072	-4.920
101	C	2.633	-3.130	-3.698
102	C	1.394	-3.845	-3.698
103	C	3.124	-2.616	-2.462
104	C	2.625	-3.131	-1.226
105	C	3.851	-1.399	0.000
106	C	3.137	-2.635	0.000
107	C	4.024	-0.708	1.226

		108	C	3.828	-1.397	2.462
		109	C	4.027	0.715	3.698
		110	C	4.027	-0.715	3.698
		111	C	3.885	1.415	4.920
		112	C	4.151	0.683	6.118
		113	C	2.667	-3.254	-6.118
		114	C	3.885	-1.415	-4.920
		115	C	3.168	-2.657	-4.920
		116	C	4.027	-0.715	-3.698
		117	C	3.828	-1.397	-2.462
		118	C	4.024	0.708	-1.226
		119	C	4.024	-0.708	-1.226
		120	C	3.851	1.399	0.000
		121	C	4.024	0.708	1.226
		122	C	3.124	2.616	2.463
		123	C	3.828	1.397	2.462
		124	C	2.633	3.130	3.698
		125	C	3.168	2.657	4.920
		126	C	2.667	3.254	6.118
		127	C	4.151	0.683	-6.118
		128	C	4.151	-0.683	-6.118
		129	C	3.885	1.415	-4.920
		130	C	4.027	0.715	-3.698
		131	C	3.124	2.616	-2.462
		132	C	3.828	1.397	-2.462
		133	C	2.625	3.131	-1.226
		134	C	3.137	2.635	0.000
		135	C	2.625	3.132	1.226
		136	C	2.667	3.254	-6.118
		137	C	3.168	2.657	-4.920
		138	C	2.633	3.130	-3.698
		139	H	1.073	4.274	7.064
		140	H	-1.073	4.274	7.064
		141	H	-3.165	3.066	7.064
		142	H	1.073	4.274	-7.064
		143	H	-4.237	-1.208	7.064
		144	H	-4.237	1.208	7.064
		145	H	-3.165	3.066	-7.064
		146	H	-1.073	4.274	-7.064
		147	H	-3.165	-3.066	7.064
		148	H	-4.237	1.208	-7.064
		149	H	-1.073	-4.274	7.064
		150	H	-4.237	-1.208	-7.064
		151	H	3.165	-3.066	7.064
		152	H	1.073	-4.274	7.064
		153	H	-1.073	-4.274	-7.064
		154	H	-3.165	-3.066	-7.064
		155	H	4.237	-1.208	7.064
		156	H	1.073	-4.274	-7.064
		157	H	4.237	1.208	7.064
		158	H	3.165	-3.066	-7.064
		159	H	3.165	3.066	7.064
		160	H	4.237	1.208	-7.064
		161	H	4.237	-1.208	-7.064
		162	H	3.165	3.066	-7.064
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(6, 6) CNT_3	0.000030	1	O	0.720	-0.465	1.115
		2	H	1.003	0.513	1.134
		3	H	0.310	-0.473	0.167

4	O	-0.354	-0.503	-1.278
5	H	-1.351	-0.586	-1.109
6	H	-0.176	-1.445	-1.609
7	C	1.484	3.946	6.118
8	C	1.399	3.849	1.226
9	C	0.704	4.023	2.463
10	C	1.394	3.855	3.698
11	C	-0.717	4.081	4.920
12	C	0.718	4.081	4.920
13	C	-1.484	3.946	6.118
14	C	1.394	3.855	-3.698
15	C	0.704	4.023	-2.462
16	C	1.399	3.848	-1.226
17	C	-0.713	4.044	0.000
18	C	0.714	4.044	0.000
19	C	-1.399	3.849	1.226
20	C	-0.704	4.023	2.462
21	C	-2.633	3.139	3.698
22	C	-1.394	3.855	3.698
23	C	-3.168	2.667	4.920
24	C	-2.667	3.263	6.118
25	C	1.484	3.946	-6.118
26	C	-0.717	4.081	-4.920
27	C	0.718	4.081	-4.920
28	C	-1.394	3.855	-3.698
29	C	-0.704	4.023	-2.462
30	C	-2.625	3.141	-1.226
31	C	-1.399	3.849	-1.226
32	C	-3.137	2.645	0.000
33	C	-2.625	3.141	1.226
34	C	-3.828	1.407	2.462
35	C	-3.124	2.626	2.462
36	C	-4.027	0.725	3.698
37	C	-3.885	1.424	4.920
38	C	-4.151	-0.673	6.118
39	C	-4.151	0.692	6.118
40	C	-2.667	3.263	-6.118
41	C	-1.484	3.946	-6.118
42	C	-3.168	2.667	-4.920
43	C	-2.633	3.139	-3.698
44	C	-3.828	1.406	-2.463
45	C	-3.124	2.626	-2.462
46	C	-4.025	0.718	-1.226
47	C	-3.851	1.409	0.000
48	C	-4.024	-0.698	1.226
49	C	-4.024	0.717	1.226
50	C	-3.828	-1.388	2.462
51	C	-4.027	-0.706	3.698
52	C	-3.168	-2.648	4.920
53	C	-3.885	-1.405	4.920
54	C	-2.667	-3.244	6.118
55	C	-4.151	0.692	-6.118
56	C	-3.885	1.424	-4.920
57	C	-4.027	-0.706	-3.698
58	C	-4.027	0.725	-3.698
59	C	-3.828	-1.388	-2.462
60	C	-4.024	-0.698	-1.226
61	C	-3.137	-2.626	0.000
62	C	-3.851	-1.390	0.000

63	C	-2.625	-3.122	1.226
64	C	-3.124	-2.607	2.462
65	C	-1.394	-3.836	3.698
66	C	-2.633	-3.120	3.698
67	C	-0.717	-4.062	4.920
68	C	-1.484	-3.927	6.118
69	C	-4.151	-0.673	-6.118
70	C	-3.168	-2.648	-4.920
71	C	-3.885	-1.405	-4.920
72	C	-2.633	-3.120	-3.698
73	C	-3.124	-2.607	-2.462
74	C	-1.399	-3.829	-1.226
75	C	-2.625	-3.122	-1.226
76	C	-0.713	-4.025	0.000
77	C	-1.399	-3.829	1.226
78	C	0.704	-4.004	2.462
79	C	-0.704	-4.004	2.462
80	C	1.394	-3.836	3.698
81	C	0.718	-4.062	4.920
82	C	2.667	-3.244	6.118
83	C	1.484	-3.927	6.118
84	C	-1.484	-3.927	-6.118
85	C	-2.667	-3.244	-6.118
86	C	-0.717	-4.062	-4.920
87	C	-1.394	-3.836	-3.698
88	C	0.704	-4.004	-2.462
89	C	-0.704	-4.004	-2.462
90	C	1.399	-3.829	-1.226
91	C	0.714	-4.025	0.000
92	C	2.625	-3.122	1.226
93	C	1.399	-3.829	1.226
94	C	3.124	-2.607	2.462
95	C	2.633	-3.120	3.698
96	C	3.885	-1.405	4.920
97	C	3.168	-2.648	4.920
98	C	4.151	-0.673	6.118
99	C	1.484	-3.927	-6.118
100	C	0.718	-4.062	-4.920
101	C	2.633	-3.120	-3.698
102	C	1.394	-3.836	-3.698
103	C	3.124	-2.607	-2.462
104	C	2.625	-3.122	-1.226
105	C	3.851	-1.390	0.000
106	C	3.137	-2.626	0.000
107	C	4.024	-0.698	1.226
108	C	3.828	-1.388	2.462
109	C	4.027	0.725	3.698
110	C	4.027	-0.706	3.698
111	C	3.885	1.424	4.920
112	C	4.151	0.692	6.118
113	C	2.667	-3.244	-6.118
114	C	3.885	-1.405	-4.920
115	C	3.168	-2.648	-4.920
116	C	4.027	-0.706	-3.698
117	C	3.828	-1.388	-2.462
118	C	4.024	0.717	-1.226
119	C	4.024	-0.698	-1.226
120	C	3.851	1.409	0.000
121	C	4.024	0.717	1.226

		122	C	3.124	2.626	2.462
		123	C	3.828	1.407	2.462
		124	C	2.633	3.139	3.698
		125	C	3.168	2.667	4.920
		126	C	2.667	3.263	6.118
		127	C	4.151	0.692	-6.118
		128	C	4.151	-0.673	-6.118
		129	C	3.885	1.424	-4.920
		130	C	4.027	0.725	-3.698
		131	C	3.124	2.626	-2.462
		132	C	3.828	1.407	-2.462
		133	C	2.625	3.141	-1.226
		134	C	3.137	2.645	0.000
		135	C	2.625	3.140	1.227
		136	C	2.667	3.263	-6.118
		137	C	3.168	2.667	-4.920
		138	C	2.633	3.139	-3.698
		139	H	1.073	4.283	7.064
		140	H	-1.073	4.283	7.064
		141	H	-3.165	3.075	7.064
		142	H	1.073	4.283	-7.064
		143	H	-4.237	-1.198	7.064
		144	H	-4.237	1.217	7.064
		145	H	-3.165	3.075	-7.064
		146	H	-1.073	4.283	-7.064
		147	H	-3.165	-3.056	7.064
		148	H	-4.237	1.217	-7.064
		149	H	-1.073	-4.264	7.064
		150	H	-4.237	-1.198	-7.064
		151	H	3.165	-3.056	7.064
		152	H	1.073	-4.264	7.064
		153	H	-1.073	-4.264	-7.064
		154	H	-3.165	-3.056	-7.064
		155	H	4.237	-1.198	7.064
		156	H	1.073	-4.264	-7.064
		157	H	4.237	1.217	7.064
		158	H	3.165	-3.056	-7.064
		159	H	3.165	3.075	7.064
		160	H	4.237	1.217	-7.064
		161	H	4.237	-1.198	-7.064
		162	H	3.165	3.075	-7.064
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(6, 6) CNT_4	0.000085	1	O	0.448	-0.447	1.346
		2	H	0.432	-1.386	1.732
		3	H	1.454	-0.311	1.321
		4	O	-0.198	-0.831	-1.165
		5	H	0.047	-0.662	-0.176
		6	H	-0.990	-0.195	-1.222
		7	C	1.484	3.946	6.118
		8	C	1.399	3.849	1.226
		9	C	0.704	4.023	2.463
		10	C	1.394	3.855	3.698
		11	C	-0.717	4.081	4.920
		12	C	0.718	4.081	4.920
		13	C	-1.484	3.946	6.118
		14	C	1.394	3.855	-3.698
		15	C	0.704	4.023	-2.462
		16	C	1.399	3.848	-1.226
		17	C	-0.713	4.044	0.000

18	C	0.714	4.044	0.000
19	C	-1.399	3.849	1.226
20	C	-0.704	4.023	2.462
21	C	-2.633	3.139	3.698
22	C	-1.394	3.855	3.698
23	C	-3.168	2.667	4.920
24	C	-2.667	3.263	6.118
25	C	1.484	3.946	-6.118
26	C	-0.717	4.081	-4.920
27	C	0.718	4.081	-4.920
28	C	-1.394	3.855	-3.698
29	C	-0.704	4.023	-2.462
30	C	-2.625	3.141	-1.226
31	C	-1.399	3.849	-1.226
32	C	-3.137	2.645	0.000
33	C	-2.625	3.141	1.226
34	C	-3.828	1.407	2.462
35	C	-3.124	2.626	2.462
36	C	-4.027	0.725	3.698
37	C	-3.885	1.424	4.920
38	C	-4.151	-0.673	6.118
39	C	-4.151	0.692	6.118
40	C	-2.667	3.263	-6.118
41	C	-1.484	3.946	-6.118
42	C	-3.168	2.667	-4.920
43	C	-2.633	3.139	-3.698
44	C	-3.828	1.406	-2.463
45	C	-3.124	2.626	-2.462
46	C	-4.024	0.718	-1.226
47	C	-3.851	1.409	0.000
48	C	-4.024	-0.698	1.226
49	C	-4.024	0.717	1.226
50	C	-3.828	-1.388	2.462
51	C	-4.027	-0.706	3.698
52	C	-3.168	-2.648	4.920
53	C	-3.885	-1.405	4.920
54	C	-2.667	-3.244	6.118
55	C	-4.151	0.692	-6.118
56	C	-3.885	1.424	-4.920
57	C	-4.027	-0.706	-3.698
58	C	-4.027	0.725	-3.698
59	C	-3.828	-1.388	-2.462
60	C	-4.024	-0.698	-1.226
61	C	-3.137	-2.626	0.000
62	C	-3.851	-1.390	0.000
63	C	-2.625	-3.122	1.226
64	C	-3.124	-2.607	2.462
65	C	-1.394	-3.836	3.698
66	C	-2.633	-3.120	3.698
67	C	-0.717	-4.062	4.920
68	C	-1.484	-3.927	6.118
69	C	-4.151	-0.673	-6.118
70	C	-3.168	-2.648	-4.920
71	C	-3.885	-1.405	-4.920
72	C	-2.633	-3.120	-3.698
73	C	-3.124	-2.607	-2.462
74	C	-1.399	-3.829	-1.226
75	C	-2.625	-3.122	-1.226
76	C	-0.713	-4.025	0.000

77	C	-1.399	-3.829	1.226
78	C	0.704	-4.004	2.463
79	C	-0.704	-4.004	2.462
80	C	1.394	-3.836	3.698
81	C	0.718	-4.062	4.920
82	C	2.667	-3.244	6.118
83	C	1.484	-3.927	6.118
84	C	-1.484	-3.927	-6.118
85	C	-2.667	-3.244	-6.118
86	C	-0.717	-4.062	-4.920
87	C	-1.394	-3.836	-3.698
88	C	0.704	-4.004	-2.462
89	C	-0.704	-4.004	-2.462
90	C	1.399	-3.830	-1.226
91	C	0.713	-4.025	0.000
92	C	2.625	-3.122	1.226
93	C	1.399	-3.829	1.226
94	C	3.124	-2.607	2.462
95	C	2.633	-3.120	3.698
96	C	3.885	-1.405	4.920
97	C	3.168	-2.648	4.920
98	C	4.151	-0.673	6.118
99	C	1.484	-3.927	-6.118
100	C	0.718	-4.062	-4.920
101	C	2.633	-3.120	-3.698
102	C	1.394	-3.836	-3.698
103	C	3.124	-2.607	-2.462
104	C	2.625	-3.122	-1.226
105	C	3.851	-1.390	0.000
106	C	3.137	-2.626	0.000
107	C	4.024	-0.698	1.226
108	C	3.828	-1.388	2.462
109	C	4.027	0.725	3.698
110	C	4.027	-0.706	3.698
111	C	3.885	1.424	4.920
112	C	4.151	0.692	6.118
113	C	2.667	-3.244	-6.118
114	C	3.885	-1.405	-4.920
115	C	3.168	-2.648	-4.920
116	C	4.027	-0.706	-3.698
117	C	3.828	-1.388	-2.462
118	C	4.024	0.717	-1.226
119	C	4.024	-0.698	-1.226
120	C	3.851	1.409	0.000
121	C	4.024	0.717	1.226
122	C	3.124	2.626	2.462
123	C	3.828	1.407	2.462
124	C	2.633	3.139	3.698
125	C	3.168	2.667	4.920
126	C	2.667	3.263	6.118
127	C	4.151	0.692	-6.118
128	C	4.151	-0.673	-6.118
129	C	3.885	1.424	-4.920
130	C	4.027	0.725	-3.698
131	C	3.124	2.626	-2.462
132	C	3.828	1.407	-2.462
133	C	2.625	3.141	-1.226
134	C	3.137	2.645	0.000
135	C	2.625	3.140	1.227

136	C	2.667	3.263	-6.118
137	C	3.168	2.667	-4.920
138	C	2.633	3.139	-3.698
139	H	1.073	4.283	7.064
140	H	-1.073	4.283	7.064
141	H	-3.165	3.075	7.064
142	H	1.073	4.283	-7.064
143	H	-4.237	-1.198	7.064
144	H	-4.237	1.217	7.064
145	H	-3.165	3.075	-7.064
146	H	-1.073	4.283	-7.064
147	H	-3.165	-3.056	7.064
148	H	-4.237	1.217	-7.064
149	H	-1.073	-4.264	7.064
150	H	-4.237	-1.198	-7.064
151	H	3.165	-3.056	7.064
152	H	1.073	-4.264	7.064
153	H	-1.073	-4.264	-7.064
154	H	-3.165	-3.056	-7.064
155	H	4.237	-1.198	7.064
156	H	1.073	-4.264	-7.064
157	H	4.237	1.217	7.064
158	H	3.165	-3.056	-7.064
159	H	3.165	3.075	7.064
160	H	4.237	1.217	-7.064
161	H	4.237	-1.198	-7.064
162	H	3.165	3.075	-7.064

Table S13. The coordinates and energies of the sampled structures of confined water dimer in (7, 7) CNT. The first structure which is highlighted with underline was used in the paper.

Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$\underline{(H_2O)_2}$@(7, 7) CNT_1	0.000000	1	O	0.972	1.023	0.813
		2	H	1.850	1.195	1.292
		3	H	0.816	1.956	0.445
		4	O	1.691	-0.411	-1.259
		5	H	1.393	0.149	-0.444
		6	H	1.059	-1.197	-1.126
		7	C	0.599	-4.856	6.115
		8	C	0.625	-4.711	1.225
		9	C	1.322	-4.550	2.461
		10	C	0.632	-4.717	3.697
		11	C	2.639	-4.011	4.919
		12	C	1.338	-4.619	4.919
		13	C	3.296	-3.597	6.115
		14	C	0.632	-4.717	-3.700
		15	C	1.322	-4.550	-2.464
		16	C	0.625	-4.711	-1.229
		17	C	2.613	-3.967	-0.002
		18	C	1.322	-4.570	-0.002
		19	C	3.168	-3.523	1.226
		20	C	2.597	-3.955	2.461
		21	C	4.073	-2.427	3.697
		22	C	3.169	-3.533	3.697
		23	C	4.436	-1.813	4.919
		24	C	4.161	-2.538	6.115
		25	C	0.599	-4.856	-6.118
		26	C	2.639	-4.011	-4.923
		27	C	1.338	-4.619	-4.923

28	C	3.169	-3.533	-3.700
29	C	2.597	-3.955	-2.464
30	C	4.063	-2.428	-1.229
31	C	3.168	-3.523	-1.229
32	C	4.388	-1.795	-0.002
33	C	4.063	-2.428	1.225
34	C	4.702	-0.414	2.461
35	C	4.372	-1.783	2.461
36	C	4.728	0.295	3.697
37	C	4.772	-0.417	4.919
38	C	4.569	1.691	6.115
39	C	4.857	0.355	6.115
40	C	4.161	-2.538	-6.118
41	C	3.296	-3.597	-6.118
42	C	4.436	-1.813	-4.923
43	C	4.073	-2.427	-3.700
44	C	4.702	-0.414	-2.464
45	C	4.372	-1.783	-2.464
46	C	4.720	0.301	-1.229
47	C	4.721	-0.410	-0.002
48	C	4.422	1.684	1.225
49	C	4.720	0.301	1.225
50	C	4.110	2.328	2.461
51	C	4.427	1.692	3.697
52	C	3.292	3.492	4.919
53	C	4.173	2.359	4.919
54	C	2.742	4.040	6.115
55	C	4.857	0.355	-6.118
56	C	4.772	-0.417	-4.923
57	C	4.427	1.692	-3.700
58	C	4.728	0.295	-3.700
59	C	4.110	2.328	-2.464
60	C	4.422	1.684	-1.229
61	C	3.255	3.456	-0.002
62	C	4.130	2.332	-0.002
63	C	2.698	3.899	1.225
64	C	3.246	3.438	2.461
65	C	1.428	4.537	3.697
66	C	2.708	3.901	3.697
67	C	0.748	4.754	4.919
68	C	1.517	4.647	6.115
69	C	4.569	1.691	-6.118
70	C	3.292	3.492	-4.923
71	C	4.173	2.359	-4.923
72	C	2.708	3.901	-3.700
73	C	3.246	3.438	-2.464
74	C	1.431	4.528	-1.229
75	C	2.698	3.899	-1.229
76	C	0.742	4.703	-0.002
77	C	1.431	4.528	1.225
78	C	-0.674	4.702	2.461
79	C	0.733	4.685	2.461
80	C	-1.372	4.570	3.697
81	C	-0.687	4.771	4.919
82	C	-2.697	4.104	6.115
83	C	-1.458	4.683	6.115
84	C	1.517	4.647	-6.118
85	C	2.742	4.040	-6.118
86	C	0.748	4.754	-4.923

87	C	1.428	4.537	-3.700
88	C	-0.674	4.702	-2.464
89	C	0.733	4.685	-2.464
90	C	-1.375	4.561	-1.229
91	C	-0.682	4.720	-0.002
92	C	-2.657	3.963	1.225
93	C	-1.375	4.561	1.225
94	C	-3.216	3.515	2.461
95	C	-2.666	3.965	3.697
96	C	-4.168	2.458	4.919
97	C	-3.260	3.570	4.919
98	C	-4.580	1.800	6.115
99	C	-1.458	4.683	-6.118
100	C	-0.687	4.771	-4.923
101	C	-2.666	3.965	-3.700
102	C	-1.372	4.570	-3.700
103	C	-3.216	3.515	-2.464
104	C	-2.657	3.963	-1.229
105	C	-4.125	2.430	-0.002
106	C	-3.224	3.533	-0.002
107	C	-4.433	1.789	1.225
108	C	-4.106	2.426	2.461
109	C	-4.772	0.409	3.697
110	C	-4.438	1.798	3.697
111	C	-4.833	-0.302	4.919
112	C	-4.900	0.471	6.115
113	C	-2.697	4.104	-6.118
114	C	-4.168	2.458	-4.923
115	C	-3.260	3.570	-4.923
116	C	-4.438	1.798	-3.700
117	C	-4.106	2.426	-2.464
118	C	-4.764	0.414	-1.229
119	C	-4.433	1.789	-1.229
120	C	-4.782	-0.297	-0.002
121	C	-4.764	0.414	1.225
122	C	-4.466	-1.677	2.461
123	C	-4.763	-0.302	2.461
124	C	-4.182	-2.328	3.697
125	C	-4.530	-1.706	4.919
126	C	-3.433	-3.517	6.115
127	C	-4.273	-2.438	6.115
128	C	-4.900	0.471	-6.118
129	C	-4.580	1.800	-6.118
130	C	-4.833	-0.302	-4.923
131	C	-4.772	0.409	-3.700
132	C	-4.466	-1.677	-2.464
133	C	-4.763	-0.302	-2.464
134	C	-4.172	-2.330	-1.229
135	C	-4.482	-1.689	-0.002
136	C	-3.304	-3.446	1.225
137	C	-4.172	-2.330	1.225
138	C	-2.743	-3.891	2.461
139	C	-3.304	-3.456	3.697
140	C	-1.501	-4.585	4.919
141	C	-2.787	-3.947	4.919
142	C	-0.767	-4.840	6.115
143	C	-4.273	-2.438	-6.118
144	C	-4.530	-1.706	-4.923
145	C	-3.304	-3.456	-3.700

		146	C	-4.182	-2.328	-3.700
		147	C	-2.743	-3.891	-2.464
		148	C	-3.304	-3.446	-1.229
		149	C	-1.483	-4.537	-0.002
		150	C	-2.759	-3.903	-0.002
		151	C	-0.789	-4.694	1.225
		152	C	-1.483	-4.517	2.461
		153	C	-0.797	-4.701	3.697
		154	C	-3.433	-3.517	-6.118
		155	C	-1.501	-4.585	-4.923
		156	C	-2.787	-3.947	-4.923
		157	C	-0.797	-4.701	-3.700
		158	C	-1.483	-4.517	-2.464
		159	C	-0.789	-4.694	-1.229
		160	C	-0.767	-4.840	-6.118
		161	H	1.120	-4.948	7.063
		162	H	3.032	-4.055	7.063
		163	H	4.557	-2.188	7.063
		164	H	1.120	-4.948	-7.066
		165	H	4.543	2.219	7.063
		166	H	5.051	-0.138	7.063
		167	H	4.557	-2.188	-7.066
		168	H	3.032	-4.055	-7.066
		169	H	3.247	3.884	7.063
		170	H	5.051	-0.138	-7.066
		171	H	1.088	4.956	7.063
		172	H	4.543	2.219	-7.066
		173	H	-3.206	3.961	7.063
		174	H	-1.022	4.981	7.063
		175	H	1.088	4.956	-7.066
		176	H	3.247	3.884	-7.066
		177	H	-4.541	2.328	7.063
		178	H	-1.022	4.981	-7.066
		179	H	-5.105	-0.016	7.063
		180	H	-3.206	3.961	-7.066
		181	H	-3.180	-3.981	7.063
		182	H	-4.660	-2.078	7.063
		183	H	-5.105	-0.016	-7.066
		184	H	-4.541	2.328	-7.066
		185	H	-1.290	-4.919	7.063
		186	H	-4.660	-2.078	-7.066
		187	H	-3.180	-3.981	-7.066
		188	H	-1.290	-4.919	-7.066
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(7, 7) CNT_2	0.000003	1	O	1.353	1.100	1.263
		2	H	0.450	1.549	1.126
		3	H	1.321	0.467	0.447
		4	O	1.312	-0.500	-0.812
		5	H	1.563	-1.413	-0.446
		6	H	2.183	-0.284	-1.287
		7	C	0.599	-4.856	6.115
		8	C	0.625	-4.711	1.225
		9	C	1.322	-4.550	2.461
		10	C	0.632	-4.717	3.697
		11	C	2.639	-4.011	4.919
		12	C	1.338	-4.619	4.919
		13	C	3.296	-3.597	6.115
		14	C	0.632	-4.717	-3.700
		15	C	1.322	-4.550	-2.464

16	C	0.625	-4.711	-1.229
17	C	2.613	-3.968	-0.002
18	C	1.322	-4.570	-0.002
19	C	3.168	-3.523	1.225
20	C	2.597	-3.955	2.461
21	C	4.073	-2.427	3.697
22	C	3.169	-3.533	3.697
23	C	4.436	-1.813	4.919
24	C	4.161	-2.538	6.115
25	C	0.599	-4.856	-6.118
26	C	2.639	-4.011	-4.923
27	C	1.338	-4.619	-4.923
28	C	3.169	-3.533	-3.700
29	C	2.597	-3.955	-2.464
30	C	4.063	-2.428	-1.229
31	C	3.168	-3.523	-1.229
32	C	4.388	-1.795	-0.002
33	C	4.063	-2.428	1.225
34	C	4.702	-0.414	2.461
35	C	4.372	-1.783	2.461
36	C	4.728	0.295	3.697
37	C	4.772	-0.417	4.919
38	C	4.569	1.691	6.115
39	C	4.857	0.355	6.115
40	C	4.161	-2.538	-6.118
41	C	3.296	-3.597	-6.118
42	C	4.436	-1.813	-4.923
43	C	4.073	-2.427	-3.700
44	C	4.702	-0.414	-2.464
45	C	4.372	-1.783	-2.464
46	C	4.720	0.301	-1.229
47	C	4.721	-0.410	-0.002
48	C	4.422	1.684	1.225
49	C	4.720	0.301	1.225
50	C	4.110	2.328	2.461
51	C	4.427	1.692	3.697
52	C	3.292	3.492	4.919
53	C	4.173	2.359	4.919
54	C	2.742	4.040	6.115
55	C	4.857	0.355	-6.118
56	C	4.772	-0.417	-4.923
57	C	4.427	1.692	-3.700
58	C	4.728	0.295	-3.700
59	C	4.110	2.328	-2.464
60	C	4.422	1.684	-1.229
61	C	3.255	3.456	-0.002
62	C	4.130	2.332	-0.002
63	C	2.698	3.899	1.225
64	C	3.246	3.438	2.461
65	C	1.428	4.537	3.697
66	C	2.708	3.901	3.697
67	C	0.748	4.754	4.919
68	C	1.517	4.647	6.115
69	C	4.569	1.691	-6.118
70	C	3.292	3.492	-4.923
71	C	4.173	2.359	-4.923
72	C	2.708	3.901	-3.700
73	C	3.246	3.438	-2.464
74	C	1.431	4.528	-1.229

75	C	2.698	3.899	-1.229
76	C	0.742	4.703	-0.002
77	C	1.431	4.528	1.225
78	C	-0.674	4.702	2.461
79	C	0.733	4.685	2.461
80	C	-1.372	4.570	3.697
81	C	-0.687	4.771	4.919
82	C	-2.697	4.104	6.115
83	C	-1.458	4.683	6.115
84	C	1.517	4.647	-6.118
85	C	2.742	4.040	-6.118
86	C	0.748	4.754	-4.923
87	C	1.428	4.537	-3.700
88	C	-0.674	4.702	-2.464
89	C	0.733	4.685	-2.464
90	C	-1.375	4.561	-1.229
91	C	-0.682	4.720	-0.002
92	C	-2.657	3.963	1.225
93	C	-1.375	4.561	1.225
94	C	-3.216	3.515	2.461
95	C	-2.666	3.965	3.697
96	C	-4.168	2.458	4.919
97	C	-3.260	3.570	4.919
98	C	-4.580	1.800	6.115
99	C	-1.458	4.683	-6.118
100	C	-0.687	4.771	-4.923
101	C	-2.666	3.965	-3.700
102	C	-1.372	4.570	-3.700
103	C	-3.216	3.515	-2.464
104	C	-2.657	3.963	-1.229
105	C	-4.125	2.430	-0.002
106	C	-3.224	3.533	-0.002
107	C	-4.433	1.789	1.225
108	C	-4.106	2.426	2.461
109	C	-4.772	0.409	3.697
110	C	-4.438	1.798	3.697
111	C	-4.833	-0.302	4.919
112	C	-4.900	0.471	6.115
113	C	-2.697	4.104	-6.118
114	C	-4.168	2.458	-4.923
115	C	-3.260	3.570	-4.923
116	C	-4.438	1.798	-3.700
117	C	-4.106	2.426	-2.464
118	C	-4.764	0.414	-1.229
119	C	-4.433	1.789	-1.229
120	C	-4.782	-0.297	-0.002
121	C	-4.764	0.414	1.225
122	C	-4.466	-1.677	2.461
123	C	-4.763	-0.302	2.461
124	C	-4.182	-2.328	3.697
125	C	-4.530	-1.706	4.919
126	C	-3.433	-3.517	6.115
127	C	-4.273	-2.438	6.115
128	C	-4.900	0.471	-6.118
129	C	-4.580	1.800	-6.118
130	C	-4.833	-0.302	-4.923
131	C	-4.772	0.409	-3.700
132	C	-4.466	-1.677	-2.464
133	C	-4.763	-0.302	-2.464

		134	C	-4.172	-2.330	-1.229
		135	C	-4.482	-1.689	-0.002
		136	C	-3.304	-3.446	1.225
		137	C	-4.172	-2.330	1.225
		138	C	-2.743	-3.891	2.461
		139	C	-3.304	-3.456	3.697
		140	C	-1.501	-4.585	4.919
		141	C	-2.787	-3.947	4.919
		142	C	-0.767	-4.840	6.115
		143	C	-4.273	-2.438	-6.118
		144	C	-4.530	-1.706	-4.923
		145	C	-3.304	-3.456	-3.700
		146	C	-4.182	-2.328	-3.700
		147	C	-2.743	-3.891	-2.464
		148	C	-3.304	-3.446	-1.229
		149	C	-1.483	-4.537	-0.002
		150	C	-2.759	-3.903	-0.002
		151	C	-0.789	-4.694	1.225
		152	C	-1.483	-4.517	2.461
		153	C	-0.797	-4.701	3.697
		154	C	-3.433	-3.517	-6.118
		155	C	-1.501	-4.585	-4.923
		156	C	-2.787	-3.947	-4.923
		157	C	-0.797	-4.701	-3.700
		158	C	-1.483	-4.517	-2.464
		159	C	-0.789	-4.694	-1.229
		160	C	-0.767	-4.840	-6.118
		161	H	1.120	-4.948	7.063
		162	H	3.032	-4.055	7.063
		163	H	4.557	-2.188	7.063
		164	H	1.120	-4.948	-7.066
		165	H	4.543	2.219	7.063
		166	H	5.051	-0.138	7.063
		167	H	4.557	-2.188	-7.066
		168	H	3.032	-4.055	-7.066
		169	H	3.247	3.884	7.063
		170	H	5.051	-0.138	-7.066
		171	H	1.088	4.956	7.063
		172	H	4.543	2.219	-7.066
		173	H	-3.206	3.961	7.063
		174	H	-1.022	4.981	7.063
		175	H	1.088	4.956	-7.066
		176	H	3.247	3.884	-7.066
		177	H	-4.541	2.328	7.063
		178	H	-1.022	4.981	-7.066
		179	H	-5.105	-0.016	7.063
		180	H	-3.206	3.961	-7.066
		181	H	-3.180	-3.981	7.063
		182	H	-4.660	-2.078	7.063
		183	H	-5.105	-0.016	-7.066
		184	H	-4.541	2.328	-7.066
		185	H	-1.290	-4.919	7.063
		186	H	-4.660	-2.078	-7.066
		187	H	-3.180	-3.981	-7.066
		188	H	-1.290	-4.919	-7.066
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(7, 7) CNT_3	0.000036	1	O	0.045	1.747	1.249
		2	H	0.952	1.305	1.114
		3	H	-0.435	1.338	0.431

4	O	-1.194	0.742	-0.830
5	H	-1.552	1.564	-1.305
6	H	-2.071	0.385	-0.465
7	C	0.643	-4.874	6.111
8	C	0.668	-4.729	1.222
9	C	1.366	-4.568	2.457
10	C	0.675	-4.735	3.693
11	C	2.683	-4.029	4.916
12	C	1.382	-4.636	4.916
13	C	3.339	-3.615	6.111
14	C	0.675	-4.735	-3.704
15	C	1.366	-4.568	-2.468
16	C	0.668	-4.729	-1.232
17	C	2.656	-3.985	-0.005
18	C	1.365	-4.588	-0.005
19	C	3.212	-3.541	1.222
20	C	2.641	-3.973	2.457
21	C	4.116	-2.444	3.693
22	C	3.212	-3.551	3.693
23	C	4.479	-1.830	4.916
24	C	4.204	-2.556	6.111
25	C	0.643	-4.874	-6.122
26	C	2.683	-4.029	-4.926
27	C	1.382	-4.636	-4.926
28	C	3.212	-3.551	-3.704
29	C	2.641	-3.973	-2.468
30	C	4.107	-2.446	-1.232
31	C	3.212	-3.541	-1.232
32	C	4.431	-1.813	-0.005
33	C	4.107	-2.446	1.222
34	C	4.745	-0.432	2.457
35	C	4.416	-1.800	2.457
36	C	4.772	0.278	3.693
37	C	4.816	-0.434	4.916
38	C	4.613	1.673	6.111
39	C	4.901	0.337	6.111
40	C	4.204	-2.556	-6.122
41	C	3.339	-3.615	-6.122
42	C	4.479	-1.830	-4.926
43	C	4.116	-2.444	-3.704
44	C	4.745	-0.432	-2.468
45	C	4.416	-1.800	-2.468
46	C	4.764	0.283	-1.232
47	C	4.765	-0.428	-0.005
48	C	4.465	1.666	1.222
49	C	4.764	0.283	1.222
50	C	4.154	2.310	2.457
51	C	4.470	1.674	3.693
52	C	3.335	3.474	4.916
53	C	4.217	2.341	4.916
54	C	2.785	4.022	6.111
55	C	4.901	0.337	-6.122
56	C	4.816	-0.434	-4.926
57	C	4.470	1.674	-3.704
58	C	4.772	0.278	-3.704
59	C	4.154	2.310	-2.468
60	C	4.465	1.666	-1.232
61	C	3.298	3.439	-0.006
62	C	4.173	2.314	-0.005

63	C	2.742	3.880	1.221
64	C	3.290	3.421	2.457
65	C	1.471	4.519	3.693
66	C	2.751	3.884	3.693
67	C	0.792	4.736	4.916
68	C	1.561	4.630	6.111
69	C	4.613	1.673	-6.122
70	C	3.335	3.474	-4.926
71	C	4.217	2.341	-4.926
72	C	2.751	3.884	-3.704
73	C	3.289	3.421	-2.468
74	C	1.475	4.510	-1.232
75	C	2.742	3.881	-1.232
76	C	0.786	4.685	-0.006
77	C	1.474	4.510	1.223
78	C	-0.631	4.685	2.458
79	C	0.777	4.668	2.457
80	C	-1.329	4.552	3.693
81	C	-0.644	4.754	4.916
82	C	-2.654	4.087	6.111
83	C	-1.415	4.665	6.111
84	C	1.561	4.630	-6.122
85	C	2.785	4.022	-6.122
86	C	0.792	4.737	-4.926
87	C	1.471	4.519	-3.704
88	C	-0.631	4.685	-2.468
89	C	0.777	4.668	-2.468
90	C	-1.332	4.544	-1.232
91	C	-0.639	4.703	-0.005
92	C	-2.614	3.945	1.222
93	C	-1.331	4.544	1.221
94	C	-3.172	3.498	2.457
95	C	-2.623	3.948	3.693
96	C	-4.125	2.441	4.916
97	C	-3.217	3.552	4.916
98	C	-4.537	1.782	6.111
99	C	-1.415	4.665	-6.122
100	C	-0.644	4.754	-4.926
101	C	-2.623	3.948	-3.704
102	C	-1.328	4.552	-3.704
103	C	-3.172	3.498	-2.468
104	C	-2.614	3.945	-1.232
105	C	-4.082	2.413	-0.005
106	C	-3.181	3.515	-0.005
107	C	-4.390	1.772	1.222
108	C	-4.063	2.408	2.457
109	C	-4.729	0.391	3.693
110	C	-4.394	1.780	3.693
111	C	-4.790	-0.320	4.916
112	C	-4.857	0.454	6.111
113	C	-2.654	4.087	-6.122
114	C	-4.125	2.441	-4.926
115	C	-3.217	3.552	-4.926
116	C	-4.394	1.780	-3.704
117	C	-4.063	2.408	-2.468
118	C	-4.721	0.396	-1.232
119	C	-4.390	1.771	-1.233
120	C	-4.739	-0.315	-0.005
121	C	-4.721	0.396	1.222

122	C	-4.423	-1.695	2.457
123	C	-4.719	-0.319	2.457
124	C	-4.139	-2.346	3.693
125	C	-4.487	-1.723	4.916
126	C	-3.390	-3.534	6.111
127	C	-4.229	-2.456	6.111
128	C	-4.857	0.454	-6.122
129	C	-4.537	1.782	-6.122
130	C	-4.790	-0.320	-4.926
131	C	-4.729	0.391	-3.704
132	C	-4.423	-1.695	-2.468
133	C	-4.719	-0.319	-2.468
134	C	-4.129	-2.347	-1.232
135	C	-4.438	-1.707	-0.005
136	C	-3.260	-3.464	1.222
137	C	-4.129	-2.347	1.222
138	C	-2.700	-3.909	2.457
139	C	-3.261	-3.473	3.693
140	C	-1.457	-4.603	4.916
141	C	-2.743	-3.964	4.916
142	C	-0.724	-4.857	6.111
143	C	-4.229	-2.456	-6.122
144	C	-4.487	-1.723	-4.926
145	C	-3.261	-3.473	-3.704
146	C	-4.139	-2.346	-3.704
147	C	-2.700	-3.909	-2.468
148	C	-3.260	-3.464	-1.232
149	C	-1.440	-4.554	-0.005
150	C	-2.715	-3.921	-0.005
151	C	-0.746	-4.712	1.222
152	C	-1.439	-4.535	2.457
153	C	-0.753	-4.718	3.693
154	C	-3.390	-3.534	-6.122
155	C	-1.457	-4.603	-4.926
156	C	-2.743	-3.964	-4.926
157	C	-0.753	-4.718	-3.704
158	C	-1.439	-4.535	-2.468
159	C	-0.746	-4.712	-1.232
160	C	-0.724	-4.857	-6.122
161	H	1.164	-4.965	7.059
162	H	3.075	-4.073	7.059
163	H	4.600	-2.206	7.059
164	H	1.164	-4.965	-7.070
165	H	4.586	2.202	7.059
166	H	5.094	-0.155	7.059
167	H	4.600	-2.206	-7.070
168	H	3.075	-4.073	-7.070
169	H	3.291	3.866	7.059
170	H	5.094	-0.155	-7.070
171	H	1.131	4.938	7.059
172	H	4.586	2.202	-7.070
173	H	-3.163	3.943	7.059
174	H	-0.978	4.963	7.059
175	H	1.131	4.938	-7.070
176	H	3.291	3.866	-7.070
177	H	-4.497	2.310	7.059
178	H	-0.978	4.963	-7.070
179	H	-5.062	-0.034	7.059
180	H	-3.163	3.943	-7.070

		181	H	-3.136	-3.999	7.059
		182	H	-4.617	-2.096	7.059
		183	H	-5.062	-0.034	-7.070
		184	H	-4.497	2.310	-7.070
		185	H	-1.247	-4.937	7.059
		186	H	-4.617	-2.096	-7.070
		187	H	-3.136	-3.999	-7.070
		188	H	-1.247	-4.937	-7.070
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(7, 7) CNT_4	0.000048	1	O	0.219	1.397	0.803
		2	H	-0.180	2.198	1.281
		3	H	1.054	1.841	0.436
		4	O	-1.355	1.093	-1.271
		5	H	-0.729	1.198	-0.455
		6	H	-1.595	0.114	-1.137
		7	C	0.643	-4.874	6.111
		8	C	0.668	-4.729	1.222
		9	C	1.366	-4.568	2.457
		10	C	0.675	-4.735	3.693
		11	C	2.683	-4.029	4.916
		12	C	1.382	-4.636	4.916
		13	C	3.339	-3.615	6.111
		14	C	0.675	-4.735	-3.704
		15	C	1.366	-4.568	-2.468
		16	C	0.668	-4.729	-1.232
		17	C	2.656	-3.985	-0.005
		18	C	1.365	-4.588	-0.005
		19	C	3.212	-3.541	1.222
		20	C	2.641	-3.973	2.457
		21	C	4.116	-2.444	3.693
		22	C	3.212	-3.551	3.693
		23	C	4.479	-1.830	4.916
		24	C	4.204	-2.556	6.111
		25	C	0.643	-4.874	-6.122
		26	C	2.683	-4.029	-4.926
		27	C	1.382	-4.636	-4.926
		28	C	3.212	-3.551	-3.704
		29	C	2.641	-3.973	-2.468
		30	C	4.107	-2.446	-1.232
		31	C	3.212	-3.541	-1.232
		32	C	4.431	-1.813	-0.005
		33	C	4.107	-2.446	1.222
		34	C	4.745	-0.432	2.457
		35	C	4.416	-1.800	2.457
		36	C	4.772	0.278	3.693
		37	C	4.816	-0.434	4.916
		38	C	4.613	1.673	6.111
		39	C	4.901	0.337	6.111
		40	C	4.204	-2.556	-6.122
		41	C	3.339	-3.615	-6.122
		42	C	4.479	-1.830	-4.926
		43	C	4.116	-2.444	-3.704
		44	C	4.745	-0.432	-2.468
		45	C	4.416	-1.800	-2.468
		46	C	4.764	0.283	-1.232
		47	C	4.765	-0.428	-0.005
		48	C	4.465	1.666	1.222
		49	C	4.764	0.283	1.222
		50	C	4.154	2.310	2.457

51	C	4.470	1.674	3.693
52	C	3.335	3.474	4.916
53	C	4.217	2.341	4.916
54	C	2.785	4.022	6.111
55	C	4.901	0.337	-6.122
56	C	4.816	-0.434	-4.926
57	C	4.470	1.674	-3.704
58	C	4.772	0.278	-3.704
59	C	4.154	2.310	-2.468
60	C	4.465	1.666	-1.232
61	C	3.298	3.439	-0.006
62	C	4.173	2.314	-0.005
63	C	2.742	3.880	1.221
64	C	3.290	3.421	2.457
65	C	1.471	4.519	3.693
66	C	2.751	3.884	3.693
67	C	0.792	4.736	4.916
68	C	1.561	4.630	6.111
69	C	4.613	1.673	-6.122
70	C	3.335	3.474	-4.926
71	C	4.217	2.341	-4.926
72	C	2.751	3.884	-3.704
73	C	3.289	3.421	-2.468
74	C	1.475	4.510	-1.232
75	C	2.742	3.881	-1.232
76	C	0.786	4.685	-0.006
77	C	1.474	4.511	1.223
78	C	-0.631	4.685	2.458
79	C	0.777	4.668	2.457
80	C	-1.329	4.552	3.693
81	C	-0.644	4.754	4.916
82	C	-2.654	4.087	6.111
83	C	-1.415	4.665	6.111
84	C	1.561	4.630	-6.122
85	C	2.785	4.022	-6.122
86	C	0.792	4.737	-4.926
87	C	1.471	4.519	-3.704
88	C	-0.631	4.685	-2.468
89	C	0.777	4.668	-2.468
90	C	-1.332	4.544	-1.232
91	C	-0.639	4.703	-0.005
92	C	-2.614	3.945	1.222
93	C	-1.331	4.544	1.221
94	C	-3.172	3.498	2.457
95	C	-2.623	3.948	3.693
96	C	-4.125	2.441	4.916
97	C	-3.217	3.552	4.916
98	C	-4.537	1.782	6.111
99	C	-1.415	4.665	-6.122
100	C	-0.644	4.754	-4.926
101	C	-2.623	3.948	-3.704
102	C	-1.328	4.552	-3.704
103	C	-3.172	3.498	-2.468
104	C	-2.614	3.945	-1.232
105	C	-4.082	2.413	-0.005
106	C	-3.181	3.516	-0.005
107	C	-4.390	1.772	1.222
108	C	-4.063	2.408	2.457
109	C	-4.729	0.391	3.693

110	C	-4.394	1.780	3.693
111	C	-4.790	-0.320	4.916
112	C	-4.857	0.454	6.111
113	C	-2.654	4.087	-6.122
114	C	-4.125	2.441	-4.926
115	C	-3.217	3.552	-4.926
116	C	-4.394	1.780	-3.704
117	C	-4.063	2.408	-2.468
118	C	-4.721	0.396	-1.232
119	C	-4.390	1.772	-1.232
120	C	-4.739	-0.315	-0.005
121	C	-4.721	0.396	1.222
122	C	-4.423	-1.695	2.457
123	C	-4.719	-0.319	2.457
124	C	-4.139	-2.346	3.693
125	C	-4.487	-1.723	4.916
126	C	-3.390	-3.534	6.111
127	C	-4.229	-2.456	6.111
128	C	-4.857	0.454	-6.122
129	C	-4.537	1.782	-6.122
130	C	-4.790	-0.320	-4.926
131	C	-4.729	0.391	-3.704
132	C	-4.423	-1.695	-2.468
133	C	-4.719	-0.319	-2.468
134	C	-4.129	-2.347	-1.232
135	C	-4.438	-1.707	-0.005
136	C	-3.260	-3.464	1.222
137	C	-4.129	-2.347	1.222
138	C	-2.700	-3.909	2.457
139	C	-3.261	-3.473	3.693
140	C	-1.457	-4.603	4.916
141	C	-2.743	-3.964	4.916
142	C	-0.724	-4.857	6.111
143	C	-4.229	-2.456	-6.122
144	C	-4.487	-1.723	-4.926
145	C	-3.261	-3.473	-3.704
146	C	-4.139	-2.346	-3.704
147	C	-2.700	-3.909	-2.468
148	C	-3.260	-3.464	-1.232
149	C	-1.440	-4.554	-0.005
150	C	-2.715	-3.921	-0.005
151	C	-0.746	-4.712	1.222
152	C	-1.439	-4.535	2.457
153	C	-0.753	-4.718	3.693
154	C	-3.390	-3.534	-6.122
155	C	-1.457	-4.603	-4.926
156	C	-2.743	-3.964	-4.926
157	C	-0.753	-4.718	-3.704
158	C	-1.439	-4.535	-2.468
159	C	-0.746	-4.712	-1.232
160	C	-0.724	-4.857	-6.122
161	H	1.164	-4.965	7.059
162	H	3.075	-4.073	7.059
163	H	4.600	-2.206	7.059
164	H	1.164	-4.965	-7.070
165	H	4.586	2.202	7.059
166	H	5.094	-0.155	7.059
167	H	4.600	-2.206	-7.070
168	H	3.075	-4.073	-7.070

169	H	3.291	3.866	7.059
170	H	5.094	-0.155	-7.070
171	H	1.131	4.938	7.059
172	H	4.586	2.202	-7.070
173	H	-3.163	3.943	7.059
174	H	-0.978	4.963	7.059
175	H	1.131	4.938	-7.070
176	H	3.291	3.866	-7.070
177	H	-4.497	2.310	7.059
178	H	-0.978	4.963	-7.070
179	H	-5.062	-0.034	7.059
180	H	-3.163	3.943	-7.070
181	H	-3.136	-3.999	7.059
182	H	-4.617	-2.096	7.059
183	H	-5.062	-0.034	-7.070
184	H	-4.497	2.310	-7.070
185	H	-1.247	-4.937	7.059
186	H	-4.617	-2.096	-7.070
187	H	-3.136	-3.999	-7.070
188	H	-1.247	-4.937	-7.070

Table S14. The coordinates and energies of the sampled structures of confined water dimer in (8, 8) CNT. The first structure which is highlighted with underline was used in the paper.

Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$\underline{(H_2O)_2}$@(8, 8) CNT_1	0.000000	1	O	2.114	0.035	0.731
		2	H	2.879	-0.369	1.262
		3	H	2.625	0.792	0.287
		4	O	1.742	-1.720	-1.180
		5	H	1.869	-1.019	-0.432
		6	H	0.794	-2.007	-0.945
		7	C	-1.520	-5.365	6.098
		8	C	-1.436	-5.224	1.210
		9	C	-0.734	-5.356	2.445
		10	C	-1.434	-5.238	3.681
		11	C	0.688	-5.435	4.904
		12	C	-0.748	-5.435	4.904
		13	C	1.459	-5.365	6.098
		14	C	-1.434	-5.238	-3.716
		15	C	-0.734	-5.356	-2.480
		16	C	-1.436	-5.224	-1.245
		17	C	0.681	-5.370	-0.018
		18	C	-0.741	-5.370	-0.018
		19	C	1.376	-5.224	1.210
		20	C	0.674	-5.356	2.445
		21	C	2.693	-4.691	3.681
		22	C	1.374	-5.238	3.681
		23	C	3.318	-4.346	4.904
		24	C	2.723	-4.842	6.098
		25	C	-1.520	-5.365	-6.133
		26	C	0.688	-5.435	-4.939
		27	C	-0.748	-5.435	-4.939
		28	C	1.374	-5.238	-3.716
		29	C	0.674	-5.356	-2.480
		30	C	2.682	-4.683	-1.245
		31	C	1.376	-5.224	-1.245
		32	C	3.277	-4.295	-0.018
		33	C	2.682	-4.683	1.210
		34	C	4.267	-3.284	2.445

35	C	3.272	-4.280	2.445
36	C	4.679	-2.705	3.681
37	C	4.333	-3.330	4.904
38	C	5.353	-1.472	6.098
39	C	4.830	-2.735	6.098
40	C	2.723	-4.842	-6.133
41	C	1.459	-5.365	-6.133
42	C	3.318	-4.346	-4.939
43	C	2.693	-4.691	-3.716
44	C	4.267	-3.284	-2.480
45	C	3.272	-4.280	-2.480
46	C	4.670	-2.694	-1.245
47	C	4.283	-3.289	-0.018
48	C	5.211	-1.388	1.210
49	C	4.671	-2.694	1.210
50	C	5.344	-0.685	2.445
51	C	5.226	-1.386	3.681
52	C	5.423	0.736	4.904
53	C	5.423	-0.700	4.904
54	C	5.353	1.508	6.098
55	C	4.830	-2.735	-6.133
56	C	4.333	-3.330	-4.939
57	C	5.226	-1.386	-3.716
58	C	4.679	-2.706	-3.716
59	C	5.344	-0.686	-2.480
60	C	5.212	-1.388	-1.245
61	C	5.358	0.729	-0.018
62	C	5.358	-0.693	-0.018
63	C	5.212	1.424	1.210
64	C	5.344	0.722	2.445
65	C	4.679	2.741	3.681
66	C	5.225	1.422	3.681
67	C	4.333	3.366	4.904
68	C	4.830	2.771	6.098
69	C	5.353	-1.472	-6.133
70	C	5.423	0.736	-4.939
71	C	5.423	-0.700	-4.939
72	C	5.226	1.422	-3.716
73	C	5.344	0.722	-2.480
74	C	4.670	2.730	-1.245
75	C	5.212	1.424	-1.245
76	C	4.283	3.325	-0.018
77	C	4.670	2.730	1.210
78	C	3.272	4.315	2.445
79	C	4.267	3.320	2.445
80	C	2.693	4.727	3.681
81	C	3.318	4.381	4.904
82	C	1.459	5.401	6.098
83	C	2.723	4.878	6.098
84	C	4.830	2.771	-6.133
85	C	5.353	1.508	-6.133
86	C	4.333	3.366	-4.939
87	C	4.679	2.741	-3.716
88	C	3.272	4.315	-2.480
89	C	4.267	3.320	-2.480
90	C	2.682	4.718	-1.245
91	C	3.277	4.331	-0.018
92	C	1.376	5.260	1.210
93	C	2.682	4.718	1.210

94	C	0.674	5.392	2.445
95	C	1.374	5.274	3.681
96	C	-0.748	5.471	4.904
97	C	0.688	5.471	4.904
98	C	-1.520	5.401	6.098
99	C	2.723	4.878	-6.133
100	C	3.318	4.381	-4.939
101	C	1.374	5.274	-3.716
102	C	2.693	4.727	-3.716
103	C	0.674	5.392	-2.480
104	C	1.376	5.260	-1.245
105	C	-0.741	5.406	-0.018
106	C	0.681	5.406	-0.018
107	C	-1.436	5.260	1.210
108	C	-0.734	5.392	2.445
109	C	-2.754	4.727	3.681
110	C	-1.434	5.274	3.681
111	C	-3.378	4.381	4.904
112	C	-2.783	4.878	6.098
113	C	1.459	5.401	-6.133
114	C	-0.748	5.471	-4.939
115	C	0.688	5.471	-4.939
116	C	-1.434	5.274	-3.716
117	C	-0.734	5.392	-2.480
118	C	-2.742	4.718	-1.245
119	C	-1.436	5.260	-1.245
120	C	-3.337	4.331	-0.018
121	C	-2.742	4.718	1.210
122	C	-4.328	3.320	2.445
123	C	-3.332	4.315	2.445
124	C	-4.739	2.741	3.681
125	C	-4.394	3.366	4.904
126	C	-5.413	1.508	6.098
127	C	-4.890	2.771	6.098
128	C	-2.783	4.878	-6.133
129	C	-1.520	5.401	-6.133
130	C	-3.378	4.381	-4.939
131	C	-2.754	4.727	-3.716
132	C	-4.328	3.320	-2.480
133	C	-3.332	4.315	-2.480
134	C	-4.731	2.730	-1.245
135	C	-4.343	3.325	-0.018
136	C	-5.272	1.424	1.210
137	C	-4.731	2.730	1.210
138	C	-5.404	0.722	2.445
139	C	-5.286	1.422	3.681
140	C	-5.483	-0.700	4.904
141	C	-5.483	0.736	4.904
142	C	-5.413	-1.472	6.098
143	C	-4.890	2.771	-6.133
144	C	-4.394	3.366	-4.939
145	C	-5.286	1.422	-3.716
146	C	-4.739	2.741	-3.716
147	C	-5.404	0.722	-2.480
148	C	-5.272	1.424	-1.245
149	C	-5.418	-0.693	-0.018
150	C	-5.418	0.729	-0.018
151	C	-5.272	-1.388	1.210
152	C	-5.404	-0.686	2.445

153	C	-4.739	-2.706	3.681
154	C	-5.286	-1.386	3.681
155	C	-4.394	-3.330	4.904
156	C	-4.890	-2.735	6.098
157	C	-5.413	1.508	-6.133
158	C	-5.483	-0.700	-4.939
159	C	-5.483	0.736	-4.939
160	C	-5.286	-1.386	-3.716
161	C	-5.404	-0.686	-2.480
162	C	-4.731	-2.694	-1.245
163	C	-5.272	-1.388	-1.245
164	C	-4.343	-3.289	-0.018
165	C	-4.731	-2.694	1.210
166	C	-3.332	-4.280	2.445
167	C	-4.328	-3.284	2.445
168	C	-2.754	-4.691	3.681
169	C	-3.378	-4.346	4.904
170	C	-2.783	-4.842	6.098
171	C	-4.890	-2.735	-6.133
172	C	-5.413	-1.472	-6.133
173	C	-4.394	-3.330	-4.939
174	C	-4.739	-2.706	-3.716
175	C	-3.332	-4.280	-2.480
176	C	-4.328	-3.284	-2.480
177	C	-2.742	-4.683	-1.245
178	C	-3.337	-4.295	-0.018
179	C	-2.742	-4.683	1.210
180	C	-2.783	-4.842	-6.133
181	C	-3.378	-4.346	-4.939
182	C	-2.754	-4.691	-3.716
183	H	-1.072	-5.644	7.047
184	H	1.012	-5.644	7.047
185	H	3.236	-4.722	7.047
186	H	-1.072	-5.644	-7.082
187	H	5.631	-1.024	7.047
188	H	4.710	-3.249	7.047
189	H	3.236	-4.722	-7.082
190	H	1.012	-5.644	-7.082
191	H	5.631	1.060	7.047
192	H	4.710	-3.249	-7.082
193	H	4.710	3.284	7.047
194	H	5.631	-1.024	-7.082
195	H	1.012	5.680	7.047
196	H	3.236	4.758	7.047
197	H	4.710	3.284	-7.082
198	H	5.631	1.060	-7.082
199	H	-1.072	5.680	7.047
200	H	3.236	4.758	-7.082
201	H	-3.297	4.758	7.047
202	H	1.012	5.680	-7.082
203	H	-5.692	1.060	7.047
204	H	-4.770	3.284	7.047
205	H	-3.297	4.758	-7.082
206	H	-1.072	5.680	-7.082
207	H	-5.692	-1.024	7.047
208	H	-4.770	3.284	-7.082
209	H	-4.770	-3.249	7.047
210	H	-5.692	1.060	-7.082
211	H	-3.297	-4.722	7.047

		212	H	-4.770	-3.249	-7.082
		213	H	-5.692	-1.024	-7.082
		214	H	-3.297	-4.722	-7.082
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(8, 8) CNT_2	0.000006	1	O	-1.478	1.508	0.769
		2	H	-2.306	1.760	1.300
		3	H	-1.302	2.408	0.333
		4	O	-2.454	0.021	-1.158
		5	H	-2.049	0.600	-0.404
		6	H	-1.985	-0.853	-0.931
		7	C	-1.461	-5.401	6.123
		8	C	-1.377	-5.259	1.235
		9	C	-0.675	-5.392	2.469
		10	C	-1.375	-5.273	3.706
		11	C	0.747	-5.470	4.928
		12	C	-0.689	-5.470	4.928
		13	C	1.519	-5.401	6.123
		14	C	-1.375	-5.273	-3.691
		15	C	-0.675	-5.392	-2.455
		16	C	-1.377	-5.259	-1.221
		17	C	0.740	-5.405	0.007
		18	C	-0.682	-5.405	0.007
		19	C	1.435	-5.259	1.235
		20	C	0.733	-5.392	2.469
		21	C	2.752	-4.727	3.706
		22	C	1.433	-5.273	3.706
		23	C	3.377	-4.381	4.928
		24	C	2.782	-4.877	6.123
		25	C	-1.461	-5.401	-6.109
		26	C	0.747	-5.470	-4.914
		27	C	-0.689	-5.470	-4.914
		28	C	1.433	-5.273	-3.691
		29	C	0.733	-5.392	-2.455
		30	C	2.741	-4.718	-1.221
		31	C	1.435	-5.259	-1.221
		32	C	3.336	-4.330	0.007
		33	C	2.741	-4.718	1.235
		34	C	4.327	-3.320	2.469
		35	C	3.331	-4.315	2.469
		36	C	4.738	-2.741	3.706
		37	C	4.392	-3.365	4.928
		38	C	5.412	-1.507	6.123
		39	C	4.889	-2.771	6.123
		40	C	2.782	-4.877	-6.109
		41	C	1.519	-5.401	-6.109
		42	C	3.377	-4.381	-4.914
		43	C	2.752	-4.727	-3.691
		44	C	4.327	-3.320	-2.455
		45	C	3.331	-4.315	-2.455
		46	C	4.730	-2.730	-1.221
		47	C	4.342	-3.325	0.007
		48	C	5.271	-1.424	1.235
		49	C	4.730	-2.730	1.235
		50	C	5.403	-0.721	2.469
		51	C	5.285	-1.422	3.706
		52	C	5.482	0.701	4.928
		53	C	5.482	-0.736	4.928
		54	C	5.412	1.472	6.123
		55	C	4.889	-2.771	-6.109

56	C	4.392	-3.365	-4.914
57	C	5.285	-1.422	-3.691
58	C	4.738	-2.741	-3.691
59	C	5.403	-0.721	-2.455
60	C	5.271	-1.424	-1.221
61	C	5.417	0.693	0.007
62	C	5.417	-0.729	0.007
63	C	5.271	1.388	1.235
64	C	5.403	0.686	2.469
65	C	4.738	2.706	3.706
66	C	5.285	1.386	3.706
67	C	4.392	3.330	4.928
68	C	4.889	2.736	6.123
69	C	5.412	-1.507	-6.109
70	C	5.482	0.701	-4.914
71	C	5.482	-0.736	-4.914
72	C	5.285	1.386	-3.691
73	C	5.403	0.686	-2.455
74	C	4.730	2.695	-1.221
75	C	5.271	1.388	-1.221
76	C	4.342	3.289	0.007
77	C	4.730	2.695	1.235
78	C	3.331	4.280	2.469
79	C	4.327	3.285	2.469
80	C	2.752	4.692	3.706
81	C	3.377	4.346	4.928
82	C	1.519	5.365	6.123
83	C	2.782	4.842	6.123
84	C	4.889	2.736	-6.109
85	C	5.412	1.472	-6.109
86	C	4.392	3.330	-4.914
87	C	4.738	2.706	-3.691
88	C	3.331	4.280	-2.455
89	C	4.327	3.285	-2.455
90	C	2.741	4.683	-1.221
91	C	3.336	4.295	0.007
92	C	1.435	5.224	1.235
93	C	2.741	4.683	1.235
94	C	0.733	5.356	2.469
95	C	1.433	5.238	3.706
96	C	-0.689	5.435	4.928
97	C	0.747	5.435	4.928
98	C	-1.461	5.365	6.123
99	C	2.782	4.842	-6.109
100	C	3.377	4.346	-4.914
101	C	1.433	5.238	-3.691
102	C	2.752	4.692	-3.691
103	C	0.733	5.356	-2.455
104	C	1.435	5.224	-1.221
105	C	-0.682	5.370	0.007
106	C	0.740	5.370	0.007
107	C	-1.377	5.224	1.235
108	C	-0.675	5.356	2.469
109	C	-2.695	4.692	3.706
110	C	-1.375	5.238	3.706
111	C	-3.319	4.346	4.928
112	C	-2.724	4.842	6.123
113	C	1.519	5.365	-6.109
114	C	-0.689	5.435	-4.914

115	C	0.747	5.435	-4.914
116	C	-1.375	5.238	-3.691
117	C	-0.675	5.356	-2.455
118	C	-2.683	4.683	-1.221
119	C	-1.377	5.224	-1.221
120	C	-3.278	4.295	0.007
121	C	-2.683	4.683	1.235
122	C	-4.269	3.285	2.469
123	C	-3.273	4.280	2.469
124	C	-4.680	2.706	3.706
125	C	-4.335	3.330	4.928
126	C	-5.354	1.472	6.123
127	C	-4.831	2.736	6.123
128	C	-2.724	4.842	-6.109
129	C	-1.461	5.365	-6.109
130	C	-3.319	4.346	-4.914
131	C	-2.695	4.692	-3.691
132	C	-4.269	3.285	-2.455
133	C	-3.273	4.280	-2.455
134	C	-4.672	2.695	-1.221
135	C	-4.284	3.289	0.007
136	C	-5.213	1.388	1.235
137	C	-4.672	2.695	1.235
138	C	-5.345	0.686	2.469
139	C	-5.227	1.386	3.706
140	C	-5.424	-0.736	4.928
141	C	-5.424	0.701	4.928
142	C	-5.354	-1.507	6.123
143	C	-4.831	2.736	-6.109
144	C	-4.335	3.330	-4.914
145	C	-5.227	1.386	-3.691
146	C	-4.680	2.706	-3.691
147	C	-5.345	0.686	-2.455
148	C	-5.213	1.388	-1.221
149	C	-5.359	-0.729	0.007
150	C	-5.359	0.693	0.007
151	C	-5.213	-1.424	1.235
152	C	-5.345	-0.721	2.469
153	C	-4.680	-2.741	3.706
154	C	-5.227	-1.422	3.706
155	C	-4.335	-3.365	4.928
156	C	-4.831	-2.771	6.123
157	C	-5.354	1.472	-6.109
158	C	-5.424	-0.736	-4.914
159	C	-5.424	0.701	-4.914
160	C	-5.227	-1.422	-3.691
161	C	-5.345	-0.721	-2.455
162	C	-4.672	-2.730	-1.221
163	C	-5.213	-1.424	-1.221
164	C	-4.284	-3.325	0.007
165	C	-4.672	-2.730	1.235
166	C	-3.273	-4.315	2.469
167	C	-4.269	-3.320	2.469
168	C	-2.695	-4.727	3.706
169	C	-3.319	-4.381	4.928
170	C	-2.724	-4.877	6.123
171	C	-4.831	-2.771	-6.109
172	C	-5.354	-1.507	-6.109
173	C	-4.335	-3.365	-4.914

		174	C	-4.680	-2.741	-3.691
		175	C	-3.273	-4.315	-2.455
		176	C	-4.269	-3.320	-2.455
		177	C	-2.683	-4.718	-1.221
		178	C	-3.278	-4.330	0.007
		179	C	-2.683	-4.718	1.235
		180	C	-2.724	-4.877	-6.109
		181	C	-3.319	-4.381	-4.914
		182	C	-2.695	-4.727	-3.691
		183	H	-1.013	-5.679	7.071
		184	H	1.071	-5.679	7.071
		185	H	3.295	-4.758	7.071
		186	H	-1.013	-5.679	-7.057
		187	H	5.691	-1.060	7.071
		188	H	4.769	-3.284	7.071
		189	H	3.295	-4.758	-7.057
		190	H	1.071	-5.679	-7.057
		191	H	5.691	1.024	7.071
		192	H	4.769	-3.284	-7.057
		193	H	4.769	3.249	7.071
		194	H	5.691	-1.060	-7.057
		195	H	1.071	5.644	7.071
		196	H	3.295	4.723	7.071
		197	H	4.769	3.249	-7.057
		198	H	5.691	1.024	-7.057
		199	H	-1.013	5.644	7.071
		200	H	3.295	4.723	-7.057
		201	H	-3.238	4.723	7.071
		202	H	1.071	5.644	-7.057
		203	H	-5.633	1.024	7.071
		204	H	-4.711	3.249	7.071
		205	H	-3.238	4.723	-7.057
		206	H	-1.013	5.644	-7.057
		207	H	-5.633	-1.060	7.071
		208	H	-4.711	3.249	-7.057
		209	H	-4.711	-3.284	7.071
		210	H	-5.633	1.024	-7.057
		211	H	-3.238	-4.758	7.071
		212	H	-4.711	-3.284	-7.057
		213	H	-5.633	-1.060	-7.057
		214	H	-3.238	-4.758	-7.057
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(8, 8) CNT_3	0.000007	1	O	-1.743	1.720	1.170
		2	H	-0.796	2.007	0.934
		3	H	-1.870	1.019	0.422
		4	O	-2.115	-0.036	-0.740
		5	H	-2.880	0.367	-1.272
		6	H	-2.626	-0.793	-0.297
		7	C	-1.461	-5.401	6.123
		8	C	-1.377	-5.259	1.235
		9	C	-0.675	-5.392	2.469
		10	C	-1.375	-5.273	3.706
		11	C	0.747	-5.470	4.928
		12	C	-0.689	-5.470	4.928
		13	C	1.519	-5.401	6.123
		14	C	-1.375	-5.273	-3.691
		15	C	-0.675	-5.392	-2.455
		16	C	-1.377	-5.259	-1.221
		17	C	0.740	-5.405	0.007

18	C	-0.682	-5.405	0.007
19	C	1.435	-5.259	1.235
20	C	0.733	-5.392	2.469
21	C	2.752	-4.727	3.706
22	C	1.433	-5.273	3.706
23	C	3.377	-4.381	4.928
24	C	2.782	-4.877	6.123
25	C	-1.461	-5.401	-6.109
26	C	0.747	-5.470	-4.914
27	C	-0.689	-5.470	-4.914
28	C	1.433	-5.273	-3.691
29	C	0.733	-5.392	-2.455
30	C	2.741	-4.718	-1.221
31	C	1.435	-5.259	-1.221
32	C	3.336	-4.330	0.007
33	C	2.741	-4.718	1.235
34	C	4.327	-3.320	2.469
35	C	3.331	-4.315	2.469
36	C	4.738	-2.741	3.706
37	C	4.392	-3.365	4.928
38	C	5.412	-1.507	6.123
39	C	4.889	-2.771	6.123
40	C	2.782	-4.877	-6.109
41	C	1.519	-5.401	-6.109
42	C	3.377	-4.381	-4.914
43	C	2.752	-4.727	-3.691
44	C	4.327	-3.320	-2.455
45	C	3.331	-4.315	-2.455
46	C	4.730	-2.730	-1.221
47	C	4.342	-3.325	0.007
48	C	5.271	-1.424	1.235
49	C	4.730	-2.730	1.235
50	C	5.403	-0.721	2.469
51	C	5.285	-1.422	3.706
52	C	5.482	0.701	4.928
53	C	5.482	-0.736	4.928
54	C	5.412	1.472	6.123
55	C	4.889	-2.771	-6.109
56	C	4.392	-3.365	-4.914
57	C	5.285	-1.422	-3.691
58	C	4.738	-2.741	-3.691
59	C	5.403	-0.721	-2.455
60	C	5.271	-1.424	-1.221
61	C	5.417	0.693	0.007
62	C	5.417	-0.729	0.007
63	C	5.271	1.388	1.235
64	C	5.403	0.686	2.469
65	C	4.738	2.706	3.706
66	C	5.285	1.386	3.706
67	C	4.392	3.330	4.928
68	C	4.889	2.736	6.123
69	C	5.412	-1.507	-6.109
70	C	5.482	0.701	-4.914
71	C	5.482	-0.736	-4.914
72	C	5.285	1.386	-3.691
73	C	5.403	0.686	-2.455
74	C	4.730	2.695	-1.221
75	C	5.271	1.388	-1.221
76	C	4.342	3.289	0.007

77	C	4.730	2.695	1.235
78	C	3.331	4.280	2.469
79	C	4.327	3.285	2.469
80	C	2.752	4.692	3.706
81	C	3.377	4.346	4.928
82	C	1.519	5.365	6.123
83	C	2.782	4.842	6.123
84	C	4.889	2.736	-6.109
85	C	5.412	1.472	-6.109
86	C	4.392	3.330	-4.914
87	C	4.738	2.706	-3.691
88	C	3.331	4.280	-2.455
89	C	4.327	3.285	-2.455
90	C	2.741	4.683	-1.221
91	C	3.336	4.295	0.007
92	C	1.435	5.224	1.235
93	C	2.741	4.683	1.235
94	C	0.733	5.356	2.469
95	C	1.433	5.238	3.706
96	C	-0.689	5.435	4.928
97	C	0.747	5.435	4.928
98	C	-1.461	5.365	6.123
99	C	2.782	4.842	-6.109
100	C	3.377	4.346	-4.914
101	C	1.433	5.238	-3.691
102	C	2.752	4.692	-3.691
103	C	0.733	5.356	-2.455
104	C	1.435	5.224	-1.221
105	C	-0.682	5.370	0.007
106	C	0.740	5.370	0.007
107	C	-1.377	5.224	1.235
108	C	-0.675	5.356	2.469
109	C	-2.695	4.692	3.706
110	C	-1.375	5.238	3.706
111	C	-3.319	4.346	4.928
112	C	-2.724	4.842	6.123
113	C	1.519	5.365	-6.109
114	C	-0.689	5.435	-4.914
115	C	0.747	5.435	-4.914
116	C	-1.375	5.238	-3.691
117	C	-0.675	5.356	-2.455
118	C	-2.683	4.683	-1.221
119	C	-1.377	5.224	-1.221
120	C	-3.278	4.295	0.007
121	C	-2.683	4.683	1.235
122	C	-4.269	3.285	2.469
123	C	-3.273	4.280	2.469
124	C	-4.680	2.706	3.706
125	C	-4.335	3.330	4.928
126	C	-5.354	1.472	6.123
127	C	-4.831	2.736	6.123
128	C	-2.724	4.842	-6.109
129	C	-1.461	5.365	-6.109
130	C	-3.319	4.346	-4.914
131	C	-2.695	4.692	-3.691
132	C	-4.269	3.285	-2.455
133	C	-3.273	4.280	-2.455
134	C	-4.672	2.695	-1.221
135	C	-4.284	3.289	0.007

136	C	-5.213	1.388	1.235
137	C	-4.672	2.695	1.235
138	C	-5.345	0.686	2.469
139	C	-5.227	1.386	3.706
140	C	-5.424	-0.736	4.928
141	C	-5.424	0.701	4.928
142	C	-5.354	-1.507	6.123
143	C	-4.831	2.736	-6.109
144	C	-4.335	3.330	-4.914
145	C	-5.227	1.386	-3.691
146	C	-4.680	2.706	-3.691
147	C	-5.345	0.686	-2.455
148	C	-5.213	1.388	-1.221
149	C	-5.359	-0.729	0.007
150	C	-5.359	0.694	0.007
151	C	-5.213	-1.424	1.235
152	C	-5.345	-0.721	2.469
153	C	-4.680	-2.741	3.706
154	C	-5.227	-1.422	3.706
155	C	-4.335	-3.365	4.928
156	C	-4.831	-2.771	6.123
157	C	-5.354	1.472	-6.109
158	C	-5.424	-0.736	-4.914
159	C	-5.424	0.701	-4.914
160	C	-5.227	-1.422	-3.691
161	C	-5.345	-0.721	-2.455
162	C	-4.672	-2.730	-1.221
163	C	-5.213	-1.424	-1.221
164	C	-4.284	-3.325	0.007
165	C	-4.672	-2.730	1.235
166	C	-3.273	-4.315	2.469
167	C	-4.269	-3.320	2.469
168	C	-2.695	-4.727	3.706
169	C	-3.319	-4.381	4.928
170	C	-2.724	-4.877	6.123
171	C	-4.831	-2.771	-6.109
172	C	-5.354	-1.507	-6.109
173	C	-4.335	-3.365	-4.914
174	C	-4.680	-2.741	-3.691
175	C	-3.273	-4.315	-2.455
176	C	-4.269	-3.320	-2.455
177	C	-2.683	-4.718	-1.221
178	C	-3.278	-4.330	0.007
179	C	-2.683	-4.718	1.235
180	C	-2.724	-4.877	-6.109
181	C	-3.319	-4.381	-4.914
182	C	-2.695	-4.727	-3.691
183	H	-1.013	-5.679	7.071
184	H	1.071	-5.679	7.071
185	H	3.295	-4.758	7.071
186	H	-1.013	-5.679	-7.057
187	H	5.691	-1.060	7.071
188	H	4.769	-3.284	7.071
189	H	3.295	-4.758	-7.057
190	H	1.071	-5.679	-7.057
191	H	5.691	1.024	7.071
192	H	4.769	-3.284	-7.057
193	H	4.769	3.249	7.071
194	H	5.691	-1.060	-7.057

		195	H	1.071	5.644	7.071
		196	H	3.295	4.723	7.071
		197	H	4.769	3.249	-7.057
		198	H	5.691	1.024	-7.057
		199	H	-1.013	5.644	7.071
		200	H	3.295	4.723	-7.057
		201	H	-3.238	4.723	7.071
		202	H	1.071	5.644	-7.057
		203	H	-5.633	1.024	7.071
		204	H	-4.711	3.249	7.071
		205	H	-3.238	4.723	-7.057
		206	H	-1.013	5.644	-7.057
		207	H	-5.633	-1.060	7.071
		208	H	-4.711	3.249	-7.057
		209	H	-4.711	-3.284	7.071
		210	H	-5.633	1.024	-7.057
		211	H	-3.238	-4.758	7.071
		212	H	-4.711	-3.284	-7.057
		213	H	-5.633	-1.060	-7.057
		214	H	-3.238	-4.758	-7.057
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(8, 8) CNT_4	0.000009	1	O	2.453	-0.021	1.148
		2	H	1.984	0.854	0.921
		3	H	2.048	-0.599	0.393
		4	O	1.478	-1.507	-0.779
		5	H	1.302	-2.407	-0.345
		6	H	2.306	-1.758	-1.310
		7	C	-1.520	-5.365	6.098
		8	C	-1.436	-5.224	1.210
		9	C	-0.734	-5.356	2.445
		10	C	-1.434	-5.238	3.681
		11	C	0.688	-5.435	4.904
		12	C	-0.748	-5.435	4.904
		13	C	1.459	-5.365	6.098
		14	C	-1.434	-5.238	-3.716
		15	C	-0.734	-5.356	-2.480
		16	C	-1.436	-5.224	-1.245
		17	C	0.681	-5.370	-0.018
		18	C	-0.741	-5.370	-0.018
		19	C	1.376	-5.224	1.210
		20	C	0.674	-5.356	2.445
		21	C	2.693	-4.691	3.681
		22	C	1.374	-5.238	3.681
		23	C	3.318	-4.346	4.904
		24	C	2.723	-4.842	6.098
		25	C	-1.520	-5.365	-6.133
		26	C	0.688	-5.435	-4.939
		27	C	-0.748	-5.435	-4.939
		28	C	1.374	-5.238	-3.716
		29	C	0.674	-5.356	-2.480
		30	C	2.682	-4.683	-1.245
		31	C	1.376	-5.224	-1.245
		32	C	3.277	-4.295	-0.018
		33	C	2.682	-4.683	1.210
		34	C	4.267	-3.284	2.445
		35	C	3.272	-4.280	2.445
		36	C	4.679	-2.706	3.681
		37	C	4.333	-3.330	4.904
		38	C	5.353	-1.472	6.098

39	C	4.830	-2.735	6.098
40	C	2.723	-4.842	-6.133
41	C	1.459	-5.365	-6.133
42	C	3.318	-4.346	-4.939
43	C	2.693	-4.691	-3.716
44	C	4.267	-3.284	-2.480
45	C	3.272	-4.280	-2.480
46	C	4.670	-2.695	-1.246
47	C	4.283	-3.289	-0.017
48	C	5.212	-1.388	1.210
49	C	4.670	-2.694	1.210
50	C	5.344	-0.686	2.445
51	C	5.226	-1.386	3.681
52	C	5.423	0.736	4.904
53	C	5.423	-0.700	4.904
54	C	5.353	1.508	6.098
55	C	4.830	-2.735	-6.133
56	C	4.333	-3.330	-4.939
57	C	5.226	-1.386	-3.716
58	C	4.679	-2.706	-3.716
59	C	5.344	-0.686	-2.480
60	C	5.212	-1.388	-1.245
61	C	5.358	0.729	-0.018
62	C	5.358	-0.693	-0.017
63	C	5.212	1.424	1.210
64	C	5.344	0.722	2.445
65	C	4.679	2.741	3.681
66	C	5.226	1.422	3.681
67	C	4.333	3.366	4.904
68	C	4.830	2.771	6.098
69	C	5.353	-1.472	-6.133
70	C	5.423	0.736	-4.939
71	C	5.423	-0.700	-4.939
72	C	5.226	1.422	-3.716
73	C	5.344	0.722	-2.480
74	C	4.670	2.730	-1.245
75	C	5.212	1.424	-1.245
76	C	4.283	3.325	-0.018
77	C	4.670	2.730	1.210
78	C	3.272	4.315	2.445
79	C	4.267	3.320	2.445
80	C	2.693	4.727	3.681
81	C	3.318	4.381	4.904
82	C	1.459	5.401	6.098
83	C	2.723	4.878	6.098
84	C	4.830	2.771	-6.133
85	C	5.353	1.508	-6.133
86	C	4.333	3.366	-4.939
87	C	4.679	2.741	-3.716
88	C	3.272	4.315	-2.480
89	C	4.267	3.320	-2.480
90	C	2.682	4.718	-1.245
91	C	3.277	4.331	-0.018
92	C	1.376	5.260	1.210
93	C	2.682	4.718	1.210
94	C	0.674	5.392	2.445
95	C	1.374	5.274	3.681
96	C	-0.748	5.471	4.904
97	C	0.688	5.471	4.904

98	C	-1.520	5.401	6.098
99	C	2.723	4.878	-6.133
100	C	3.318	4.381	-4.939
101	C	1.374	5.274	-3.716
102	C	2.693	4.727	-3.716
103	C	0.674	5.392	-2.480
104	C	1.376	5.260	-1.245
105	C	-0.741	5.406	-0.018
106	C	0.681	5.406	-0.018
107	C	-1.436	5.260	1.210
108	C	-0.734	5.392	2.445
109	C	-2.754	4.727	3.681
110	C	-1.434	5.274	3.681
111	C	-3.378	4.381	4.904
112	C	-2.783	4.878	6.098
113	C	1.459	5.401	-6.133
114	C	-0.748	5.471	-4.939
115	C	0.688	5.471	-4.939
116	C	-1.434	5.274	-3.716
117	C	-0.734	5.392	-2.480
118	C	-2.742	4.718	-1.245
119	C	-1.436	5.260	-1.245
120	C	-3.337	4.331	-0.018
121	C	-2.742	4.718	1.210
122	C	-4.328	3.320	2.445
123	C	-3.332	4.315	2.445
124	C	-4.739	2.741	3.681
125	C	-4.394	3.366	4.904
126	C	-5.413	1.508	6.098
127	C	-4.890	2.771	6.098
128	C	-2.783	4.878	-6.133
129	C	-1.520	5.401	-6.133
130	C	-3.378	4.381	-4.939
131	C	-2.754	4.727	-3.716
132	C	-4.328	3.320	-2.480
133	C	-3.332	4.315	-2.480
134	C	-4.731	2.730	-1.245
135	C	-4.343	3.325	-0.018
136	C	-5.272	1.424	1.210
137	C	-4.731	2.730	1.210
138	C	-5.404	0.722	2.445
139	C	-5.286	1.422	3.681
140	C	-5.483	-0.700	4.904
141	C	-5.483	0.736	4.904
142	C	-5.413	-1.472	6.098
143	C	-4.890	2.771	-6.133
144	C	-4.394	3.366	-4.939
145	C	-5.286	1.422	-3.716
146	C	-4.739	2.741	-3.716
147	C	-5.404	0.722	-2.480
148	C	-5.272	1.424	-1.245
149	C	-5.418	-0.693	-0.018
150	C	-5.418	0.729	-0.018
151	C	-5.272	-1.388	1.210
152	C	-5.404	-0.686	2.445
153	C	-4.739	-2.706	3.681
154	C	-5.286	-1.386	3.681
155	C	-4.394	-3.330	4.904
156	C	-4.890	-2.735	6.098

157	C	-5.413	1.508	-6.133
158	C	-5.483	-0.700	-4.939
159	C	-5.483	0.736	-4.939
160	C	-5.286	-1.386	-3.716
161	C	-5.404	-0.686	-2.480
162	C	-4.731	-2.694	-1.245
163	C	-5.272	-1.388	-1.245
164	C	-4.343	-3.289	-0.018
165	C	-4.731	-2.694	1.210
166	C	-3.332	-4.280	2.445
167	C	-4.328	-3.284	2.445
168	C	-2.754	-4.691	3.681
169	C	-3.378	-4.346	4.904
170	C	-2.783	-4.842	6.098
171	C	-4.890	-2.735	-6.133
172	C	-5.413	-1.472	-6.133
173	C	-4.394	-3.330	-4.939
174	C	-4.739	-2.706	-3.716
175	C	-3.332	-4.280	-2.480
176	C	-4.328	-3.284	-2.480
177	C	-2.742	-4.683	-1.245
178	C	-3.337	-4.295	-0.018
179	C	-2.742	-4.683	1.210
180	C	-2.783	-4.842	-6.133
181	C	-3.378	-4.346	-4.939
182	C	-2.754	-4.691	-3.716
183	H	-1.072	-5.644	7.047
184	H	1.012	-5.644	7.047
185	H	3.236	-4.722	7.047
186	H	-1.072	-5.644	-7.082
187	H	5.631	-1.024	7.047
188	H	4.710	-3.249	7.047
189	H	3.236	-4.722	-7.082
190	H	1.012	-5.644	-7.082
191	H	5.631	1.060	7.047
192	H	4.710	-3.249	-7.082
193	H	4.710	3.284	7.047
194	H	5.631	-1.024	-7.082
195	H	1.012	5.680	7.047
196	H	3.236	4.758	7.047
197	H	4.710	3.284	-7.082
198	H	5.631	1.060	-7.082
199	H	-1.072	5.680	7.047
200	H	3.236	4.758	-7.082
201	H	-3.297	4.758	7.047
202	H	1.012	5.680	-7.082
203	H	-5.692	1.060	7.047
204	H	-4.770	3.284	7.047
205	H	-3.297	4.758	-7.082
206	H	-1.072	5.680	-7.082
207	H	-5.692	-1.024	7.047
208	H	-4.770	3.284	-7.082
209	H	-4.770	-3.249	7.047
210	H	-5.692	1.060	-7.082
211	H	-3.297	-4.722	7.047
212	H	-4.770	-3.249	-7.082
213	H	-5.692	-1.024	-7.082
214	H	-3.297	-4.722	-7.082

Table S15. The coordinates and energies of the sampled structures of confined water dimer in (9, 9) CNT. The first structure which is highlighted with underline was used in the paper.

Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$\underline{(H_2O)_2}$@(9, 9) CNT_1	0.000000	1	O	2.761	0.509	0.693
		2	H	3.571	0.286	1.263
		3	H	3.133	1.328	0.224
		4	O	2.826	-1.360	-1.144
		5	H	2.775	-0.620	-0.425
		6	H	1.982	-1.865	-0.886
		7	C	6.238	0.020	6.116
		8	C	6.063	0.062	1.230
		9	C	6.012	0.774	2.464
		10	C	6.083	0.067	3.700
		11	C	5.761	2.177	4.923
		12	C	6.101	0.781	4.923
		13	C	5.532	2.915	6.116
		14	C	6.083	0.067	-3.697
		15	C	6.012	0.774	-2.461
		16	C	6.063	0.062	-1.227
		17	C	5.686	2.150	0.002
		18	C	6.023	0.770	0.002
		19	C	5.396	2.797	1.230
		20	C	5.679	2.142	2.464
		21	C	4.623	3.989	3.700
		22	C	5.415	2.802	3.700
		23	C	4.178	4.548	4.923
		24	C	4.772	4.053	6.116
		25	C	6.238	0.020	-6.113
		26	C	5.761	2.177	-4.919
		27	C	6.101	0.781	-4.919
		28	C	5.415	2.802	-3.697
		29	C	5.679	2.142	-2.461
		30	C	4.611	3.973	-1.227
		31	C	5.396	2.797	-1.227
		32	C	4.125	4.489	0.002
		33	C	4.611	3.973	1.230
		34	C	2.980	5.318	2.464
		35	C	4.114	4.485	2.464
		36	C	2.354	5.655	3.700
		37	C	3.020	5.398	4.923
		38	C	1.057	6.200	6.116
		39	C	2.370	5.816	6.116
		40	C	4.772	4.053	-6.113
		41	C	5.532	2.915	-6.113
		42	C	4.178	4.548	-4.919
		43	C	4.623	3.989	-3.697
		44	C	2.980	5.318	-2.461
		45	C	4.114	4.485	-2.461
		46	C	2.342	5.638	-1.227
		47	C	2.980	5.330	0.002
		48	C	0.985	6.035	1.230
		49	C	2.342	5.638	1.230
		50	C	0.275	6.108	2.464
		51	C	0.983	6.055	3.700
		52	C	-1.150	6.104	4.923
		53	C	0.284	6.197	4.923
		54	C	-1.917	6.007	6.116
		55	C	2.370	5.816	-6.113

56	C	3.020	5.398	-4.919
57	C	0.983	6.055	-3.697
58	C	2.354	5.655	-3.697
59	C	0.275	6.108	-2.461
60	C	0.985	6.035	-1.227
61	C	-1.137	6.026	0.002
62	C	0.281	6.118	0.002
63	C	-1.824	5.852	1.230
64	C	-1.130	6.017	2.464
65	C	-3.133	5.298	3.700
66	C	-1.826	5.872	3.700
67	C	-3.760	4.957	4.923
68	C	-3.170	5.456	6.116
69	C	1.057	6.200	-6.113
70	C	-1.150	6.104	-4.919
71	C	0.284	6.197	-4.919
72	C	-1.826	5.872	-3.697
73	C	-1.130	6.017	-2.461
74	C	-3.119	5.284	-1.227
75	C	-1.824	5.852	-1.227
76	C	-3.711	4.895	0.002
77	C	-3.119	5.284	1.230
78	C	-4.727	3.911	2.464
79	C	-3.710	4.884	2.464
80	C	-5.167	3.353	3.700
81	C	-4.799	3.964	4.923
82	C	-5.929	2.170	6.116
83	C	-5.323	3.397	6.116
84	C	-3.170	5.456	-6.113
85	C	-1.917	6.007	-6.113
86	C	-3.760	4.957	-4.919
87	C	-3.133	5.298	-3.697
88	C	-4.727	3.911	-2.461
89	C	-3.710	4.884	-2.461
90	C	-5.153	3.338	-1.227
91	C	-4.738	3.913	0.002
92	C	-5.779	2.071	1.230
93	C	-5.153	3.338	1.230
94	C	-5.975	1.384	2.464
95	C	-5.799	2.073	3.700
96	C	-6.218	-0.020	4.923
97	C	-6.061	1.409	4.923
98	C	-6.255	-0.792	6.116
99	C	-5.323	3.397	-6.113
100	C	-4.799	3.964	-4.919
101	C	-5.799	2.073	-3.697
102	C	-5.167	3.353	-3.697
103	C	-5.975	1.384	-2.461
104	C	-5.779	2.071	-1.227
105	C	-6.139	-0.021	0.002
106	C	-5.983	1.392	0.002
107	C	-6.087	-0.727	1.230
108	C	-6.129	-0.015	2.464
109	C	-5.768	-2.112	3.700
110	C	-6.107	-0.725	3.700
111	C	-5.542	-2.789	4.923
112	C	-5.931	-2.121	6.116
113	C	-5.929	2.170	-6.113
114	C	-6.218	-0.020	-4.919

115	C	-6.061	1.409	-4.919
116	C	-6.107	-0.725	-3.697
117	C	-6.129	-0.015	-2.461
118	C	-5.752	-2.101	-1.227
119	C	-6.087	-0.727	-1.227
120	C	-5.472	-2.752	0.002
121	C	-5.752	-2.101	1.230
122	C	-4.679	-3.923	2.464
123	C	-5.460	-2.752	2.464
124	C	-4.206	-4.453	3.700
125	C	-4.744	-3.984	4.923
126	C	-3.174	-5.409	6.116
127	C	-4.276	-4.600	6.116
128	C	-5.931	-2.121	-6.113
129	C	-6.255	-0.792	-6.113
130	C	-5.542	-2.789	-4.919
131	C	-5.768	-2.112	-3.697
132	C	-4.679	-3.923	-2.461
133	C	-5.460	-2.752	-2.461
134	C	-4.189	-4.442	-1.227
135	C	-4.683	-3.934	0.002
136	C	-3.049	-5.279	1.230
137	C	-4.189	-4.442	1.230
138	C	-2.408	-5.591	2.464
139	C	-3.055	-5.298	3.700
140	C	-1.067	-6.074	4.923
141	C	-2.446	-5.671	4.923
142	C	-0.313	-6.245	6.116
143	C	-4.276	-4.600	-6.113
144	C	-4.744	-3.984	-4.919
145	C	-3.055	-5.298	-3.697
146	C	-4.206	-4.453	-3.697
147	C	-2.408	-5.591	-2.461
148	C	-3.049	-5.279	-1.227
149	C	-1.053	-5.996	0.002
150	C	-2.417	-5.598	0.002
151	C	-0.347	-6.068	1.230
152	C	-1.056	-5.985	2.464
153	C	1.071	-5.995	3.700
154	C	-0.353	-6.087	3.700
155	C	1.777	-5.889	4.923
156	C	1.052	-6.156	6.116
157	C	-3.174	-5.409	-6.113
158	C	-1.067	-6.074	-4.919
159	C	-2.446	-5.671	-4.919
160	C	-0.353	-6.087	-3.697
161	C	-1.056	-5.985	-2.461
162	C	1.063	-5.976	-1.227
163	C	-0.347	-6.068	-1.227
164	C	1.753	-5.814	0.002
165	C	1.063	-5.976	1.230
166	C	3.044	-5.236	2.464
167	C	1.756	-5.803	2.464
168	C	3.649	-4.862	3.700
169	C	3.093	-5.311	4.923
170	C	4.769	-4.012	6.116
171	C	3.780	-4.957	6.116
172	C	1.052	-6.156	-6.113
173	C	-0.313	-6.245	-6.113

174	C	1.777	-5.889	-4.919
175	C	1.071	-5.995	-3.697
176	C	3.044	-5.236	-2.461
177	C	1.756	-5.803	-2.461
178	C	3.640	-4.844	-1.227
179	C	3.054	-5.242	0.002
180	C	4.662	-3.867	1.230
181	C	3.640	-4.844	1.230
182	C	5.081	-3.289	2.464
183	C	4.680	-3.876	3.700
184	C	5.790	-2.053	4.923
185	C	5.153	-3.341	4.923
186	C	6.089	-1.340	6.116
187	C	3.780	-4.957	-6.113
188	C	3.093	-5.311	-4.919
189	C	4.680	-3.876	-3.697
190	C	3.649	-4.862	-3.697
191	C	5.081	-3.289	-2.461
192	C	4.662	-3.867	-1.227
193	C	5.716	-2.025	0.002
194	C	5.086	-3.299	0.002
195	C	5.909	-1.343	1.230
196	C	5.704	-2.027	2.464
197	C	5.927	-1.352	3.700
198	C	4.769	-4.012	-6.113
199	C	5.790	-2.052	-4.919
200	C	5.153	-3.341	-4.919
201	C	5.927	-1.352	-3.697
202	C	5.704	-2.027	-2.461
203	C	5.909	-1.343	-1.227
204	C	6.089	-1.340	-6.113
205	H	6.381	0.526	7.065
206	H	5.892	2.532	7.065
207	H	4.556	4.532	7.065
208	H	6.381	0.526	-7.062
209	H	0.583	6.429	7.065
210	H	2.892	5.754	7.065
211	H	4.556	4.532	-7.062
212	H	5.892	2.532	-7.062
213	H	-1.477	6.295	7.065
214	H	2.892	5.754	-7.062
215	H	-3.679	5.327	7.065
216	H	0.583	6.429	-7.062
217	H	-6.236	1.744	7.065
218	H	-5.171	3.900	7.065
219	H	-3.679	5.327	-7.062
220	H	-1.477	6.295	-7.062
221	H	-6.462	-0.309	7.065
222	H	-5.171	3.900	-7.062
223	H	-5.892	-2.645	7.065
224	H	-6.236	1.744	-7.062
225	H	-2.807	-5.786	7.065
226	H	-4.746	-4.363	7.065
227	H	-5.892	-2.645	-7.062
228	H	-6.462	-0.309	-7.062
229	H	-0.825	-6.365	7.065
230	H	-4.746	-4.363	-7.062
231	H	1.575	-6.209	7.065
232	H	-2.807	-5.786	-7.062

		233	H	5.204	-3.716	7.065
		234	H	3.466	-5.378	7.065
		235	H	1.575	-6.209	-7.062
		236	H	-0.825	-6.365	-7.062
		237	H	6.118	-1.865	7.065
		238	H	3.466	-5.378	-7.062
		239	H	5.204	-3.716	-7.062
		240	H	6.118	-1.865	-7.062
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(9, 9) CNT_2	0.000001	1	O	-0.215	3.134	1.158
		2	H	0.646	2.656	0.901
		3	H	-0.829	2.720	0.437
		4	O	-1.795	2.144	-0.685
		5	H	-2.009	2.958	-1.253
		6	H	-2.692	2.052	-0.217
		7	C	6.296	-0.037	6.123
		8	C	6.120	0.005	1.237
		9	C	6.070	0.717	2.471
		10	C	6.140	0.010	3.707
		11	C	5.818	2.120	4.929
		12	C	6.159	0.723	4.929
		13	C	5.589	2.858	6.123
		14	C	6.140	0.010	-3.690
		15	C	6.070	0.717	-2.454
		16	C	6.120	0.005	-1.220
		17	C	5.744	2.093	0.008
		18	C	6.080	0.713	0.008
		19	C	5.453	2.740	1.237
		20	C	5.736	2.084	2.471
		21	C	4.680	3.932	3.707
		22	C	5.473	2.744	3.707
		23	C	4.236	4.490	4.929
		24	C	4.830	3.996	6.123
		25	C	6.296	-0.037	-6.106
		26	C	5.818	2.120	-4.913
		27	C	6.159	0.723	-4.913
		28	C	5.473	2.744	-3.690
		29	C	5.736	2.084	-2.454
		30	C	4.668	3.916	-1.220
		31	C	5.453	2.740	-1.220
		32	C	4.183	4.432	0.008
		33	C	4.668	3.916	1.237
		34	C	3.037	5.261	2.471
		35	C	4.172	4.428	2.471
		36	C	2.411	5.598	3.707
		37	C	3.077	5.341	4.929
		38	C	1.114	6.143	6.123
		39	C	2.427	5.759	6.123
		40	C	4.830	3.996	-6.106
		41	C	5.589	2.858	-6.106
		42	C	4.236	4.490	-4.913
		43	C	4.680	3.932	-3.690
		44	C	3.037	5.261	-2.454
		45	C	4.172	4.428	-2.454
		46	C	2.399	5.581	-1.220
		47	C	3.037	5.273	0.008
		48	C	1.042	5.978	1.237
		49	C	2.399	5.581	1.237
		50	C	0.332	6.051	2.471

51	C	1.041	5.998	3.707
52	C	-1.093	6.047	4.929
53	C	0.341	6.140	4.929
54	C	-1.860	5.950	6.123
55	C	2.427	5.759	-6.106
56	C	3.077	5.341	-4.913
57	C	1.041	5.998	-3.690
58	C	2.411	5.598	-3.690
59	C	0.332	6.051	-2.454
60	C	1.042	5.978	-1.220
61	C	-1.080	5.969	0.008
62	C	0.338	6.061	0.008
63	C	-1.767	5.795	1.237
64	C	-1.073	5.960	2.471
65	C	-3.075	5.241	3.707
66	C	-1.768	5.815	3.707
67	C	-3.703	4.900	4.929
68	C	-3.112	5.399	6.123
69	C	1.114	6.143	-6.106
70	C	-1.093	6.047	-4.913
71	C	0.341	6.140	-4.913
72	C	-1.768	5.815	-3.690
73	C	-1.073	5.960	-2.454
74	C	-3.061	5.226	-1.220
75	C	-1.767	5.795	-1.220
76	C	-3.654	4.838	0.008
77	C	-3.061	5.226	1.237
78	C	-4.670	3.854	2.471
79	C	-3.652	4.826	2.471
80	C	-5.110	3.296	3.707
81	C	-4.741	3.907	4.929
82	C	-5.872	2.113	6.123
83	C	-5.266	3.340	6.123
84	C	-3.112	5.399	-6.106
85	C	-1.860	5.950	-6.106
86	C	-3.703	4.900	-4.913
87	C	-3.075	5.241	-3.690
88	C	-4.670	3.854	-2.454
89	C	-3.652	4.826	-2.454
90	C	-5.096	3.281	-1.220
91	C	-4.681	3.856	0.008
92	C	-5.722	2.013	1.237
93	C	-5.096	3.281	1.237
94	C	-5.917	1.327	2.471
95	C	-5.742	2.016	3.707
96	C	-6.161	-0.077	4.929
97	C	-6.003	1.351	4.929
98	C	-6.198	-0.849	6.123
99	C	-5.266	3.340	-6.106
100	C	-4.741	3.907	-4.913
101	C	-5.742	2.016	-3.690
102	C	-5.110	3.296	-3.690
103	C	-5.917	1.327	-2.454
104	C	-5.722	2.013	-1.220
105	C	-6.082	-0.078	0.008
106	C	-5.926	1.335	0.008
107	C	-6.030	-0.785	1.237
108	C	-6.071	-0.072	2.471
109	C	-5.711	-2.169	3.707

110	C	-6.050	-0.782	3.707
111	C	-5.485	-2.846	4.929
112	C	-5.874	-2.178	6.123
113	C	-5.872	2.113	-6.106
114	C	-6.161	-0.077	-4.913
115	C	-6.003	1.351	-4.913
116	C	-6.050	-0.782	-3.690
117	C	-6.071	-0.072	-2.454
118	C	-5.694	-2.158	-1.220
119	C	-6.030	-0.785	-1.220
120	C	-5.415	-2.809	0.008
121	C	-5.694	-2.158	1.237
122	C	-4.622	-3.981	2.471
123	C	-5.403	-2.810	2.471
124	C	-4.149	-4.511	3.707
125	C	-4.687	-4.042	4.929
126	C	-3.116	-5.467	6.123
127	C	-4.219	-4.657	6.123
128	C	-5.874	-2.178	-6.106
129	C	-6.198	-0.849	-6.106
130	C	-5.485	-2.846	-4.913
131	C	-5.711	-2.169	-3.690
132	C	-4.622	-3.981	-2.454
133	C	-5.403	-2.810	-2.454
134	C	-4.132	-4.499	-1.220
135	C	-4.626	-3.991	0.008
136	C	-2.992	-5.336	1.237
137	C	-4.132	-4.499	1.237
138	C	-2.350	-5.648	2.471
139	C	-2.998	-5.355	3.707
140	C	-1.010	-6.131	4.929
141	C	-2.389	-5.728	4.929
142	C	-0.256	-6.302	6.123
143	C	-4.219	-4.657	-6.106
144	C	-4.687	-4.042	-4.913
145	C	-2.998	-5.355	-3.690
146	C	-4.149	-4.511	-3.690
147	C	-2.350	-5.648	-2.454
148	C	-2.992	-5.336	-1.220
149	C	-0.995	-6.054	0.008
150	C	-2.359	-5.655	0.008
151	C	-0.290	-6.125	1.237
152	C	-0.999	-6.043	2.471
153	C	1.129	-6.052	3.707
154	C	-0.296	-6.145	3.707
155	C	1.835	-5.946	4.929
156	C	1.109	-6.213	6.123
157	C	-3.116	-5.467	-6.106
158	C	-1.010	-6.131	-4.913
159	C	-2.389	-5.728	-4.913
160	C	-0.296	-6.145	-3.690
161	C	-0.999	-6.043	-2.454
162	C	1.121	-6.033	-1.220
163	C	-0.290	-6.125	-1.220
164	C	1.811	-5.871	0.008
165	C	1.121	-6.033	1.237
166	C	3.102	-5.294	2.471
167	C	1.813	-5.860	2.471
168	C	3.706	-4.920	3.707

169	C	3.151	-5.368	4.929
170	C	4.827	-4.069	6.123
171	C	3.838	-5.015	6.123
172	C	1.109	-6.213	-6.106
173	C	-0.256	-6.302	-6.106
174	C	1.835	-5.946	-4.913
175	C	1.129	-6.052	-3.690
176	C	3.102	-5.294	-2.454
177	C	1.813	-5.860	-2.454
178	C	3.698	-4.901	-1.220
179	C	3.111	-5.300	0.008
180	C	4.719	-3.924	1.237
181	C	3.698	-4.901	1.237
182	C	5.138	-3.346	2.471
183	C	4.738	-3.933	3.707
184	C	5.847	-2.110	4.929
185	C	5.211	-3.398	4.929
186	C	6.146	-1.397	6.123
187	C	3.838	-5.015	-6.106
188	C	3.151	-5.368	-4.913
189	C	4.738	-3.933	-3.690
190	C	3.706	-4.920	-3.690
191	C	5.138	-3.346	-2.454
192	C	4.719	-3.924	-1.220
193	C	5.773	-2.082	0.008
194	C	5.144	-3.356	0.008
195	C	5.966	-1.400	1.237
196	C	5.761	-2.084	2.471
197	C	5.984	-1.409	3.707
198	C	4.827	-4.069	-6.106
199	C	5.847	-2.110	-4.913
200	C	5.211	-3.398	-4.913
201	C	5.984	-1.409	-3.690
202	C	5.761	-2.084	-2.454
203	C	5.966	-1.400	-1.220
204	C	6.146	-1.397	-6.106
205	H	6.439	0.469	7.072
206	H	5.949	2.475	7.072
207	H	4.614	4.475	7.072
208	H	6.439	0.469	-7.056
209	H	0.641	6.371	7.072
210	H	2.949	5.697	7.072
211	H	4.614	4.475	-7.056
212	H	5.949	2.475	-7.056
213	H	-1.420	6.237	7.072
214	H	2.949	5.697	-7.056
215	H	-3.622	5.270	7.072
216	H	0.641	6.371	-7.056
217	H	-6.179	1.686	7.072
218	H	-5.114	3.843	7.072
219	H	-3.622	5.270	-7.056
220	H	-1.420	6.237	-7.056
221	H	-6.405	-0.366	7.072
222	H	-5.114	3.843	-7.056
223	H	-5.835	-2.703	7.072
224	H	-6.179	1.686	-7.056
225	H	-2.750	-5.843	7.072
226	H	-4.688	-4.420	7.072
227	H	-5.835	-2.703	-7.056

		228	H	-6.405	-0.366	-7.056
		229	H	-0.768	-6.422	7.072
		230	H	-4.688	-4.420	-7.056
		231	H	1.632	-6.266	7.072
		232	H	-2.750	-5.843	-7.056
		233	H	5.261	-3.773	7.072
		234	H	3.523	-5.435	7.072
		235	H	1.632	-6.266	-7.056
		236	H	-0.768	-6.422	-7.056
		237	H	6.175	-1.922	7.072
		238	H	3.523	-5.435	-7.056
		239	H	5.261	-3.773	-7.056
		240	H	6.175	-1.922	-7.056
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(9, 9) CNT_3	0.000002	1	O	-0.336	2.780	0.699
		2	H	-0.785	3.489	1.270
		3	H	0.336	3.377	0.227
		4	O	-2.146	2.289	-1.133
		5	H	-1.421	2.459	-0.416
		6	H	-2.377	1.332	-0.873
		7	C	6.296	-0.037	6.123
		8	C	6.120	0.005	1.237
		9	C	6.070	0.717	2.471
		10	C	6.140	0.010	3.707
		11	C	5.818	2.120	4.929
		12	C	6.159	0.723	4.929
		13	C	5.589	2.858	6.123
		14	C	6.140	0.010	-3.690
		15	C	6.070	0.717	-2.454
		16	C	6.120	0.005	-1.220
		17	C	5.744	2.093	0.008
		18	C	6.080	0.713	0.008
		19	C	5.453	2.740	1.237
		20	C	5.736	2.084	2.471
		21	C	4.680	3.932	3.707
		22	C	5.473	2.744	3.707
		23	C	4.236	4.490	4.929
		24	C	4.830	3.996	6.123
		25	C	6.296	-0.037	-6.106
		26	C	5.818	2.120	-4.913
		27	C	6.159	0.723	-4.913
		28	C	5.473	2.744	-3.690
		29	C	5.736	2.084	-2.454
		30	C	4.668	3.916	-1.220
		31	C	5.453	2.740	-1.220
		32	C	4.183	4.432	0.008
		33	C	4.668	3.916	1.237
		34	C	3.037	5.261	2.471
		35	C	4.172	4.428	2.471
		36	C	2.411	5.598	3.707
		37	C	3.077	5.341	4.929
		38	C	1.114	6.143	6.123
		39	C	2.427	5.759	6.123
		40	C	4.830	3.996	-6.106
		41	C	5.589	2.858	-6.106
		42	C	4.236	4.490	-4.913
		43	C	4.680	3.932	-3.690
		44	C	3.037	5.261	-2.454
		45	C	4.172	4.428	-2.454

46	C	2.399	5.581	-1.220
47	C	3.037	5.273	0.008
48	C	1.042	5.978	1.237
49	C	2.399	5.581	1.237
50	C	0.332	6.051	2.471
51	C	1.041	5.998	3.707
52	C	-1.093	6.047	4.929
53	C	0.341	6.140	4.929
54	C	-1.860	5.950	6.123
55	C	2.427	5.759	-6.106
56	C	3.077	5.341	-4.913
57	C	1.041	5.998	-3.690
58	C	2.411	5.598	-3.690
59	C	0.332	6.051	-2.454
60	C	1.042	5.978	-1.220
61	C	-1.080	5.969	0.008
62	C	0.338	6.061	0.008
63	C	-1.767	5.795	1.237
64	C	-1.073	5.960	2.470
65	C	-3.075	5.241	3.707
66	C	-1.768	5.815	3.707
67	C	-3.703	4.900	4.929
68	C	-3.112	5.399	6.123
69	C	1.114	6.143	-6.106
70	C	-1.093	6.047	-4.913
71	C	0.341	6.140	-4.913
72	C	-1.768	5.815	-3.690
73	C	-1.073	5.960	-2.454
74	C	-3.061	5.226	-1.220
75	C	-1.767	5.795	-1.220
76	C	-3.654	4.838	0.008
77	C	-3.061	5.227	1.236
78	C	-4.670	3.854	2.471
79	C	-3.652	4.826	2.470
80	C	-5.110	3.296	3.707
81	C	-4.741	3.907	4.929
82	C	-5.872	2.113	6.123
83	C	-5.266	3.340	6.123
84	C	-3.112	5.399	-6.106
85	C	-1.860	5.950	-6.106
86	C	-3.703	4.900	-4.913
87	C	-3.075	5.241	-3.690
88	C	-4.670	3.854	-2.454
89	C	-3.652	4.826	-2.454
90	C	-5.096	3.281	-1.220
91	C	-4.681	3.856	0.008
92	C	-5.722	2.013	1.237
93	C	-5.096	3.281	1.237
94	C	-5.917	1.327	2.471
95	C	-5.742	2.016	3.707
96	C	-6.161	-0.077	4.929
97	C	-6.003	1.351	4.929
98	C	-6.198	-0.849	6.123
99	C	-5.266	3.340	-6.106
100	C	-4.741	3.907	-4.913
101	C	-5.742	2.016	-3.690
102	C	-5.110	3.296	-3.690
103	C	-5.917	1.327	-2.454
104	C	-5.722	2.013	-1.220

105	C	-6.082	-0.078	0.008
106	C	-5.926	1.335	0.008
107	C	-6.030	-0.785	1.237
108	C	-6.071	-0.072	2.471
109	C	-5.711	-2.169	3.707
110	C	-6.050	-0.782	3.707
111	C	-5.485	-2.846	4.929
112	C	-5.874	-2.178	6.123
113	C	-5.872	2.113	-6.106
114	C	-6.161	-0.077	-4.913
115	C	-6.003	1.351	-4.913
116	C	-6.050	-0.782	-3.690
117	C	-6.071	-0.072	-2.454
118	C	-5.694	-2.158	-1.220
119	C	-6.030	-0.785	-1.220
120	C	-5.415	-2.809	0.008
121	C	-5.694	-2.158	1.237
122	C	-4.622	-3.981	2.471
123	C	-5.403	-2.810	2.471
124	C	-4.149	-4.511	3.707
125	C	-4.687	-4.042	4.929
126	C	-3.116	-5.467	6.123
127	C	-4.219	-4.657	6.123
128	C	-5.874	-2.178	-6.106
129	C	-6.198	-0.849	-6.106
130	C	-5.485	-2.846	-4.913
131	C	-5.711	-2.169	-3.690
132	C	-4.622	-3.981	-2.454
133	C	-5.403	-2.810	-2.454
134	C	-4.132	-4.499	-1.220
135	C	-4.626	-3.991	0.008
136	C	-2.992	-5.336	1.237
137	C	-4.132	-4.499	1.237
138	C	-2.350	-5.648	2.471
139	C	-2.998	-5.355	3.707
140	C	-1.010	-6.131	4.929
141	C	-2.389	-5.728	4.929
142	C	-0.256	-6.302	6.123
143	C	-4.219	-4.657	-6.106
144	C	-4.687	-4.042	-4.913
145	C	-2.998	-5.355	-3.690
146	C	-4.149	-4.511	-3.690
147	C	-2.350	-5.648	-2.454
148	C	-2.992	-5.336	-1.220
149	C	-0.995	-6.054	0.008
150	C	-2.359	-5.655	0.008
151	C	-0.290	-6.125	1.237
152	C	-0.999	-6.043	2.471
153	C	1.129	-6.052	3.707
154	C	-0.296	-6.145	3.707
155	C	1.835	-5.946	4.929
156	C	1.109	-6.213	6.123
157	C	-3.116	-5.467	-6.106
158	C	-1.010	-6.131	-4.913
159	C	-2.389	-5.728	-4.913
160	C	-0.296	-6.145	-3.690
161	C	-0.999	-6.043	-2.454
162	C	1.121	-6.033	-1.220
163	C	-0.290	-6.125	-1.220

164	C	1.811	-5.871	0.008
165	C	1.121	-6.033	1.237
166	C	3.102	-5.294	2.471
167	C	1.813	-5.860	2.471
168	C	3.706	-4.920	3.707
169	C	3.151	-5.368	4.929
170	C	4.827	-4.069	6.123
171	C	3.838	-5.015	6.123
172	C	1.109	-6.213	-6.106
173	C	-0.256	-6.302	-6.106
174	C	1.835	-5.946	-4.913
175	C	1.129	-6.052	-3.690
176	C	3.102	-5.294	-2.454
177	C	1.813	-5.860	-2.454
178	C	3.698	-4.901	-1.220
179	C	3.111	-5.300	0.008
180	C	4.719	-3.924	1.237
181	C	3.698	-4.901	1.237
182	C	5.138	-3.346	2.471
183	C	4.738	-3.933	3.707
184	C	5.847	-2.110	4.929
185	C	5.211	-3.398	4.929
186	C	6.146	-1.397	6.123
187	C	3.838	-5.015	-6.106
188	C	3.151	-5.368	-4.913
189	C	4.738	-3.933	-3.690
190	C	3.706	-4.920	-3.690
191	C	5.138	-3.346	-2.454
192	C	4.719	-3.924	-1.220
193	C	5.773	-2.082	0.008
194	C	5.144	-3.356	0.008
195	C	5.966	-1.400	1.237
196	C	5.761	-2.084	2.471
197	C	5.984	-1.409	3.707
198	C	4.827	-4.069	-6.106
199	C	5.847	-2.110	-4.913
200	C	5.211	-3.398	-4.913
201	C	5.984	-1.409	-3.690
202	C	5.761	-2.084	-2.454
203	C	5.966	-1.400	-1.220
204	C	6.146	-1.397	-6.106
205	H	6.439	0.469	7.072
206	H	5.949	2.475	7.072
207	H	4.614	4.475	7.072
208	H	6.439	0.469	-7.056
209	H	0.641	6.371	7.072
210	H	2.949	5.697	7.072
211	H	4.614	4.475	-7.056
212	H	5.949	2.475	-7.056
213	H	-1.420	6.237	7.072
214	H	2.949	5.697	-7.056
215	H	-3.622	5.270	7.072
216	H	0.641	6.371	-7.056
217	H	-6.179	1.686	7.072
218	H	-5.114	3.843	7.072
219	H	-3.622	5.270	-7.056
220	H	-1.420	6.237	-7.056
221	H	-6.405	-0.366	7.072
222	H	-5.114	3.843	-7.056

		223	H	-5.835	-2.703	7.072
		224	H	-6.179	1.686	-7.056
		225	H	-2.750	-5.843	7.072
		226	H	-4.688	-4.420	7.072
		227	H	-5.835	-2.703	-7.056
		228	H	-6.405	-0.366	-7.056
		229	H	-0.768	-6.422	7.072
		230	H	-4.688	-4.420	-7.056
		231	H	1.632	-6.266	7.072
		232	H	-2.750	-5.843	-7.056
		233	H	5.261	-3.773	7.072
		234	H	3.523	-5.435	7.072
		235	H	1.632	-6.266	-7.056
		236	H	-0.768	-6.422	-7.056
		237	H	6.175	-1.922	7.072
		238	H	3.523	-5.435	-7.056
		239	H	5.261	-3.773	-7.056
		240	H	6.175	-1.922	-7.056
Opt Structure	ΔE (Hartree)	Number	Atom	x (Å)	y (Å)	z (Å)
$(H_2O)_2$@(9, 9) CNT_4	0.000161	1	O	2.911	-1.148	1.386
		2	H	2.660	-0.165	1.469
		3	H	2.671	-1.274	0.389
		4	O	2.391	-1.494	-1.156
		5	H	2.326	-2.504	-1.237
		6	H	3.303	-1.369	-1.584
		7	C	6.238	0.020	6.116
		8	C	6.063	0.062	1.230
		9	C	6.012	0.774	2.464
		10	C	6.083	0.067	3.700
		11	C	5.761	2.177	4.923
		12	C	6.101	0.781	4.923
		13	C	5.532	2.915	6.116
		14	C	6.083	0.067	-3.697
		15	C	6.012	0.774	-2.461
		16	C	6.063	0.062	-1.227
		17	C	5.686	2.150	0.002
		18	C	6.023	0.770	0.002
		19	C	5.396	2.797	1.230
		20	C	5.679	2.142	2.464
		21	C	4.623	3.989	3.700
		22	C	5.415	2.802	3.700
		23	C	4.178	4.548	4.923
		24	C	4.772	4.053	6.116
		25	C	6.238	0.020	-6.113
		26	C	5.761	2.177	-4.919
		27	C	6.101	0.781	-4.919
		28	C	5.415	2.802	-3.697
		29	C	5.679	2.142	-2.461
		30	C	4.611	3.973	-1.227
		31	C	5.396	2.797	-1.227
		32	C	4.125	4.489	0.002
		33	C	4.611	3.973	1.230
		34	C	2.980	5.318	2.464
		35	C	4.114	4.485	2.464
		36	C	2.354	5.655	3.700
		37	C	3.020	5.398	4.923
		38	C	1.057	6.200	6.116
		39	C	2.370	5.816	6.116
		40	C	4.772	4.053	-6.113

41	C	5.532	2.915	-6.113
42	C	4.178	4.548	-4.919
43	C	4.623	3.989	-3.697
44	C	2.980	5.318	-2.461
45	C	4.114	4.485	-2.461
46	C	2.342	5.638	-1.227
47	C	2.980	5.330	0.002
48	C	0.985	6.035	1.230
49	C	2.342	5.638	1.230
50	C	0.275	6.108	2.464
51	C	0.983	6.055	3.700
52	C	-1.150	6.104	4.923
53	C	0.284	6.197	4.923
54	C	-1.917	6.007	6.116
55	C	2.370	5.816	-6.113
56	C	3.020	5.398	-4.919
57	C	0.983	6.055	-3.697
58	C	2.354	5.655	-3.697
59	C	0.275	6.108	-2.461
60	C	0.985	6.035	-1.227
61	C	-1.137	6.026	0.002
62	C	0.281	6.118	0.002
63	C	-1.824	5.852	1.230
64	C	-1.130	6.017	2.464
65	C	-3.133	5.298	3.700
66	C	-1.826	5.872	3.700
67	C	-3.760	4.957	4.923
68	C	-3.170	5.456	6.116
69	C	1.057	6.200	-6.113
70	C	-1.150	6.104	-4.919
71	C	0.284	6.197	-4.919
72	C	-1.826	5.872	-3.697
73	C	-1.130	6.017	-2.461
74	C	-3.119	5.284	-1.227
75	C	-1.824	5.852	-1.227
76	C	-3.711	4.895	0.002
77	C	-3.119	5.284	1.230
78	C	-4.727	3.911	2.464
79	C	-3.710	4.884	2.464
80	C	-5.167	3.353	3.700
81	C	-4.799	3.964	4.923
82	C	-5.929	2.170	6.116
83	C	-5.323	3.397	6.116
84	C	-3.170	5.456	-6.113
85	C	-1.917	6.007	-6.113
86	C	-3.760	4.957	-4.919
87	C	-3.133	5.298	-3.697
88	C	-4.727	3.911	-2.461
89	C	-3.710	4.884	-2.461
90	C	-5.153	3.338	-1.227
91	C	-4.738	3.913	0.002
92	C	-5.779	2.071	1.230
93	C	-5.153	3.338	1.230
94	C	-5.975	1.384	2.464
95	C	-5.799	2.073	3.700
96	C	-6.218	-0.020	4.923
97	C	-6.061	1.409	4.923
98	C	-6.255	-0.792	6.116
99	C	-5.323	3.397	-6.113

100	C	-4.799	3.964	-4.919
101	C	-5.799	2.073	-3.697
102	C	-5.167	3.353	-3.697
103	C	-5.975	1.384	-2.461
104	C	-5.779	2.071	-1.227
105	C	-6.139	-0.021	0.002
106	C	-5.983	1.392	0.002
107	C	-6.087	-0.727	1.230
108	C	-6.129	-0.015	2.464
109	C	-5.768	-2.112	3.700
110	C	-6.107	-0.725	3.700
111	C	-5.542	-2.789	4.923
112	C	-5.931	-2.121	6.116
113	C	-5.929	2.170	-6.113
114	C	-6.218	-0.020	-4.919
115	C	-6.061	1.409	-4.919
116	C	-6.107	-0.725	-3.697
117	C	-6.129	-0.015	-2.461
118	C	-5.752	-2.101	-1.227
119	C	-6.087	-0.727	-1.227
120	C	-5.472	-2.752	0.002
121	C	-5.752	-2.101	1.230
122	C	-4.679	-3.923	2.464
123	C	-5.460	-2.752	2.464
124	C	-4.206	-4.453	3.700
125	C	-4.744	-3.984	4.923
126	C	-3.174	-5.409	6.116
127	C	-4.276	-4.600	6.116
128	C	-5.931	-2.121	-6.113
129	C	-6.255	-0.792	-6.113
130	C	-5.542	-2.789	-4.919
131	C	-5.768	-2.112	-3.697
132	C	-4.679	-3.923	-2.461
133	C	-5.460	-2.752	-2.461
134	C	-4.189	-4.442	-1.227
135	C	-4.683	-3.934	0.002
136	C	-3.049	-5.279	1.230
137	C	-4.189	-4.442	1.230
138	C	-2.408	-5.591	2.464
139	C	-3.055	-5.298	3.700
140	C	-1.067	-6.074	4.923
141	C	-2.446	-5.671	4.923
142	C	-0.313	-6.245	6.116
143	C	-4.276	-4.600	-6.113
144	C	-4.744	-3.984	-4.919
145	C	-3.055	-5.298	-3.697
146	C	-4.206	-4.453	-3.697
147	C	-2.408	-5.591	-2.461
148	C	-3.049	-5.279	-1.227
149	C	-1.053	-5.996	0.002
150	C	-2.417	-5.598	0.002
151	C	-0.347	-6.068	1.230
152	C	-1.056	-5.985	2.464
153	C	1.071	-5.995	3.700
154	C	-0.353	-6.087	3.700
155	C	1.777	-5.889	4.923
156	C	1.052	-6.156	6.116
157	C	-3.174	-5.409	-6.113
158	C	-1.067	-6.074	-4.919

159	C	-2.446	-5.671	-4.919
160	C	-0.353	-6.087	-3.697
161	C	-1.056	-5.985	-2.461
162	C	1.063	-5.976	-1.227
163	C	-0.347	-6.068	-1.227
164	C	1.753	-5.814	0.002
165	C	1.063	-5.976	1.230
166	C	3.044	-5.236	2.464
167	C	1.756	-5.803	2.464
168	C	3.649	-4.862	3.700
169	C	3.093	-5.311	4.923
170	C	4.769	-4.012	6.116
171	C	3.780	-4.957	6.116
172	C	1.052	-6.156	-6.113
173	C	-0.313	-6.245	-6.113
174	C	1.777	-5.889	-4.919
175	C	1.071	-5.995	-3.697
176	C	3.044	-5.236	-2.461
177	C	1.756	-5.803	-2.461
178	C	3.640	-4.844	-1.227
179	C	3.054	-5.242	0.002
180	C	4.662	-3.867	1.230
181	C	3.640	-4.844	1.230
182	C	5.081	-3.289	2.464
183	C	4.680	-3.876	3.700
184	C	5.790	-2.052	4.923
185	C	5.153	-3.341	4.923
186	C	6.089	-1.340	6.116
187	C	3.780	-4.957	-6.113
188	C	3.093	-5.311	-4.919
189	C	4.680	-3.876	-3.697
190	C	3.649	-4.862	-3.697
191	C	5.081	-3.289	-2.460
192	C	4.662	-3.867	-1.227
193	C	5.716	-2.025	0.002
194	C	5.086	-3.299	0.002
195	C	5.909	-1.343	1.230
196	C	5.704	-2.027	2.464
197	C	5.927	-1.352	3.700
198	C	4.769	-4.012	-6.113
199	C	5.790	-2.053	-4.919
200	C	5.153	-3.341	-4.919
201	C	5.927	-1.352	-3.697
202	C	5.704	-2.027	-2.460
203	C	5.908	-1.343	-1.227
204	C	6.089	-1.340	-6.113
205	H	6.381	0.526	7.065
206	H	5.892	2.532	7.065
207	H	4.556	4.532	7.065
208	H	6.381	0.526	-7.062
209	H	0.583	6.429	7.065
210	H	2.892	5.754	7.065
211	H	4.556	4.532	-7.062
212	H	5.892	2.532	-7.062
213	H	-1.477	6.295	7.065
214	H	2.892	5.754	-7.062
215	H	-3.679	5.327	7.065
216	H	0.583	6.429	-7.062
217	H	-6.236	1.744	7.065

218	H	-5.171	3.900	7.065
219	H	-3.679	5.327	-7.062
220	H	-1.477	6.295	-7.062
221	H	-6.462	-0.309	7.065
222	H	-5.171	3.900	-7.062
223	H	-5.892	-2.645	7.065
224	H	-6.236	1.744	-7.062
225	H	-2.807	-5.786	7.065
226	H	-4.746	-4.363	7.065
227	H	-5.892	-2.645	-7.062
228	H	-6.462	-0.309	-7.062
229	H	-0.825	-6.365	7.065
230	H	-4.746	-4.363	-7.062
231	H	1.575	-6.209	7.065
232	H	-2.807	-5.786	-7.062
233	H	5.204	-3.716	7.065
234	H	3.466	-5.378	7.065
235	H	1.575	-6.209	-7.062
236	H	-0.825	-6.365	-7.062
237	H	6.118	-1.865	7.065
238	H	3.466	-5.378	-7.062
239	H	5.204	-3.716	-7.062
240	H	6.118	-1.865	-7.062

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