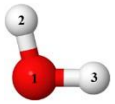
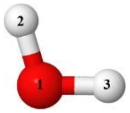
Electronic Supplementary Material (ESI) for RSC Advances.

Table S1 Structure parameters and energies of the water monomer, dimer and trimer obtained from CASPT2(4,4), (4,6) and (4,8) calculations, respectively. Distances and angles are in Å and degree, respectively.

	E^{Tot}	E^{Ex}	Distance		Angle	
G1-[1] 	-76.255865 (-75.991115) -76.255059 (-75.992457)	7.20 [7.15]	OH	0.97 [0.97]	∠HOH	104.0 [103.2]
E1-[1] 	-76.234152 (-76.003777) -76.234555 (-76.003505)	6.27 [6.28]	OH	1.09 [1.08]	∠HOH	104.9 [106.5]
E1-[2] 	-76.050102 (-76.031022) -76.045284 (-76.034444)	0.51 [0.29]	O_1H_2 O_1H_3	1.09 [1.09] 1.55 [1.55]	∠HOH	174.5 [174.5]

E^{Tot} = Total energy in au; E^{Ex} = $S_0 \rightarrow S_1$ excitation energy in eV; [..] = Values obtained from the CASPT2(6,5) method; ǂ = Transition state complex; (..) = Total energies in the S_1 state.

Table S1 (cont.)

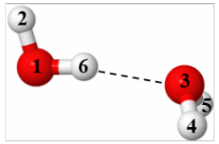
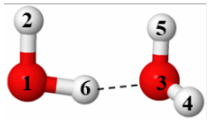
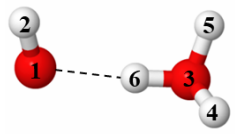
	E^{Tot}	E^{Ex}	Distance		Angle		Dihedral	
G2-[1]	-152.527356	7.29	O_1H_2	0.97	$\angle O_3O_1H_2$	109.9	$\angle H_4O_3O_1H_2$	237.2
	(-152.259461)		O_1H_6	0.97	$\angle H_4O_3O_1$	109.1	$\angle H_5O_3H_4O_1$	115.5
			O_3H_4	0.97	$\angle H_5O_3H_4$	104.0	$\angle H_6O_1H_2\ O_3$	0.0
			O_3H_5	0.97	$\angle H_6O_1H_2$	104.4		
			O_1O_3	2.94				
E2-[1]	-152.485007	5.49	O_1H_2	1.14	$\angle O_3O_1H_2$	87.9	$\angle H_4O_3O_1H_2$	105.4
	(-152.283192)		O_1H_6	1.08	$\angle H_4O_3O_1$	117.4	$\angle H_5O_3H_4O_1$	100.5
			O_3H_4	0.97	$\angle H_5O_3H_4$	104.7	$\angle H_6O_1H_2\ O_3$	1.1
			O_3H_5	0.99	$\angle H_6O_1H_2$	96.4		
			O_1O_3	2.47				
E2-[2]	-152.400416	2.61	O_1H_2	0.98	$\angle O_3O_1H_2$	104.3	$\angle H_4O_3O_1H_2$	87.0
	(-152.304451)		O_3H_6	1.01	$\angle H_4O_3O_1$	109.5	$\angle H_5O_3H_4O_1$	109.9
			O_3H_4	1.02	$\angle H_5O_3H_4$	104.1	$\angle H_6O_1H_2\ O_3$	2.0
			O_3H_5	1.04	$\angle H_6O_1H_2$	104.8		
			O_1O_3	2.82				

Table S1 (cont.)

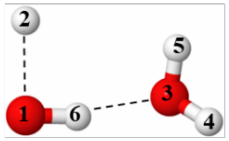
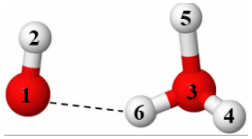
	E^{Tot}	E^{Ex}	Distance		Angle		Dihedral	
E2-[3]								
	-152.384207	1.54	O_1H_2	1.85	$\angle O_3O_1H_2$	85.3	$\angle H_4O_3O_1H_2$	129.4
	(-152.327591)		O_3H_6	1.88	$\angle H_4O_3O_1$	126.2	$\angle H_5O_3H_4O_1$	120.8
			O_3H_4	0.97	$\angle H_5O_3H_4$	104.5	$\angle H_6O_1H_2\ O_3$	0.0
			O_3H_5	0.97	$\angle H_6O_1H_2$	92.8		
			O_1O_3	2.85				
E2-[4]								
	-152.338544	0.79	O_1H_2	0.98	$\angle O_3O_1H_2$	81.7	$\angle H_4O_3O_1H_2$	105.4
	(-152.309391)		O_3H_6	0.99	$\angle H_4O_3O_1$	117.0	$\angle H_5O_3H_4O_1$	88.8
			O_3H_4	0.98	$\angle H_5O_3H_4$	104.2	$\angle H_6O_1H_2\ O_3$	3.1
			O_3H_5	1.30	$\angle H_6O_1H_2$	91.4		
			O_1O_3	2.83				

Table S1 (cont.)

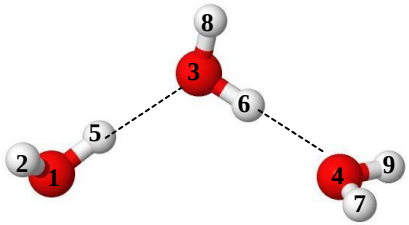
	E^{Tot}	E^{Ex}	Distance		Angle		Dihedral	
G3-[1]	-228.799506	7.17	O_1H_2	0.96	$\angle O_3O_1H_2$	107.4	$\angle O_4O_3O_1H_2$	108.0
	(-228.536069)		O_1O_3	2.92	$\angle O_4O_3O_1$	107.8	$\angle H_5O_1H_2O_3$	357.9
			O_3O_4	2.87	$\angle H_5O_1H_2$	104.1	$\angle H_6O_3O_4\ O_1$	150.0
			O_1H_5	0.97	$\angle H_6O_3O_4$	174.7	$\angle H_7O_4H_6O_3$	96.6
			O_3H_6	0.97	$\angle H_7O_4H_6$	122.6	$\angle H_8O_3H_6O_4$	168.5
			O_4H_7	0.98	$\angle H_8O_3H_6$	104.5	$\angle H_9O_4H_7O_3$	148.7
			O_3H_8	0.97	$\angle H_9O_4H_7$	104.6		
			O_4H_9	0.97				

Table S1 (cont.)

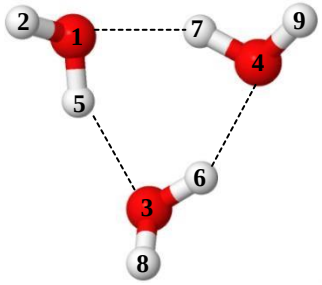
	E^{Tot}	E^{Ex}	Distance		Angle		Dihedral	
G3-[2]	-228.805785	7.62	O_1H_2	0.96	$\angle O_3O_1H_2$	121.7	$\angle O_4O_3O_1H_2$	231.3
	(-228.525698)		O_1O_3	2.82	$\angle O_4O_3O_1$	59.9	$\angle H_5O_1H_2O_3$	13.5
			O_3O_4	2.81	$\angle H_5O_1H_2$	105.3	$\angle H_6O_3O_4\ O_1$	191.0
			O_1H_5	0.98	$\angle H_6O_3O_4$	20.6	$\angle H_7O_4H_6O_3$	14.9
			O_3H_6	0.98	$\angle H_7O_4H_6$	90.0	$\angle H_8O_3H_6O_4$	215.8
			O_4H_7	0.98	$\angle H_8O_3H_6$	105.1	$\angle H_9O_4H_7O_3$	223.5
			O_3H_8	0.96	$\angle H_9O_4H$	105.1		
			O_4H_9	0.96				

Table S1 (cont.)

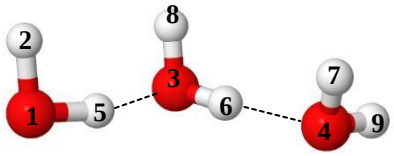
	E^{Tot}	E^{Ex}	Distance		Angle		Dihedral	
E3-[1]‡	-228.7564730	5.39	O_1H_2	1.13	$\angle O_3O_1H_2$	90.8	$\angle O_4O_3O_1H_2$	96.4
	(-228.5585441)		O_1O_3	2.47	$\angle O_4O_3O_1$	116.2	$\angle H_5O_1H_2O_3$	0.7
			O_3O_4	2.79	$\angle H_5O_1H_2$	98.3	$\angle H_6O_3O_4\ O_1$	28.8
			O_1H_5	1.10	$\angle H_6O_3O_4$	0.0	$\angle H_7O_4H_6O_3$	17.9
			O_3H_6	0.99	$\angle H_7O_4H_6$	106.5	$\angle H_8O_3H_6O_4$	326.7
			O_4H_7	0.96	$\angle H_8O_3H_6$	103.0	$\angle H_9O_4H_7O_3$	114.2
			O_3H_8	0.98	$\angle H_9O_4H_7$	107.2		
			O_4H_9	0.95				

Table S1 (cont.)

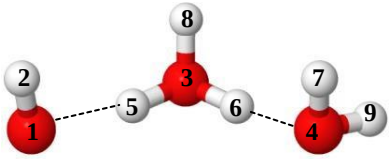
	E^{Tot}	E^{Ex}	Distance		Angle		Dihedral	
E3-[2]	-228.682179	2.75	O_1H_2	0.98	$\angle O_3O_1H_2$	97.4	$\angle O_4O_3O_1H_2$	91.0
	(-228.581076)		O_1O_3	2.78	$\angle O_4O_3O_1$	113.1	$\angle H_5O_1H_2O_3$	1.9
			O_3O_4	2.59	$\angle H_5O_1H_2$	100.2	$\angle H_6O_3O_4\ O_1$	277.2
			O_1H_5	1.79	$\angle H_6O_3O_4$	5.8	$\angle H_7O_4H_6O_3$	358.6
			O_3H_6	1.03	$\angle H_7O_4H_6$	100.8	$\angle H_8O_3H_6O_4$	5.8
			O_4H_7	0.98	$\angle H_8O_3H_6$	102.6	$\angle H_9O_4H_7O_3$	118.5
			O_3H_8	1.05	$\angle H_9O_4H_7$	104.5		
			O_4H_9	0.97				

Table S1 (cont.)

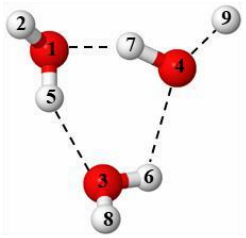
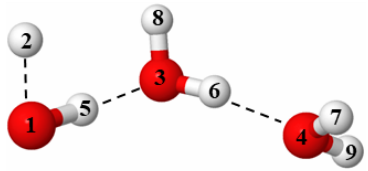
	E^{Tot}	E^{Ex}	Distance		Angle		Dihedral	
E3-[3]	-228.676045	2.49	O_1H_2	0.97	$\angle O_3O_1H_2$	121.4	$\angle O_4O_3O_1H_2$	236.3
	(-228.584499)		O_1O_4	2.52	$\angle O_4O_3O_1$	54.1	$\angle H_5O_1H_2O_3$	16.8
			O_1O_3	2.80	$\angle H_5O_1H_2$	105.9	$\angle H_6O_3O_4\ O_1$	163.9
			O_1H_5	0.97	$\angle H_6O_3O_4$	48.5	$\angle H_7O_4H_6O_3$	356.4
			O_3H_6	0.95	$\angle H_7O_4H_6$	96.6	$\angle H_8O_3H_6O_4$	228
			O_4H_7	1.04	$\angle H_8O_3H_6$	107.8	$\angle H_9O_4H_7O_3$	237.9
			O_3H_8	0.97	$\angle H_9O_4H_7$	93.7		
			O_4H_9	1.66				

Table S1 (cont.)

	E^{Tot}	E^{Ex}	Distance		Angle		Dihedral	
E3-[4]	-228.72288	4.21	O_1H_2	1.38	$\angle O_3O_1H_2$	88.3	$\angle O_4O_3O_1H_2$	104.9
	(-228.567987)		O_1O_3	2.79	$\angle O_4O_3O_1$	106.5	$\angle H_5O_1H_2O_3$	357.2
			O_3O_4	2.73	$\angle H_5O_1H_2$	91.1	$\angle H_6O_3O_4\ O_1$	123.9
			O_1H_5	1.07	$\angle H_6O_3O_4$	7.7	$\angle H_7O_4H_6O_3$	237.0
			O_3H_6	0.99	$\angle H_7O_4H_6$	123.0	$\angle H_8O_3H_6O_4$	164.6
			O_4H_7	0.97	$\angle H_8O_3H_6$	104.3	$\angle H_9O_4H_7O_3$	151.3
			O_3H_8	1.00	$\angle H_9O_4H_7$	106.1		
			O_4H_9	0.97				