SUPPORTING INFORMATION

Direct ab-initio MD study on the interaction of hydroperoxy radical (HOO) with water molecules

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1. Electron capture of defective graphene (*n*=19)

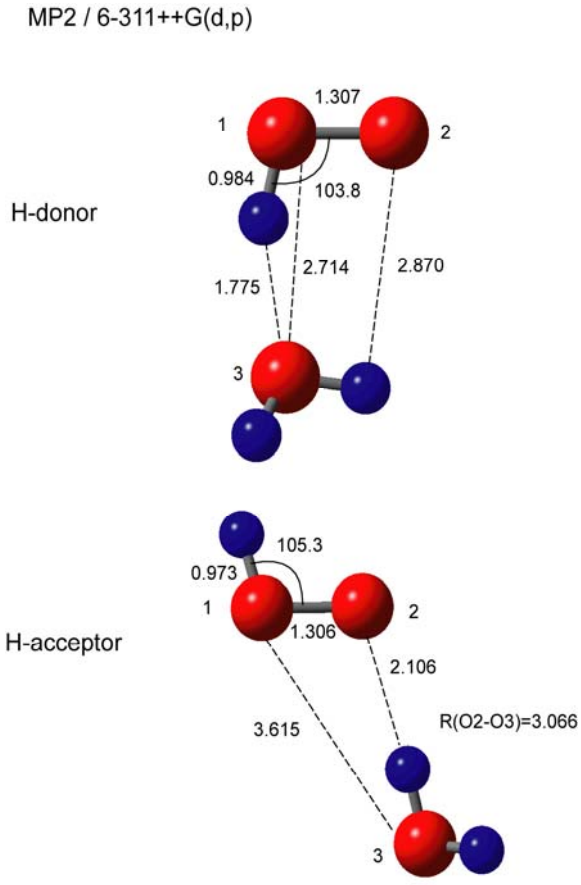


Figure S1. Optimized structure of HOO-H_2O complexes calculated at the MP2/6-311++G(d,p) level.

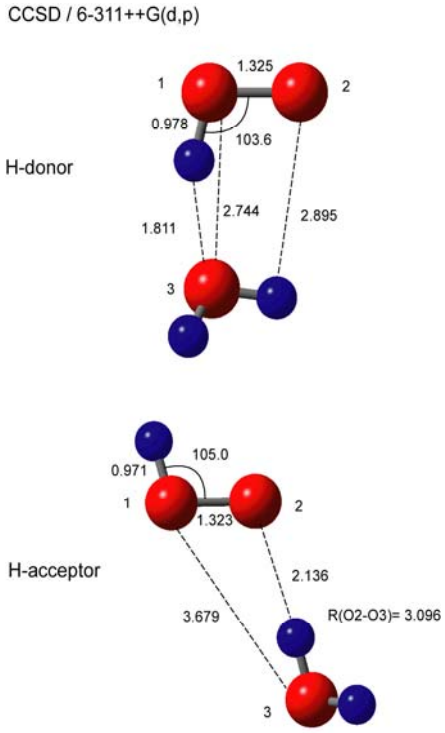


Figure S2. Optimized structure of HOO-H_2O complexes calculated at the CCSD/6-311++G(d,p) level.

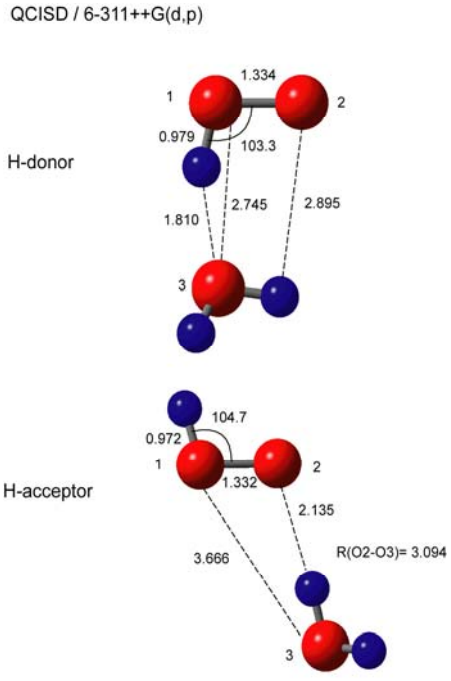


Figure S3. Optimized structure of HOO-H_2O complexes calculated at the QCISD/6-311++G(d,p) level.

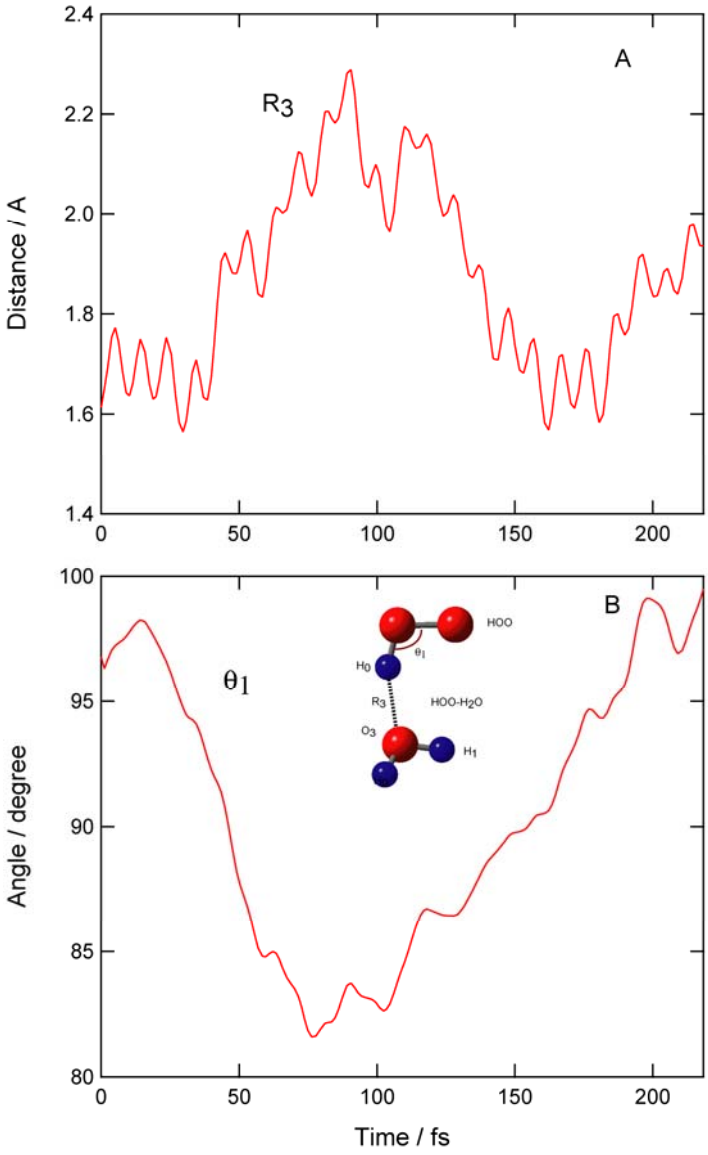


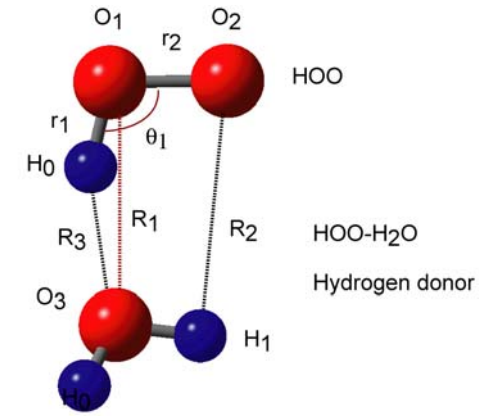
Figure S4. Time profile of bond distance and angles (R_3 and θ_1) of HOO-H_2O calculated at the MP2/6-311++G(d,p) level.

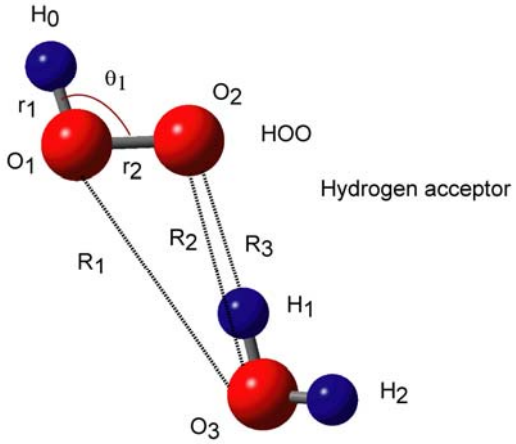
Table S1. Total energies (E in a.u), dipole moments (in Debye), number of imaginary frequencies (Im), relative energies (ΔE in kcal/mol) and types of structural forms of HOO-H_2O 1:1 complexes obtained at the B3LYP/6-311++G(d,p) level.

No	E	dipole	Im	ΔE	type
1	-227.4322055	3.882	0	0.00	H-donor
2	-227.4322043	3.8856	0	0.00	H-donor
3	-227.4322054	3.8778	0	0.00	H-donor
4	-227.4322055	3.8875	0	0.00	H-donor
5	-227.4322056	3.8849	0	0.00	H-donor
6	-227.4322052	3.8765	0	0.00	H-donor
7	-227.4322054	3.885	0	0.00	H-donor
8	-227.4322053	3.8827	0	0.00	H-donor
9	-227.4322056	3.8832	0	0.00	H-donor
10	-227.4322051	3.8873	0	0.00	H-donor
11	-227.4322055	3.8866	0	0.00	H-donor
12	-227.4322055	3.8829	0	0.00	H-donor
13	-227.4322056	3.8835	0	0.00	H-donor
14	-227.4322055	3.8763	0	0.00	H-donor
15	-227.4322056	3.8811	0	0.00	H-donor
16	-227.4218095	4.861	0	6.52	H-acceptor
17	-227.4322056	3.8817	0	0.00	H-donor
18	-227.4218922	4.7673	0	6.47	H-acceptor
19	-227.421942	4.071	0	6.44	H-acceptor
20	-227.4219417	4.0777	0	6.44	H-acceptor

Table S2. Optimized parameters of HOO--H_2O 1:1 complexes. CP means the geometrical parameters after the counterpoise correction.

	MP2	CCSD	QCISD	MP2+CP
r1	0.9836	0.9783	0.9788	0.9809
r2	1.3069	1.3254	1.3345	1.3064
r3	0.962	0.9602	0.9605	0.9611
r4	0.9605	0.9588	0.9591	0.9592
R1	2.7142	2.7444	2.7435	2.7827
R2	2.8693	2.8947	2.8962	2.8273
R3	1.7744	1.8114	1.8089	1.8672
θ_1	103.8	103.6	103.3	104.2
θ_2	104.6	104.9	104.9	105.0
θ_3	97.9	98.3	98.5	95.2





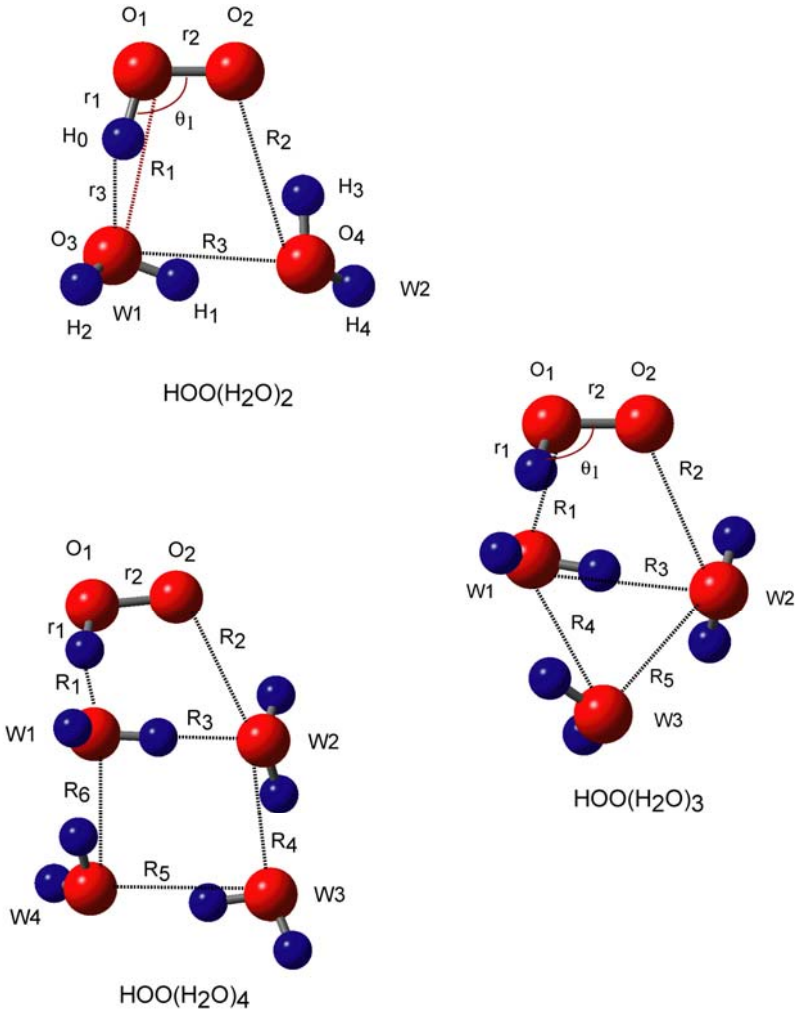


Figure S5. Optimized structure of $HOO(H_2O)_n$ complexes (n=2-4) calculated at the MP2/6-311++G(d,p) level.

Table S3. Isotropic Fermi Contact Couplings (in gauss) of HOO-H_2O (donor form) calculated at the several levels of theory with 6-311++G(d,p) and 6-311++G(2d,2p) basis sets..

No	atom	MP2	CCSD	QCISD	QCISD[a]
1	O	-20.70852	-21.20114	-20.11423	-21.09794
2	O	-16.96015	-12.85125	-12.12399	-12.50880
3	H	-13.28125	-10.16353	-10.03438	-10.22127
4	O	0.68981	0.48859	0.48868	0.43965
5	H	0.04245	0.03382	0.03368	0.09839
6	H	-0.05624	-0.03453	-0.03026	-0.03038

[a] Result of 6-311++G(2d,2p) basis set.

Table S4. Total energies (in a.u) and relative energies (ΔE_{rel} in kcal/mol) between donor and acceptor forms of the 1:1 complexes.

method	donor	acceptor	ΔE_{rel}
MP2/6-311++G(d,p)	-226.88467	-226.8743	6.50
CCSD/6-311++G(d,p)	-226.90731	-226.89767	6.05
QCISD/6-311++G(d,p)	-226.91046	-226.90084	6.04
MP2/6-311++G(2d,p)	-226.93379	-226.92364	6.37
QCISD/6-311++G(2d,2p)	-226.9648947	-226.9561799	5.47

Relative energy is defined by ΔE_{rel} =E(acceptor)-E(donor), where E(M) means total energy of M-form.