Theoretical studies on the electron capture properties of the $H_2SO_4\cdots HOO^{\bullet}$ complex and its implications as an alternative source of HOOH

Ping Li[*ab], *Zhiying Ma*[a], *Weihua Wang*[*a], *Rui Song*[a], *Yazhou Zhai*[a], *Siwei Bi*[a], *Haitao Sun*[a], *Yuxiang Bu*[*b]

[a] *Key Laboratory of Life-Organic Analysis, School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu, 273165, P. R. China*

[b] *Key Laboratory of Colloid and Interface Chemistry (Shandong University), Ministry of Education, Jinan 250100, P. R. China*

Electronic Supplementary Information

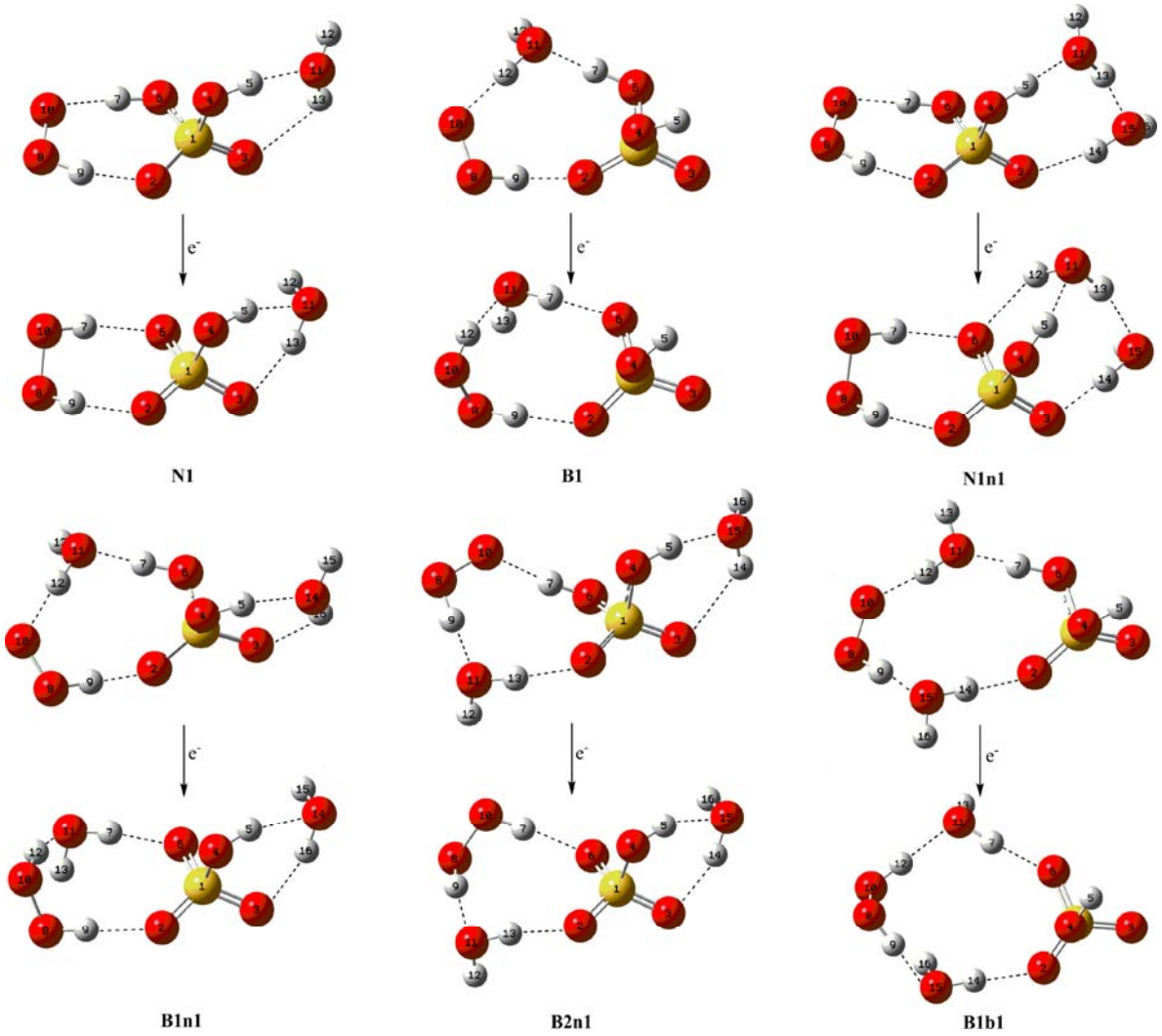

Fig. S1 The optimized radical complexes $H_2SO_4\cdots HOO^{\bullet}\cdots(H_2O)_n$(n=1-2) and their electron capture products at the B3LYP/6-311++G(3df,3pd) level of theory.

Table S1 The calculated natural charge on the H7 atom of the geometries obtained during molecular dynamical process (within 14 fs) and the optimized anionic complex **A1** [a]

Time	Natural charge
0	0.507
1	0.507
2	0.506
3	0.500
4	0.492
5	0.482
6	0.473
7	0.469
8	0.472
9	0.476
10	0.472
11	0.456
12	0.448
13	0.461
14	0.469
A1	0.477

[a] The natural charge is calculated at the MP2/6-311++G(3df,3pd) level of theory on the basis of the dynamics.