

**Table S1.** The Reaction and activated energies, enthalpies and free energies for the reaction of H<sub>2</sub>SO<sub>4</sub> with OH with zero-point correction (ZPE) included at 298k. (kcal/mol)\*

compound	$\Delta H^a$	$\Delta G^a$	$\Delta E^a$	$\Delta E^b$	$\Delta (E^b + \text{ZPE})$	$\Delta E^c (\text{Ref 10})$
H <sub>2</sub> SO <sub>4</sub> + H <sub>2</sub> O	0.00	0.00	0.00	0.00	0.00	0.00
C1'	-7.69	0.18	-7.15	-10.70	-9.11	-9.1
TS1'	-4.36	4.85	-3.25	4.18	3.95	2.5
TS2'	-3.93	4.95	-2.89	4.47	4.12	2.7
TS3'	-2.53	5.82	-1.70	6.26	4.68	2.8
TS4'	0.40	10.13	1.79	1.67	-0.29	0.7

\* a:  $\Delta H$ ,  $\Delta G$ ,  $\Delta E$  are computed at the B3LYP/6-311+G(2df,2p) level of theory; b:  $\Delta E$  is calculated at the MP2(full)/aug-cc-pv(T+d)z//B3LYP/6-311+G(2df,2p) level of theory, c: The value is obtained at the CCSD(T)/cc-pvtz// B3LYP/6-311+G(2df,2p) level of theory.