Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

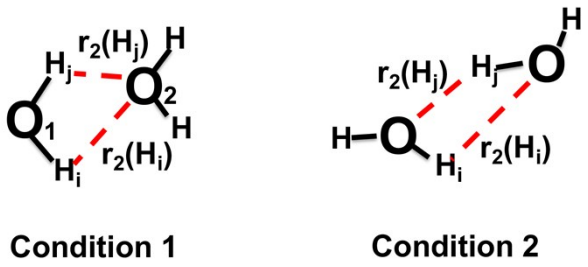

Figure S1. Schematic drawing of the configurations associated with the 2 conditions presented in equation 10. Red dashed lines indicate the H-bonds:

(1) both H_i and H_j are covalently bonded to the same O_1 and they are H-bond interacting with the same O_2, and H_j has a closer H-bond to O2 than H_i, thus H_i is dangling;

(2) the oxygen to which H_j is covalently bonded (H_j's O_1) is also the oxygen to which H_i is H-bonded (H_i's O_2)and the oxygen to which H_i is covalently bonded (H_i's O_1) is also the oxygen to which H_j is H-bonded (H_j's O_2). Again, r_2 (H_j) is shorter than r_2 (H_i), making H_i dangling.