

Supporting Information

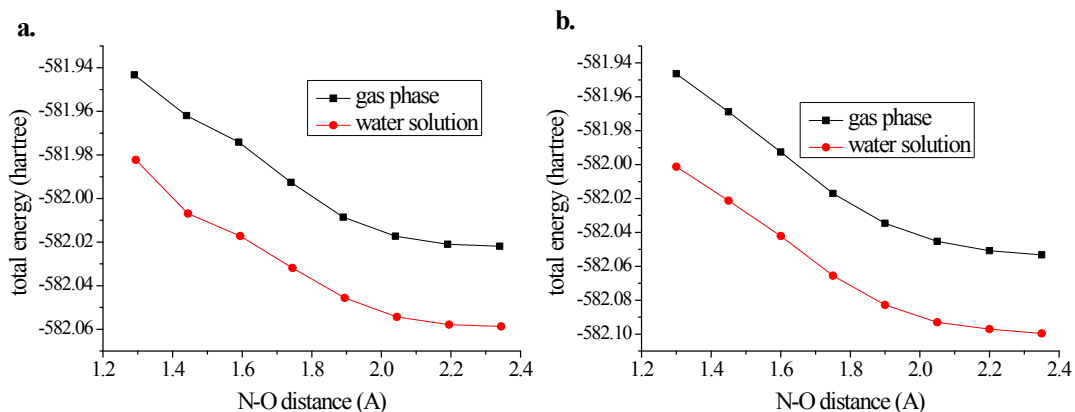


Fig. S1 The scan of N-O in the addition of $\cdot\text{OH}$ to the N-position of (a) CAe and (b) CAk.

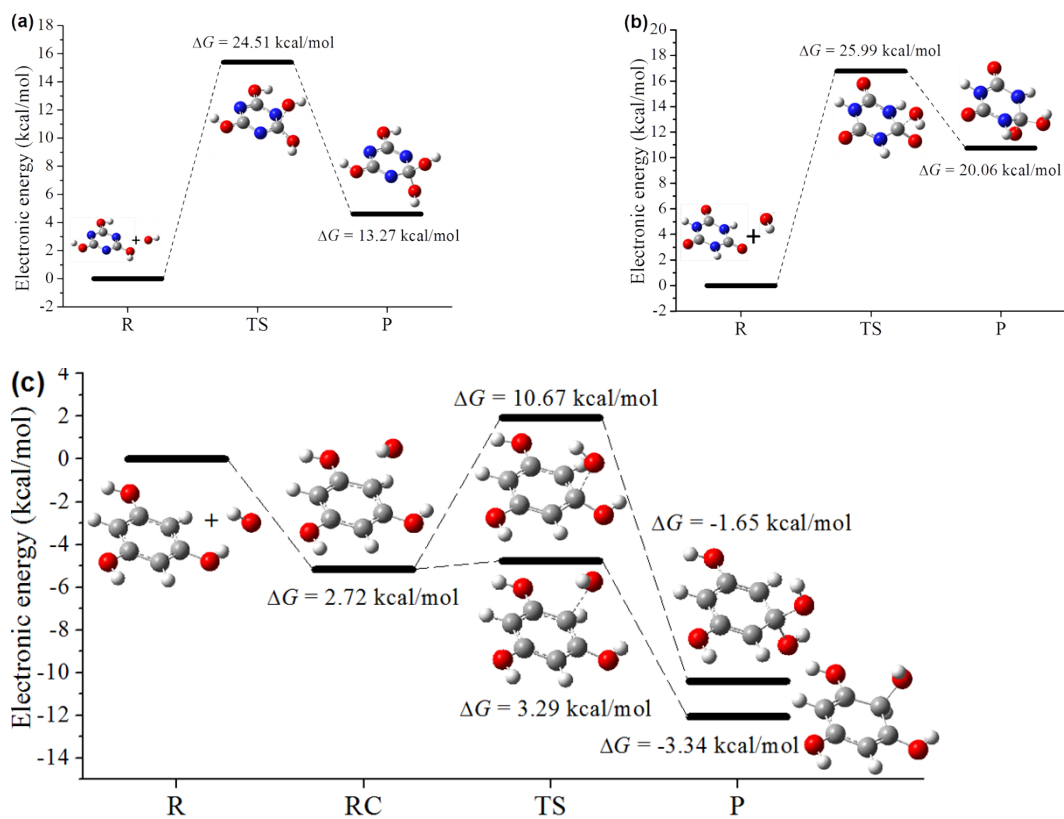


Fig. S2 Energy diagrams for $\cdot\text{OH}$ addition to (a) CAe, (b) CAk, and (c) BT in water solution.

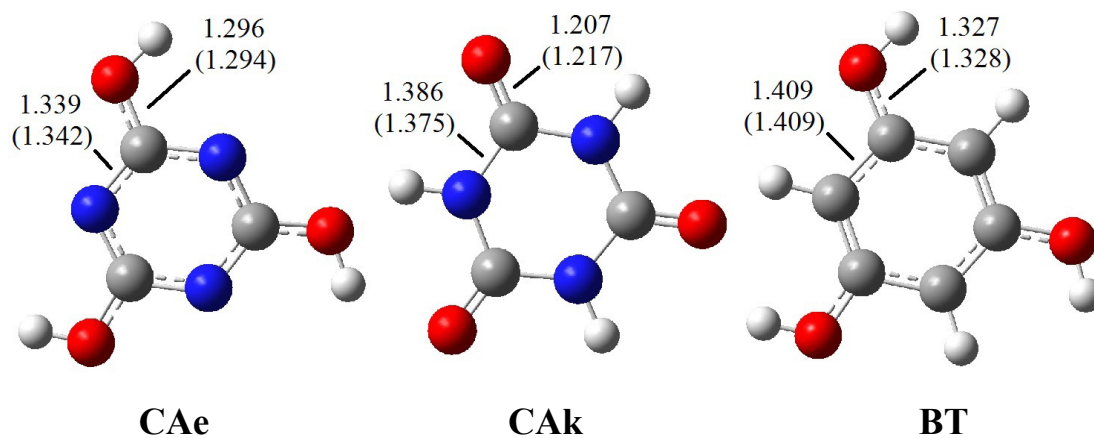


Fig. S3 Optimized structures for the cationic radicals of CAe, CAk and BT in the gas phase and water solution (in parentheses) obtained at the B3LYP/6-311++G(d,p) level of theory. Atom representation: blue for N, gray for C, red for O, and white for H.