Quantum mechanical investigation of the oxidative cleavage of the C-C backbone bonds in polyethylene in polyethylene model molecules

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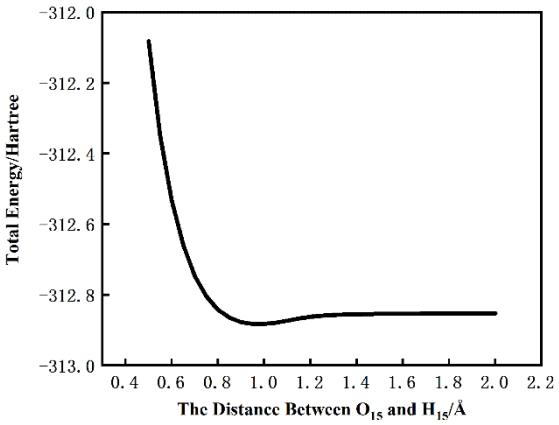

Figure S1 | Total energy change as a function of the increasing the distance between O_{15} and H_{15} during a relaxed scan based on the structure shown in **Figure 1A**. The unit used for the y-axis is Hartree with one Ha equal to 2625.50 kJ/mol.

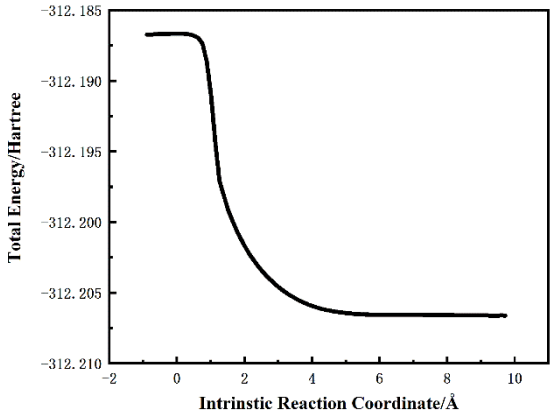

Figure S2 | IRC analysis potential energy curve.

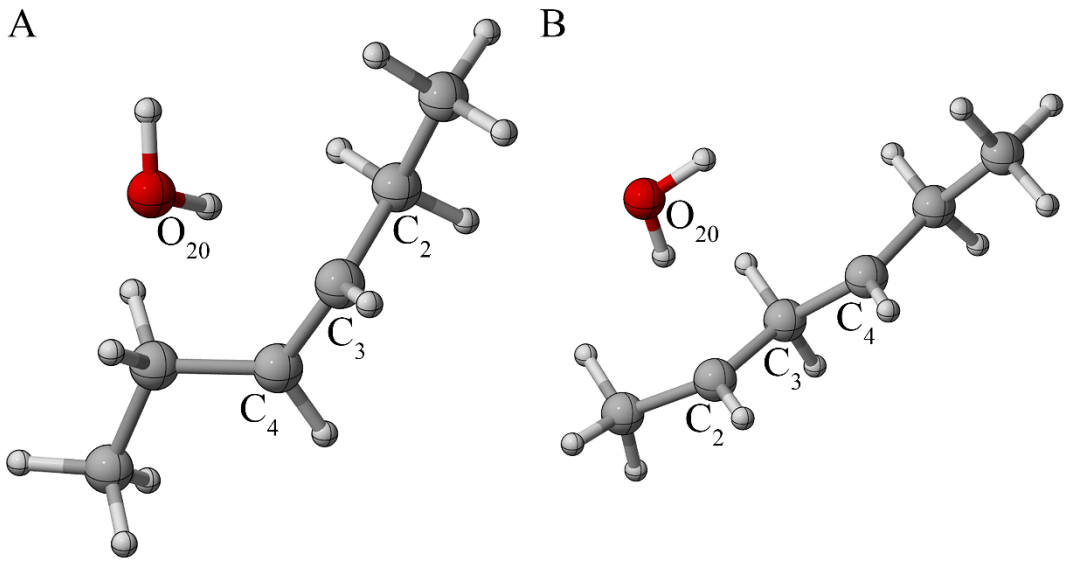

Figure S3 | (A) alkane free radical with ortho-carbon atoms each containing an unpaired electron; **(B)** alkane radical with meta-carbon atoms each containing an unpaired electron

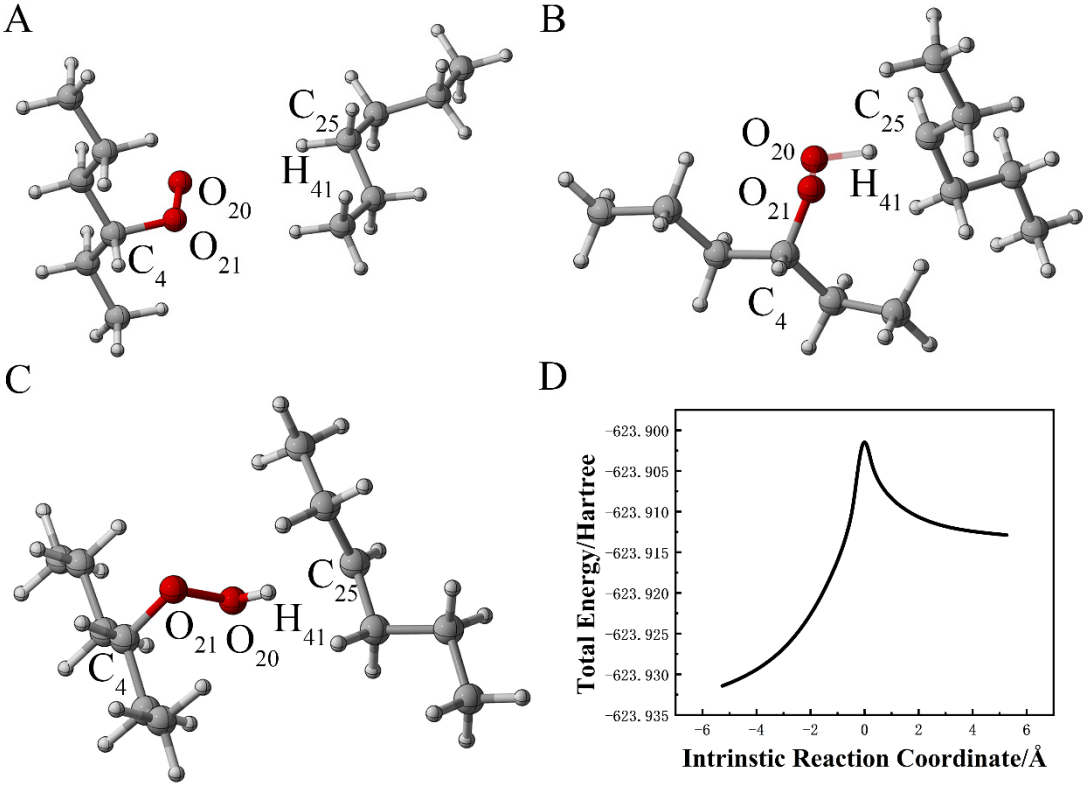

Figure S4 | (A) The structure of the reactant; **(B)** The structure of the transition state structure; **(C)** The structure of the product structure; **(D)** IRC analysis potential energy curve.

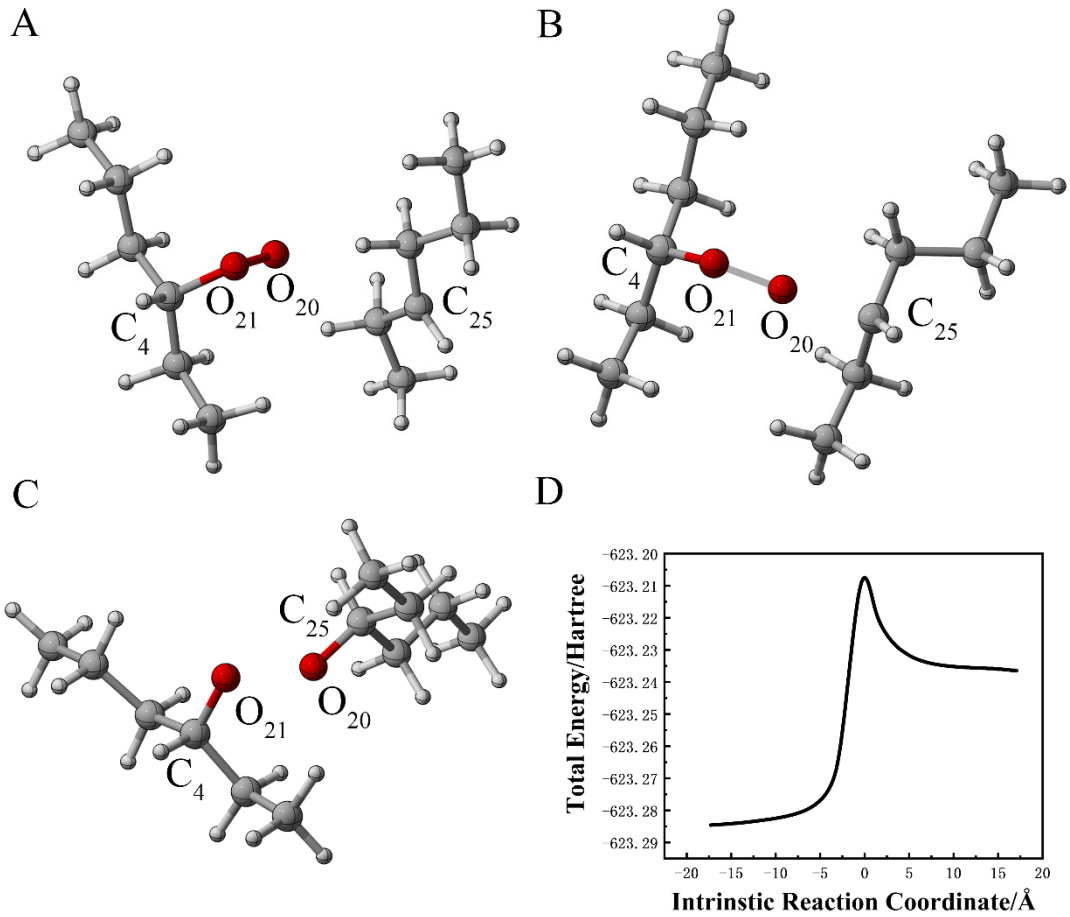

Figure S5 | (A) The structure of the reactant; **(B)** The structure of the transition state structure; **(C)** The structure of the product structure; **(D)** IRC analysis potential energy curve.

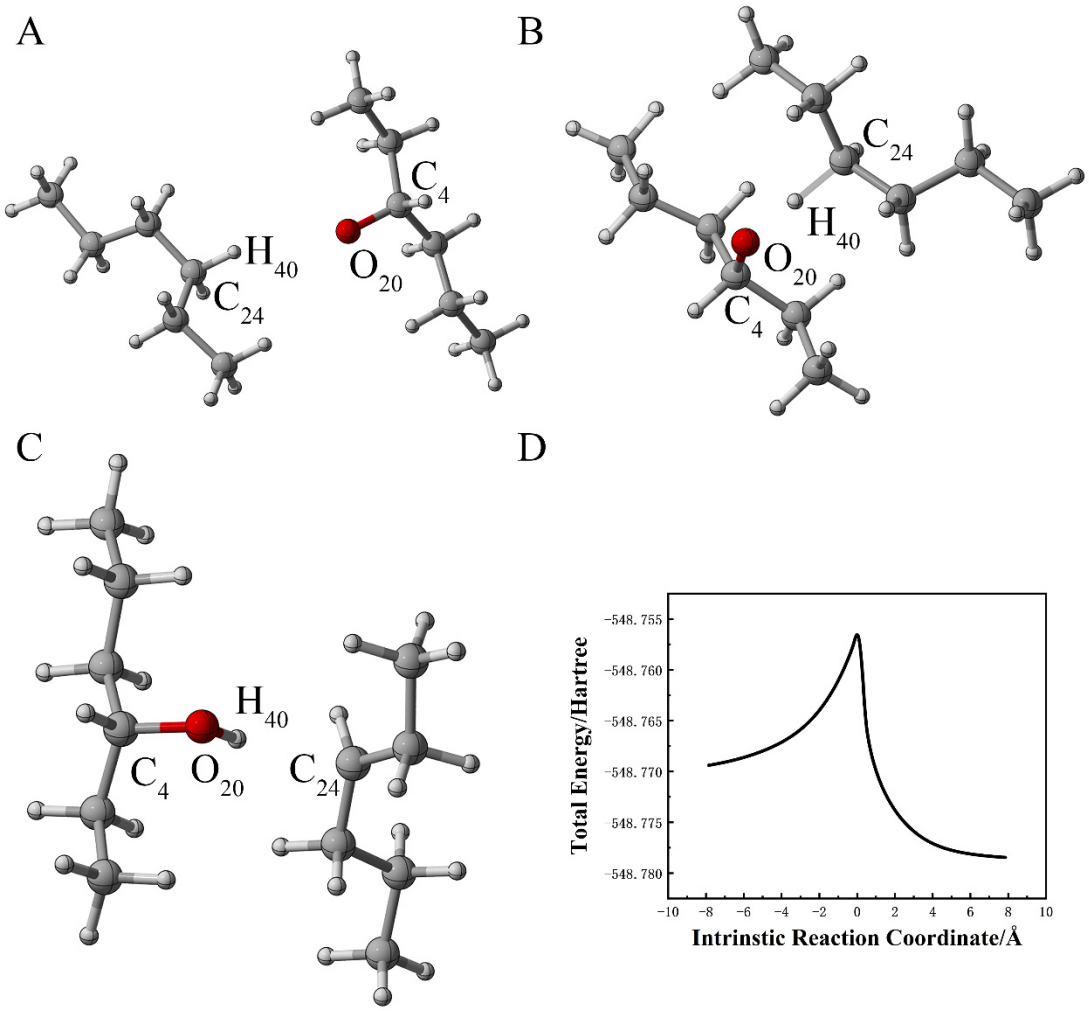

Figure S6 | (A) The structure of the reactant; **(B)** The structure of the transition state structure; **(C)** The structure of the product structure; **(D)** IRC analysis potential energy curve.

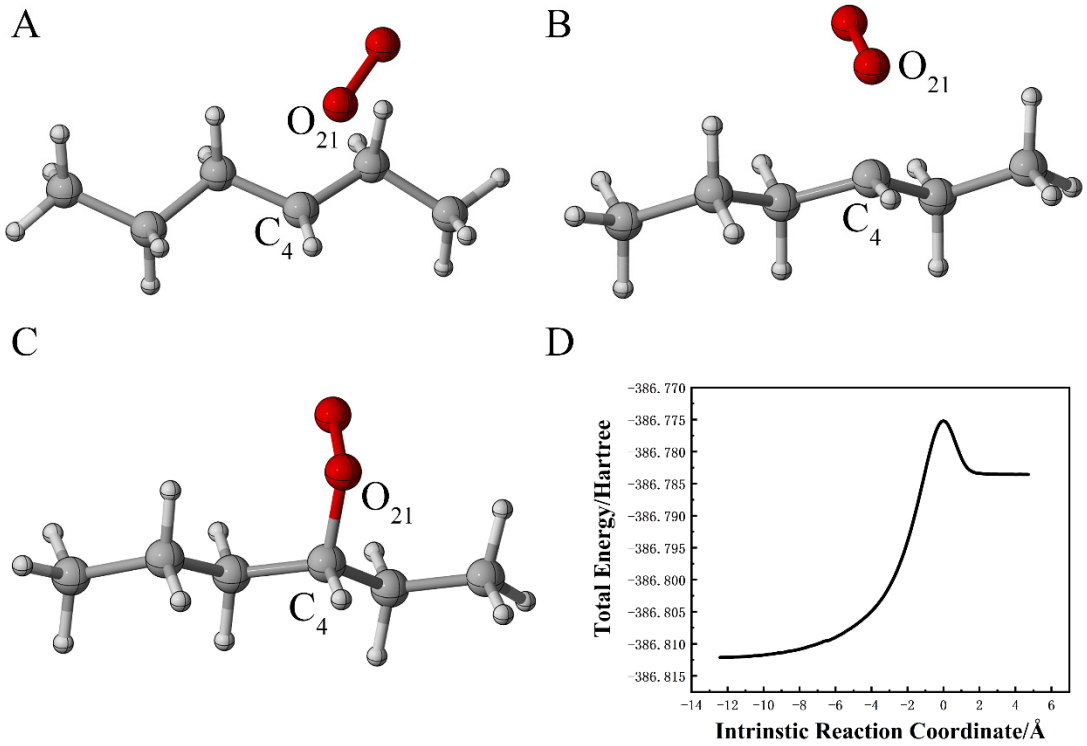

Figure S7 | (A) The structure of the reactant; **(B)** The structure of the transition state structure; **(C)** The structure of the product structure; **(D)** IRC analysis potential energy curve.