

Figure S1. Carbon number distribution of various polyethylene oxidation products at the end of simulation.

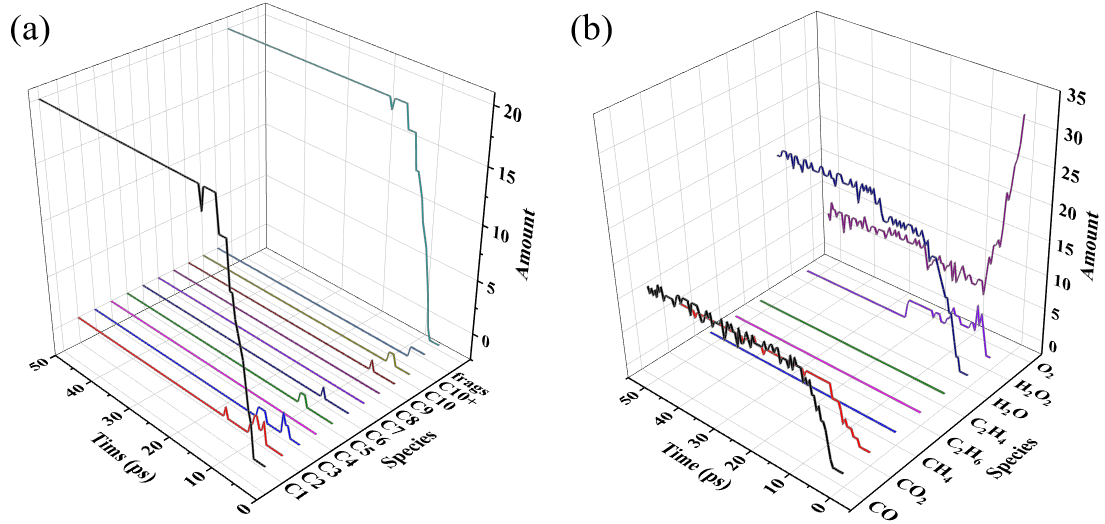


Figure S2. (a) Carbon number distribution of oxidation products and (b) variation of the amount of small molecules in the C20H42+32O2 system.

Figure S3. Evolution of carbon number distribution of thermal oxidation products of HDPE-C system at (a) 1200K, (b) 1600K, (c) 2000K.

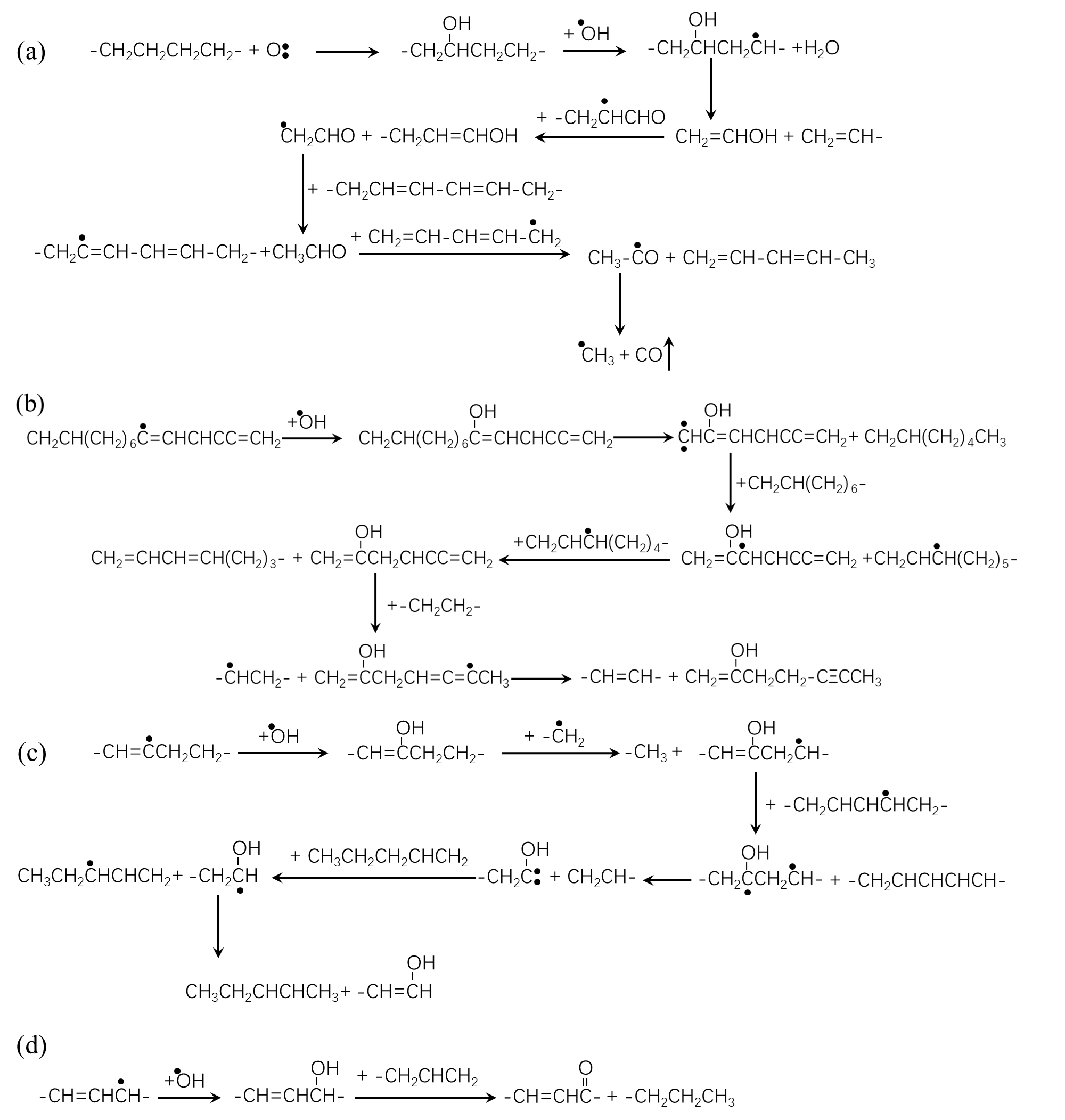
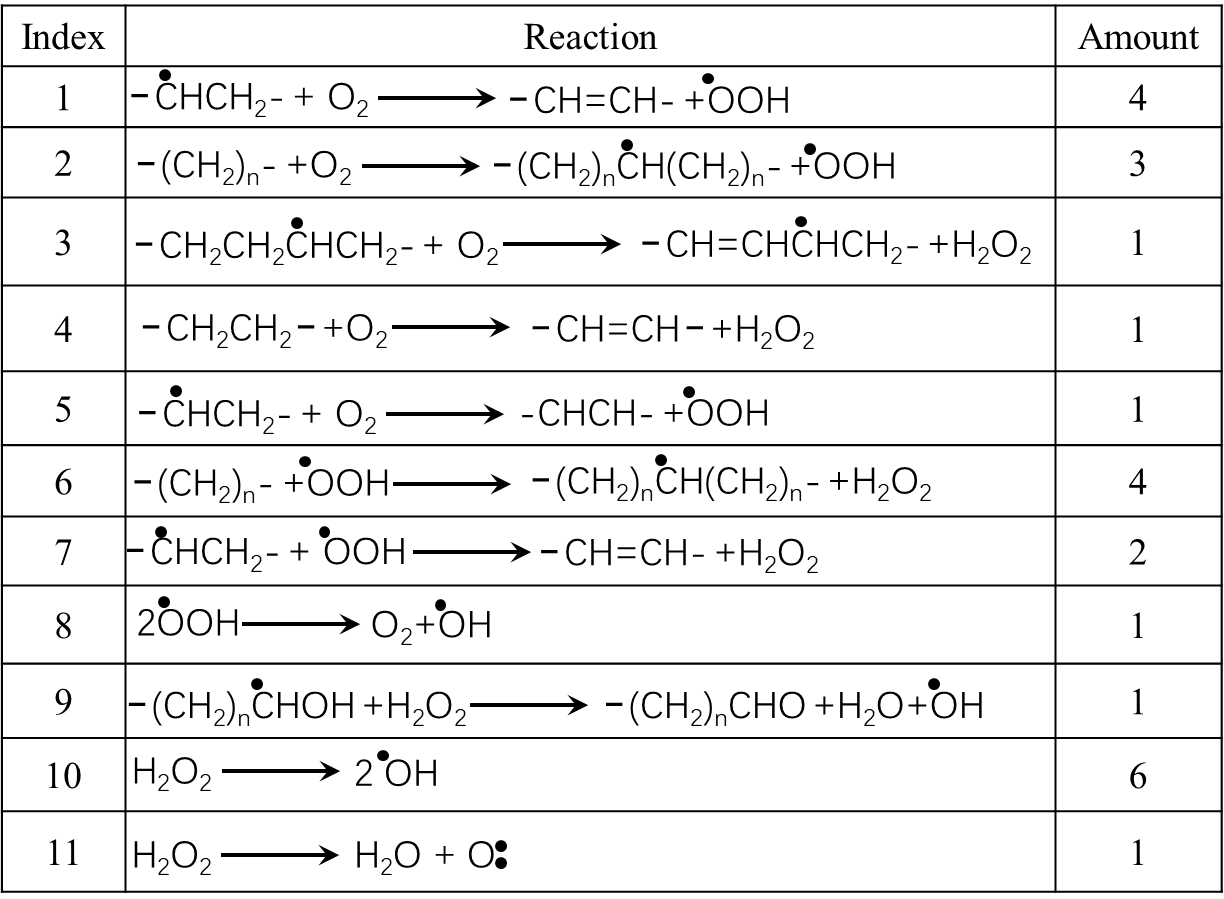


Figure S4. Complex reactions involving oxygen in HDPE-C.

**Table S1**. Generation and consumption of hydrogen peroxide in HDPE-A. 

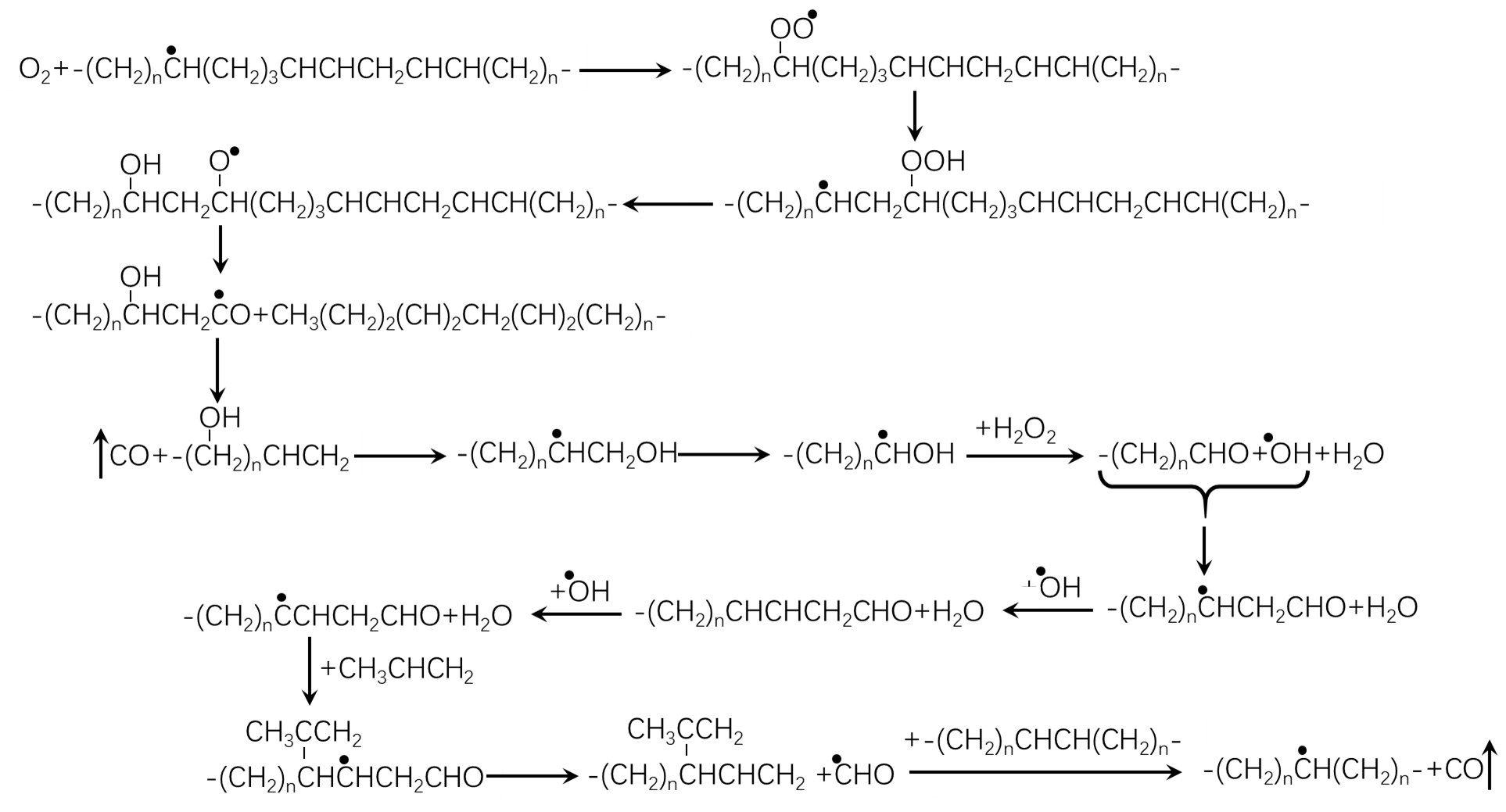
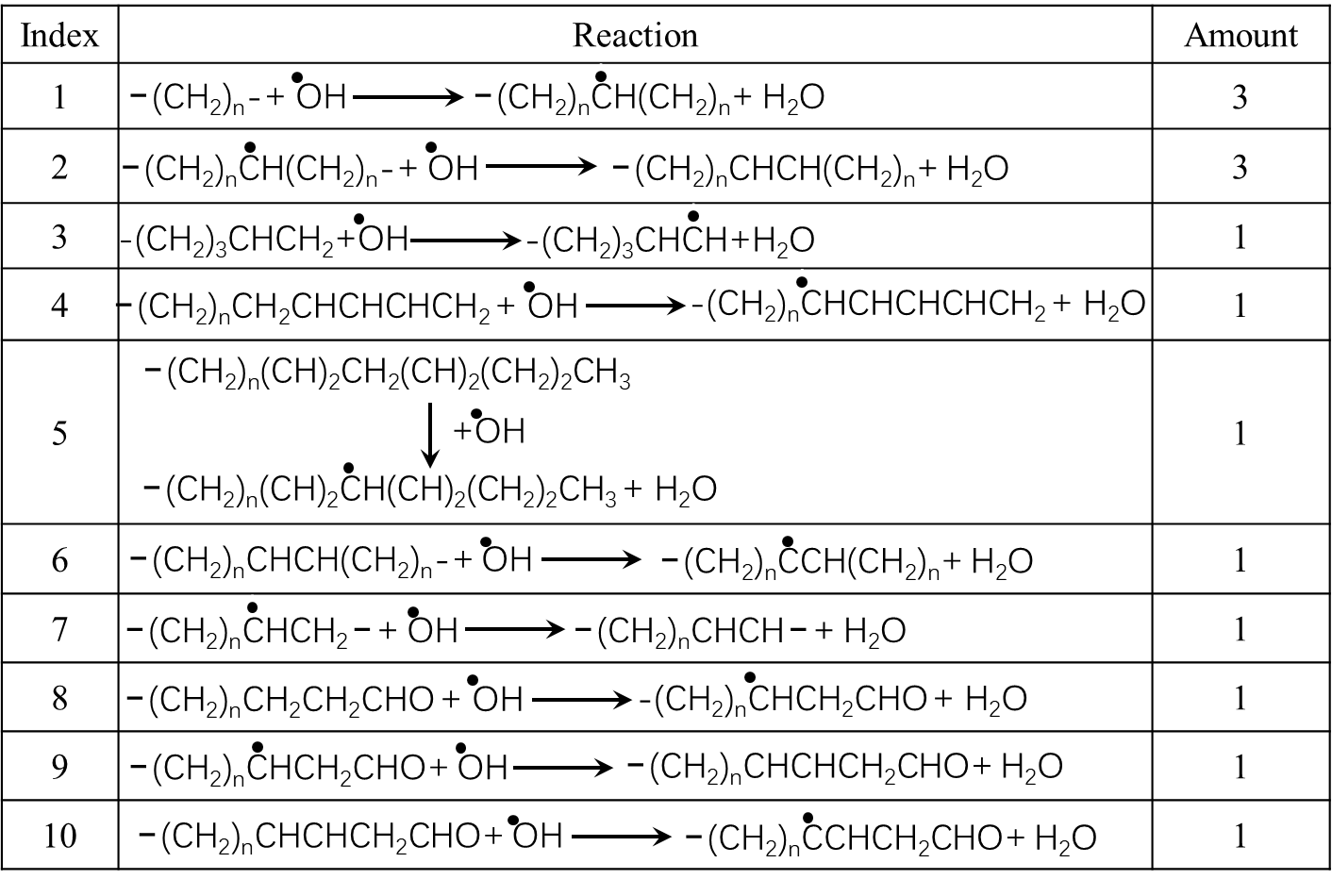


Figure S5. Complex reactions involving oxygen in HDPE-A.

**Table S2**. Simple reactions involving hydroxyl radicals in HDPE-A. 

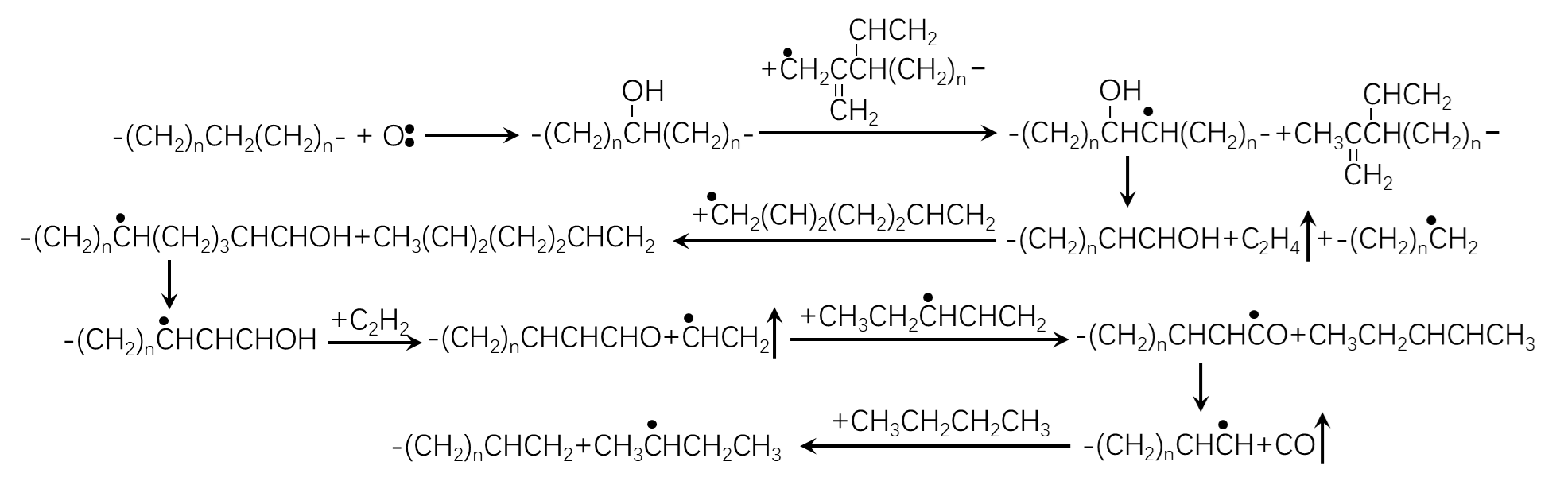
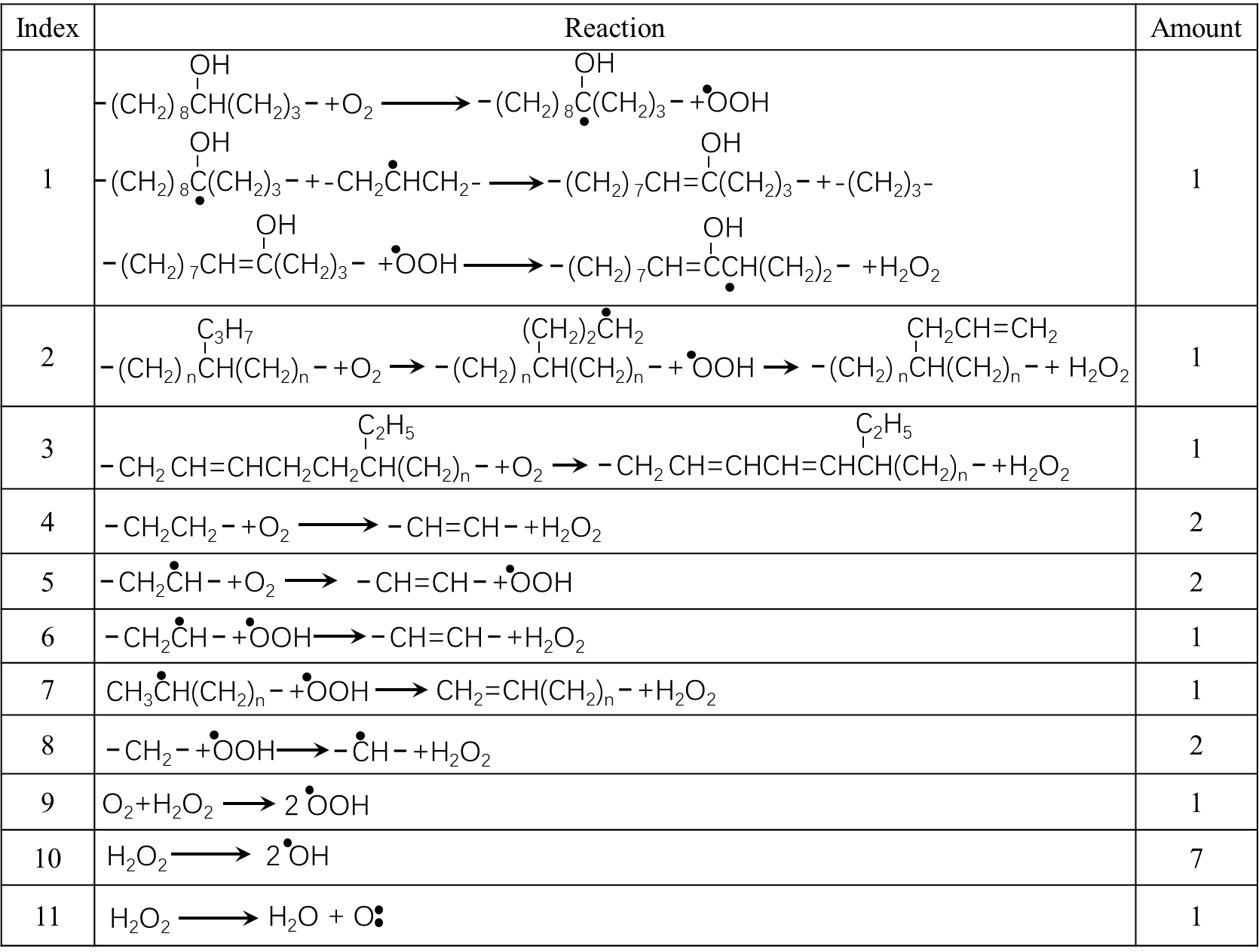


Figure S6. Complex reactions involving hydroxyl radicals in HDPE-A. **Table S3**. Formation and consumption of hydrogen peroxide in LDPE. 

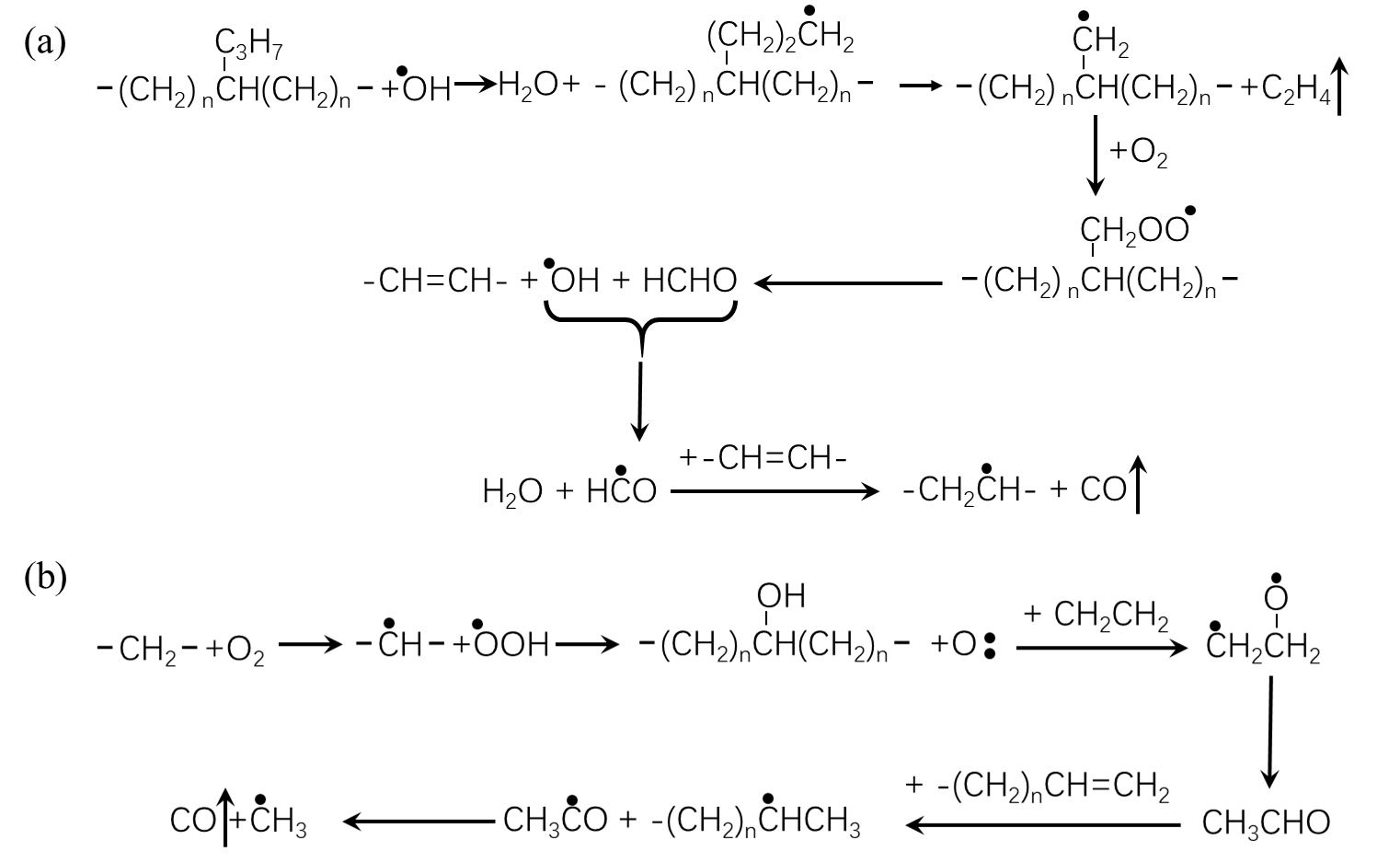
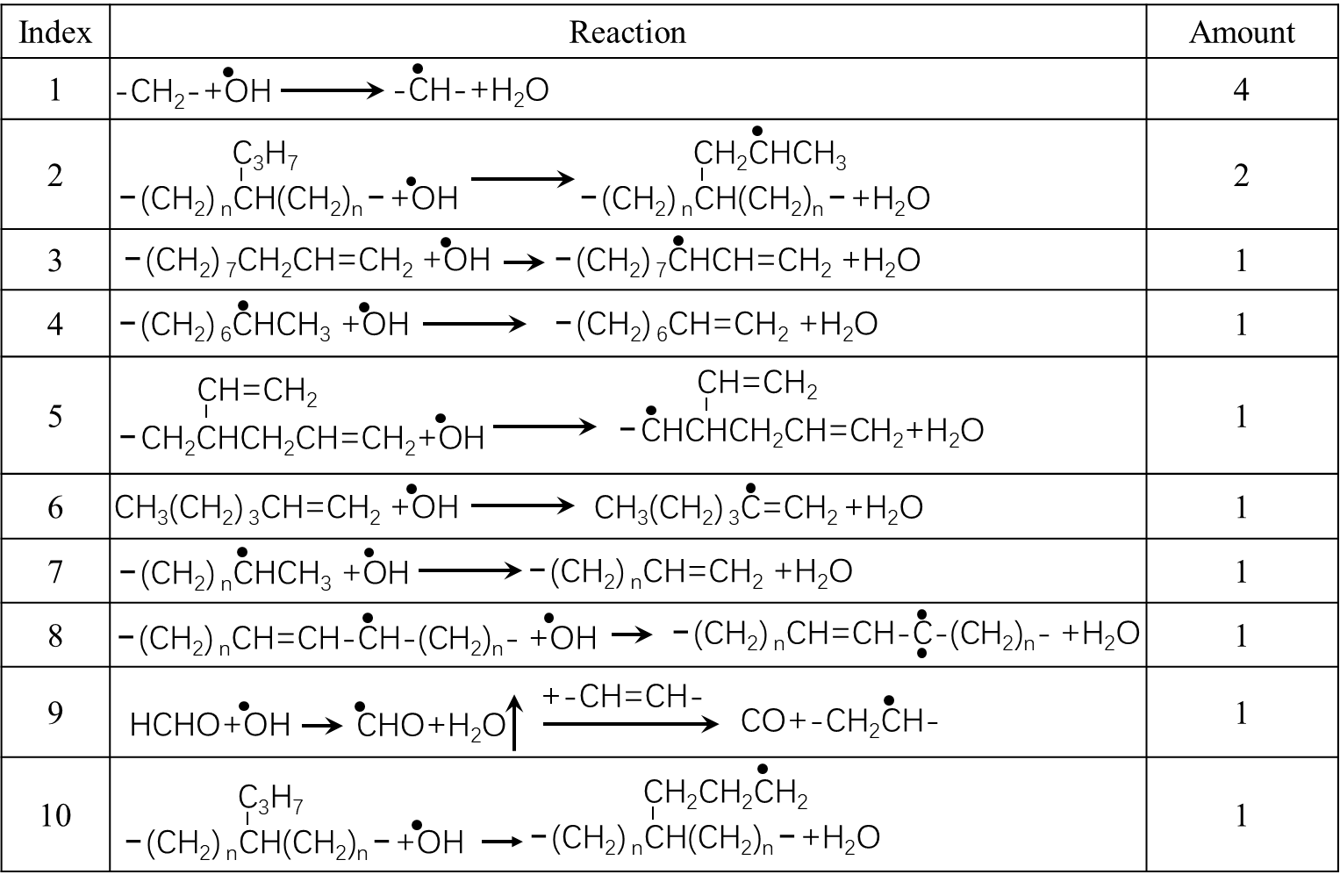


Figure S7. Complex reactions involving oxygen in LDPE.

**Table S4**. Simple reactions involving hydroxyl radicals in LDPE. 

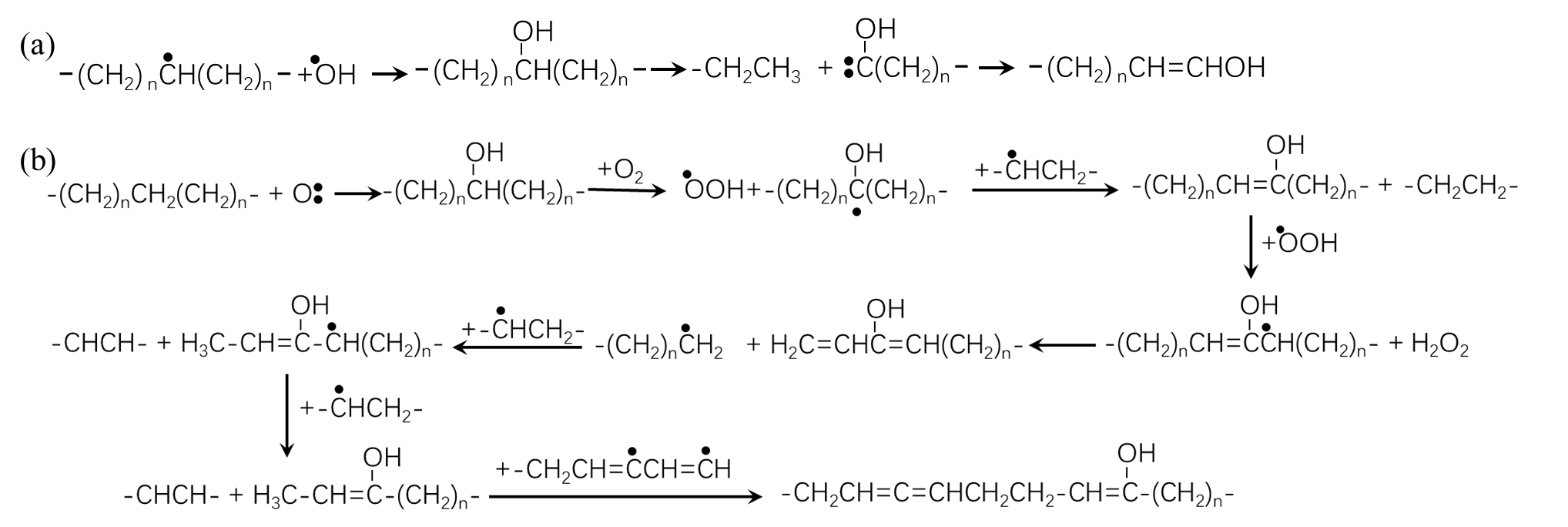
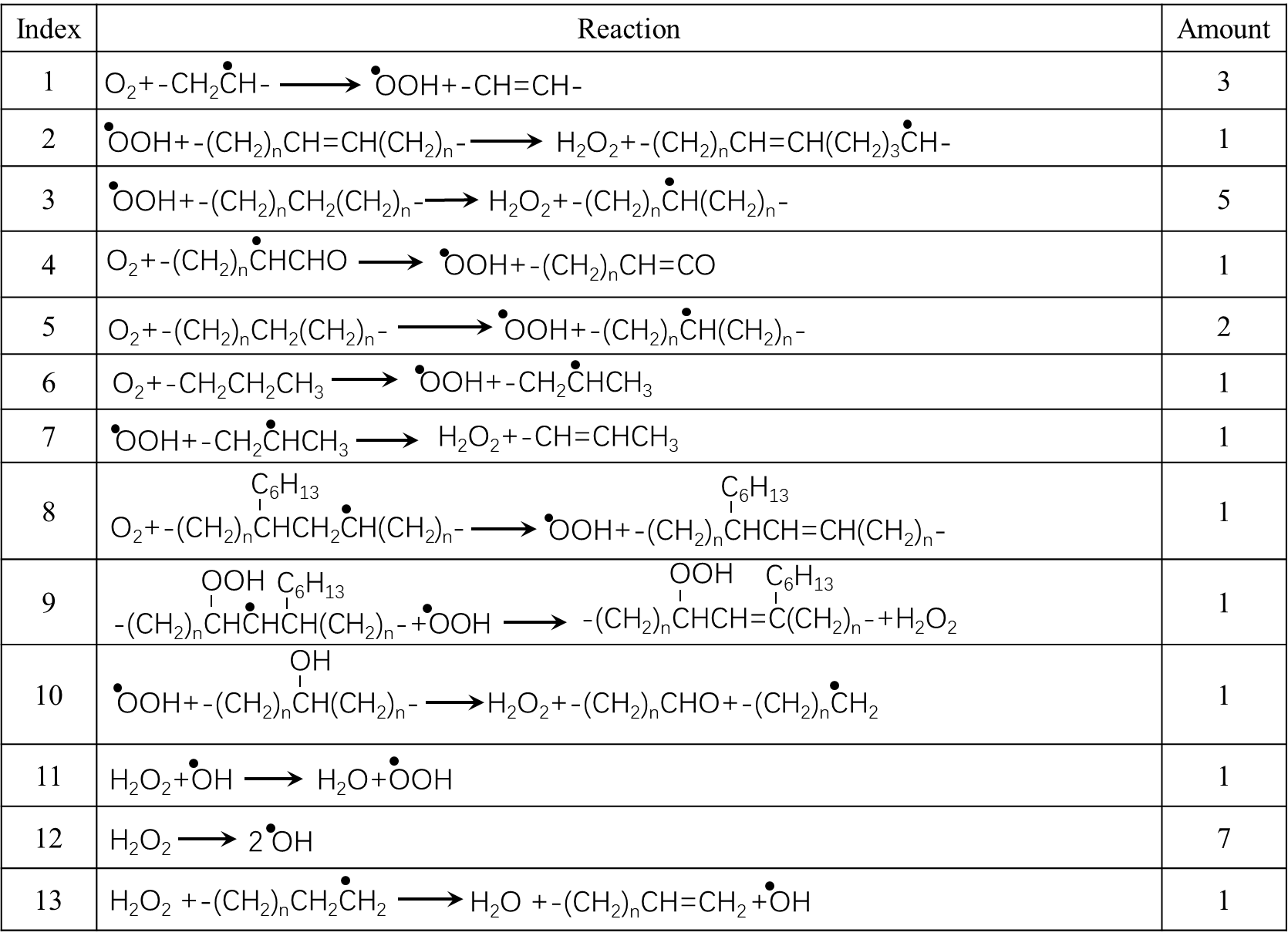


Figure S8. Complex reactions involving hydroxyl radicals in LDPE. **Table S5**. Formation and consumption of hydrogen peroxide in LLDPE. 

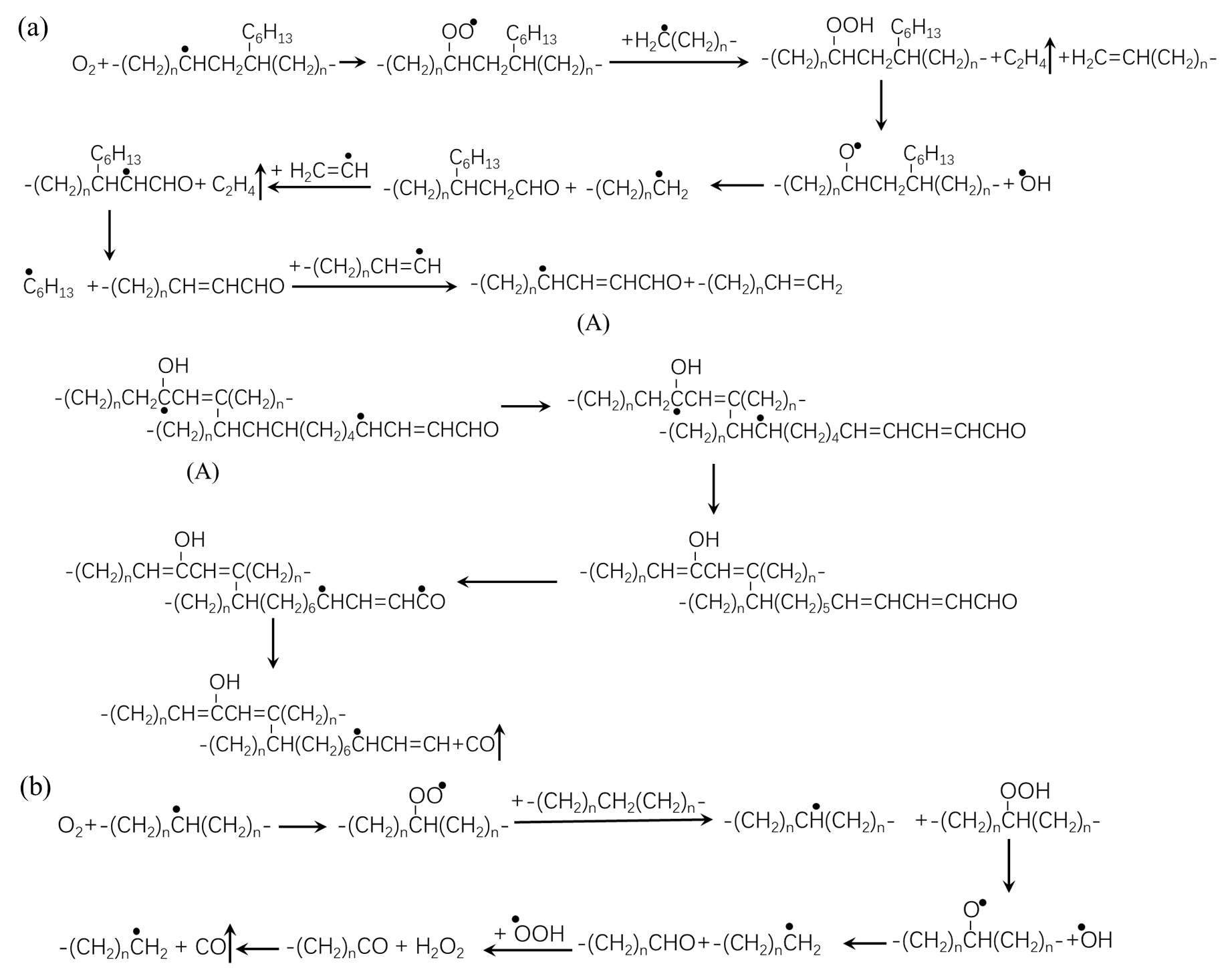
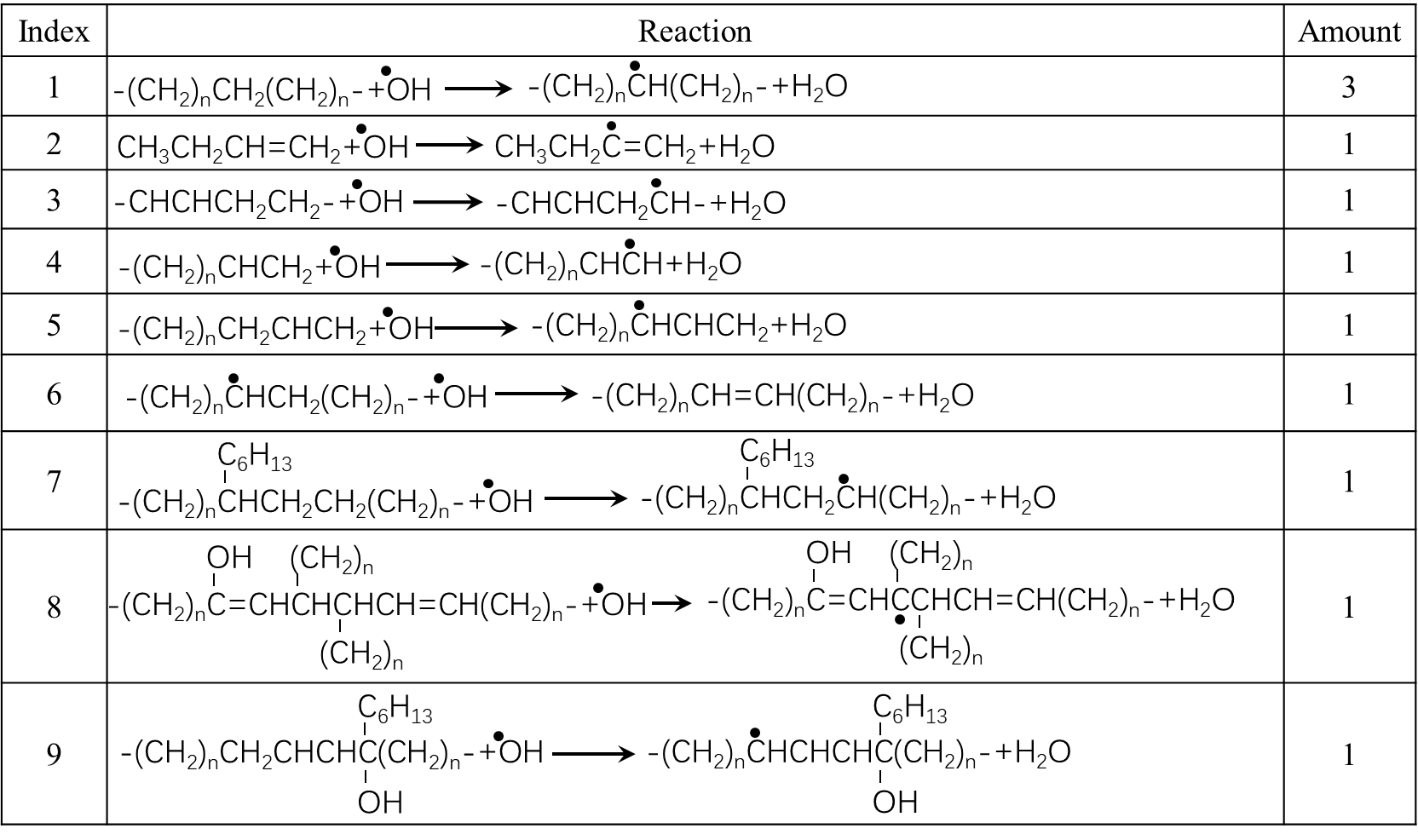


Figure S9. Complex reactions involving oxygen in LLDPE.

**Table S6**. Simple reactions involving hydroxyl radicals in LLDPE. 

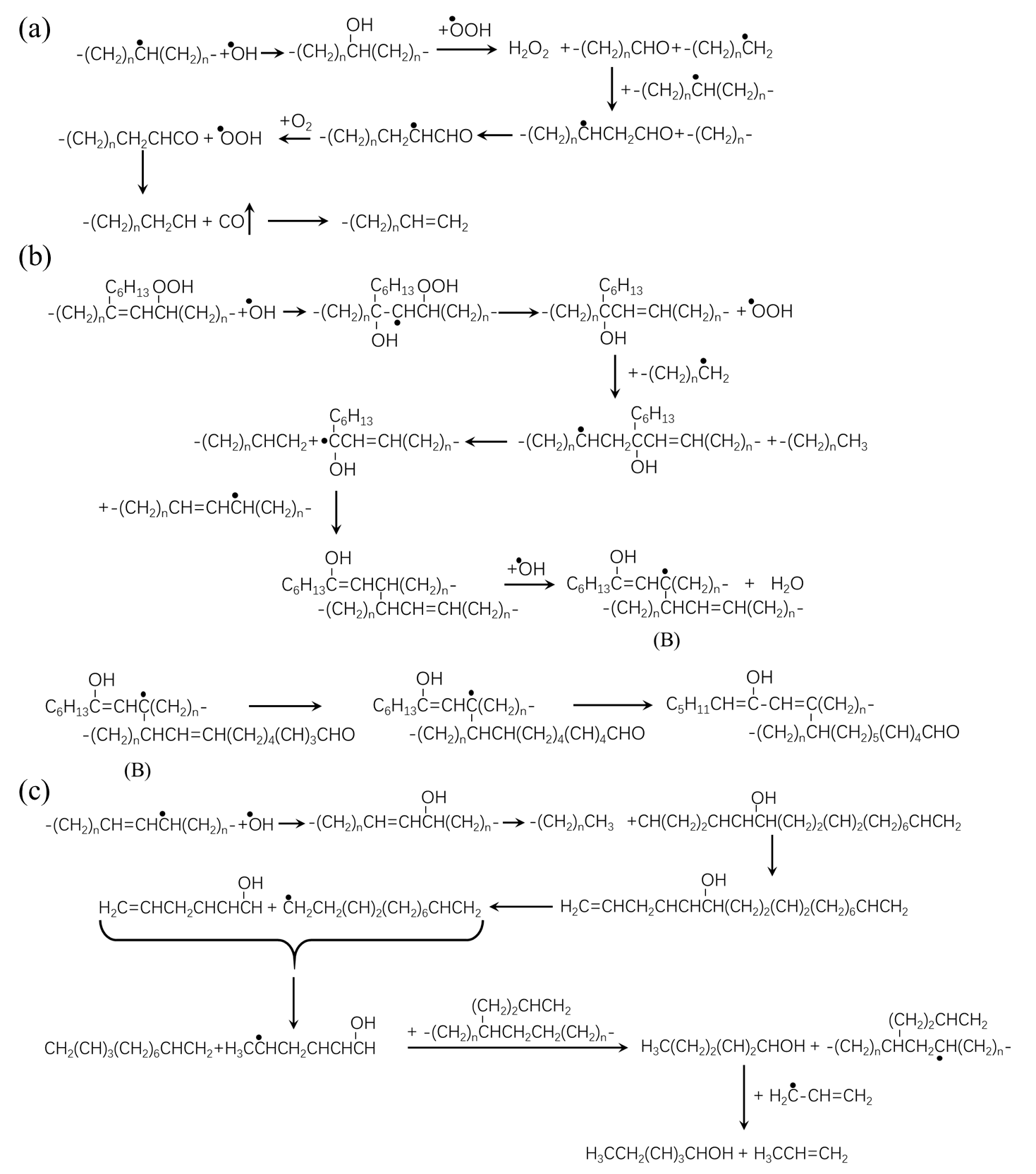


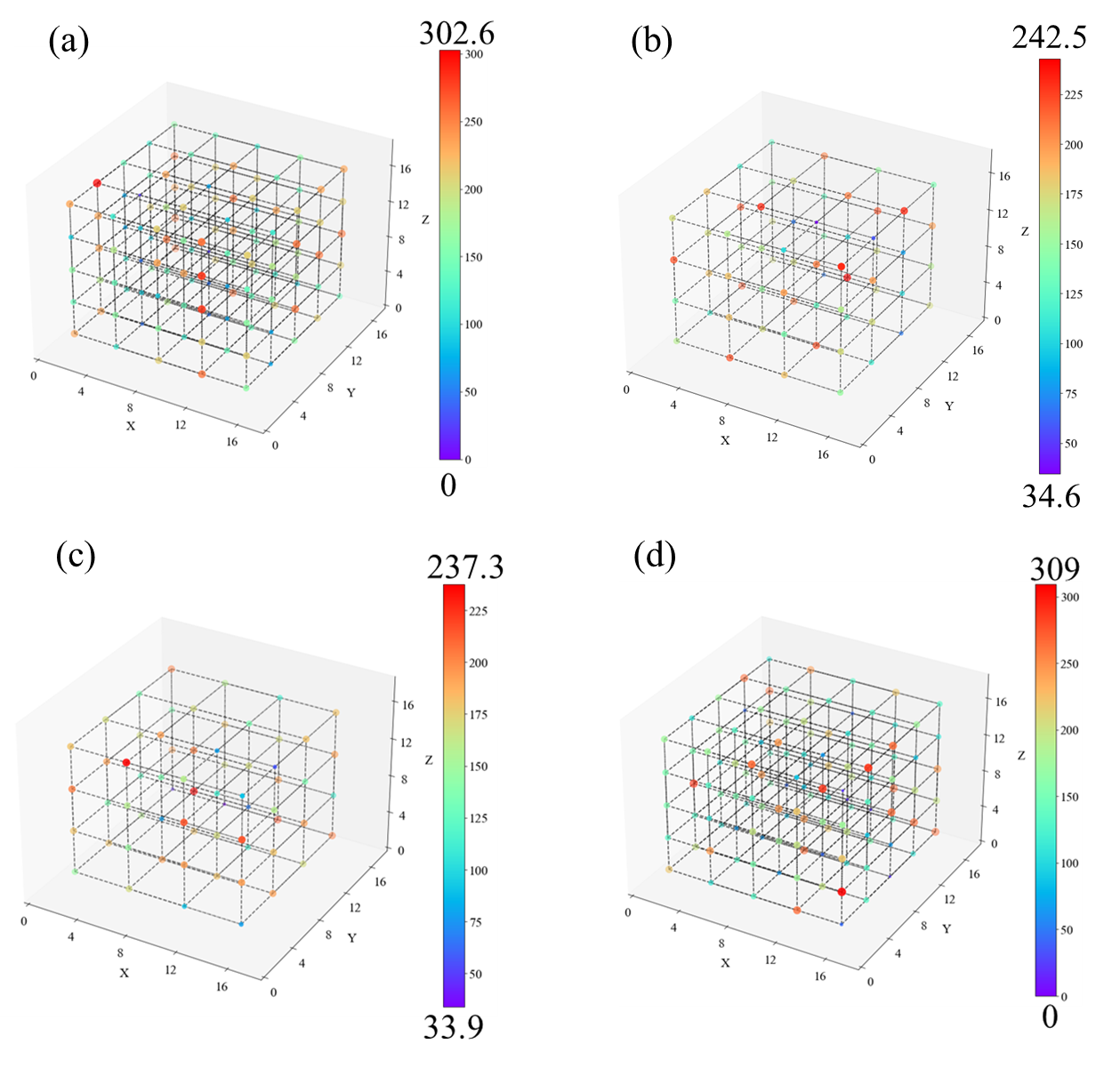
Figure S10. Complex reactions involving hydroxyl radicals in LLDPE.

Figure S11. Carbon and hydrogen atom density distribution at the initial moment in (a) HDPE-C, (b) HDPE-A, (c) LDPE, (d) LLDPE system (unit: nm-3).