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

Supplementary Material 1 for

Oxidation kinetic mechanism of n-decane under high temperature and pressure: a first-principles molecular dynamics study

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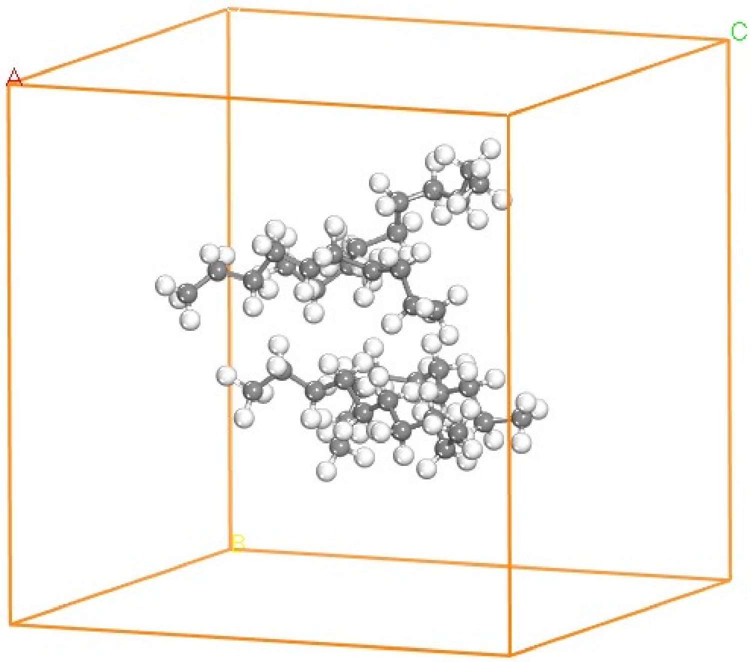


Figure S1. The computational model of $C_{10}H_{22}$ pyrolysis.

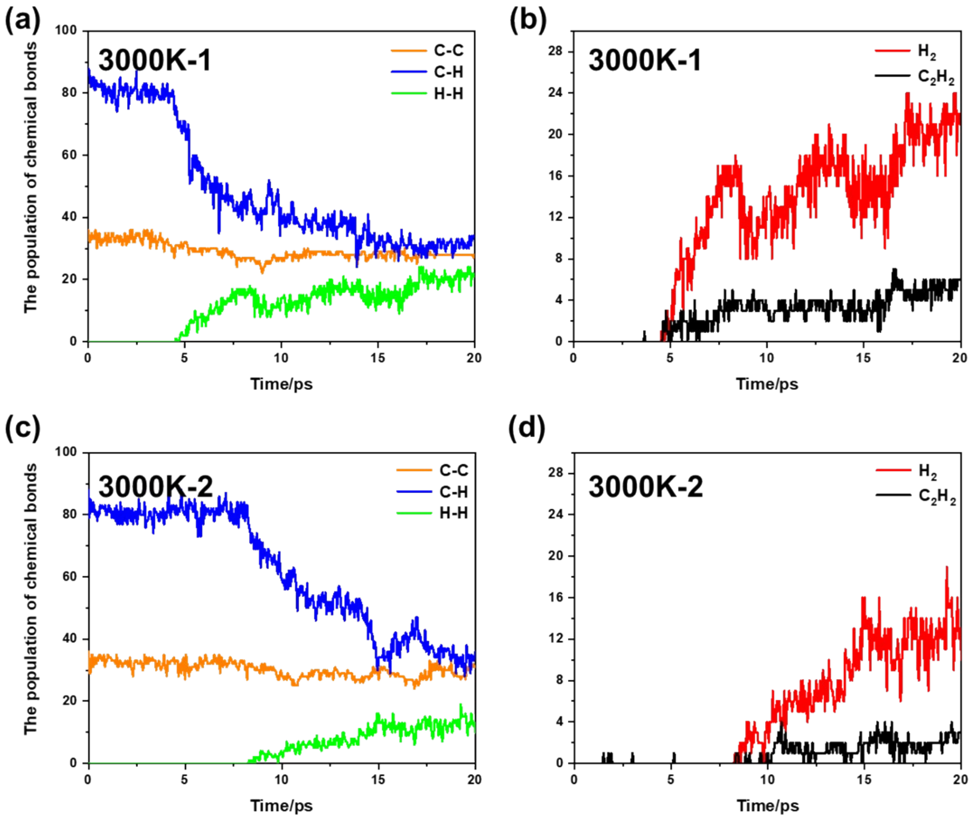
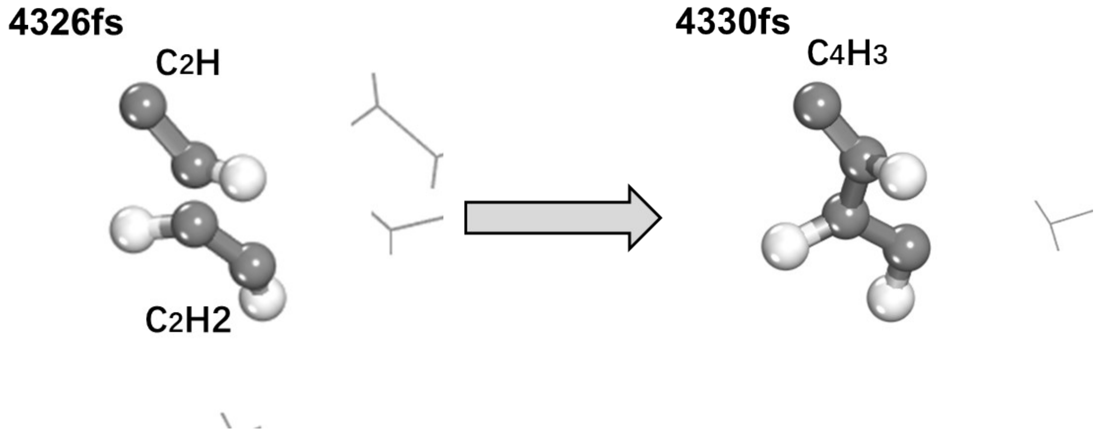


Figure S2. The time evolution of population of chemical bonds and species at 3000K.

Here, the two simulation results of $C_{10}H_{22}$ pyrolysis under 3000K and 4MPa are shown in Figure S2. In other simulation results under 2400 and 2700K, their overall rate of pyrolysis is obviously slower than that of 3000K. With only fewer short-chain CH intermediates (C_4, C_5, C_6 and C_7) formation, the time evolution of the population of chemical bonds and species under 2400 and 2700K is no clear trend. Therefore, the simulation results under 2400 and 2700K will not be shown in Figure S2.

C_2H_2+C_2H=C_4H_3



C_3H_5+C_4H_6=C_3H_6+C_4H_5

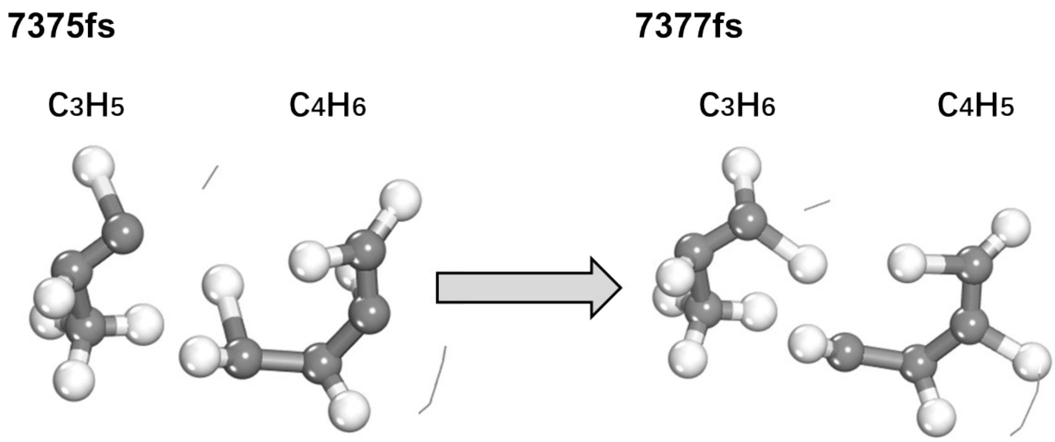


Figure S3. The reaction snapshot of $C_{10}H_{22}$ pyrolysis.

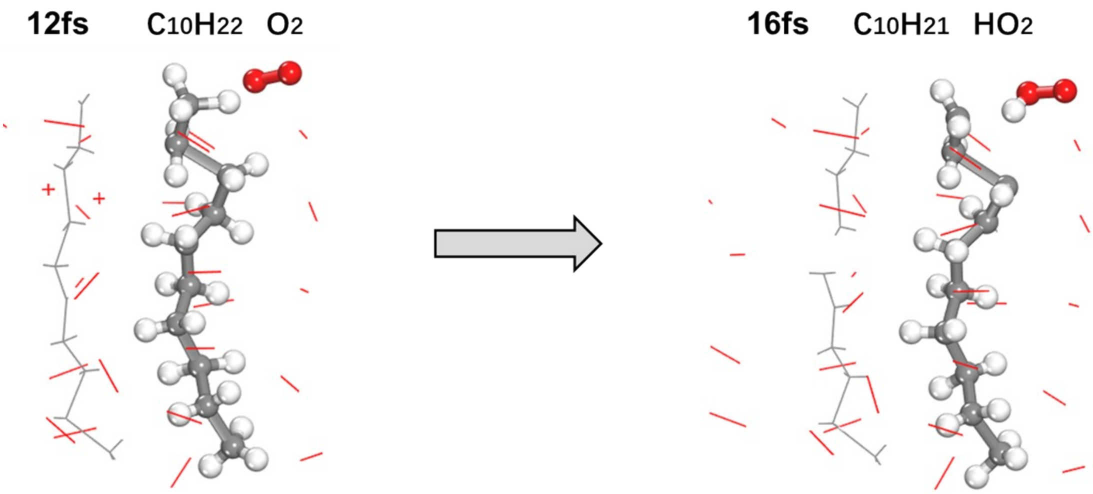
In the process of $C_{10}H_{22}$ pyrolysis, observe the C_XH_Y-related reactions. These reactions mainly include intermolecular H transfer and bimolecular complexation reactions. The reactions obtained from the pyrolysis simulations are used as a complement to that of the oxidation simulations. Figure S3 shows partial reaction snapshots.

Reaction track

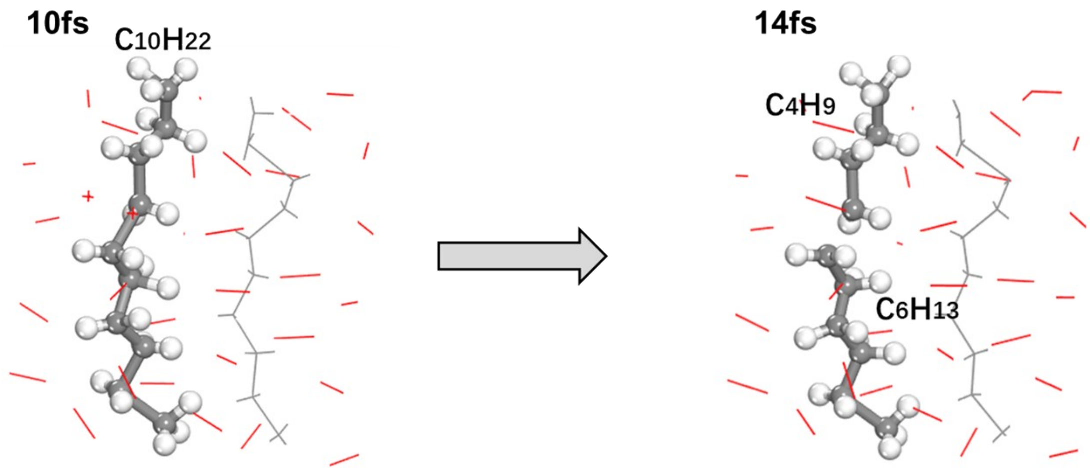
According to the atomic position at every moment, the information on breaking or forming chemical bonds of chemical species is determined by self-compiled programs. The reaction occurring within a period of time is given according to the situation of breaking or forming chemical bonds between atoms within a period of time. Finally, the detailed reaction steps are obtained by combining the reaction snapshot.

Below, five reactions are given as examples:

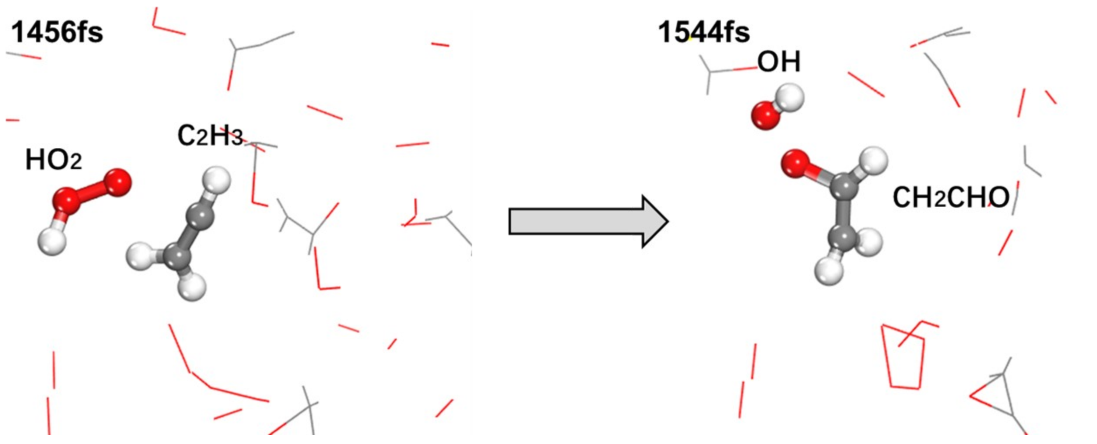
(1) Reaction: $C_{10}H_{22}+O_2=C_{10}H_{21}+HO_2$



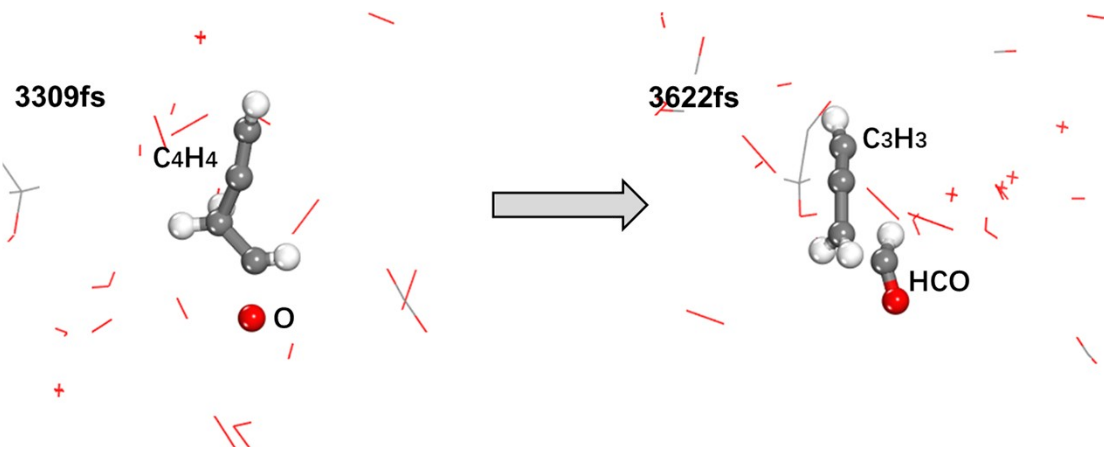
(2) Reaction: $C_{10}H_{22}=C_4H_9+C_6H_{13}$



(3) Reaction: $C_2H_3+HO_2=CH_2CHO+OH$



(4) Reaction: $C_4H_4+O=C_3H_3+HCO$



(5) Reaction: $HCO+O_2=CO+HO_2$

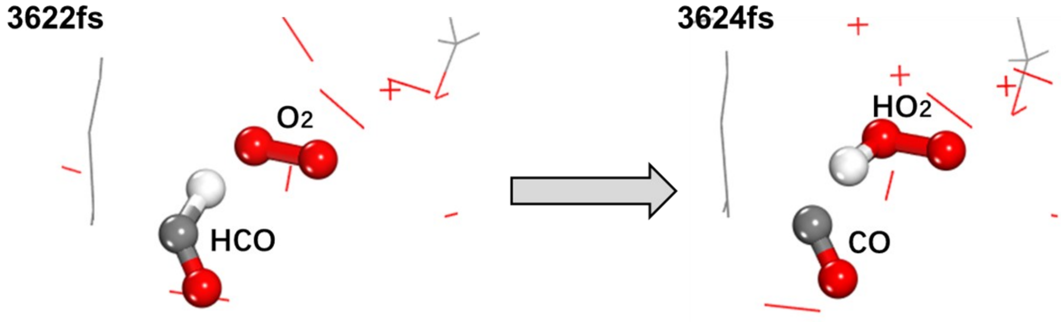


Figure S4. The reaction snapshot of $C_{10}H_{22}$ oxidation.