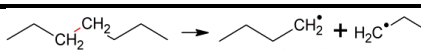
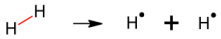
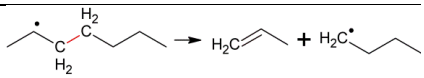
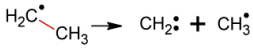
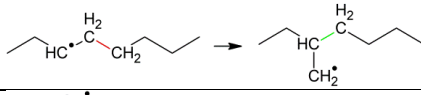
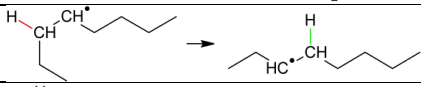
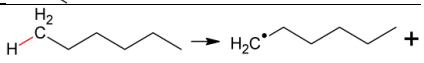
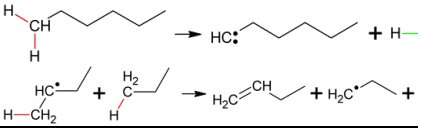
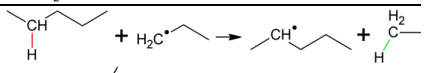
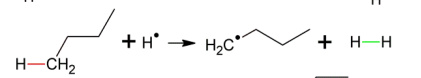
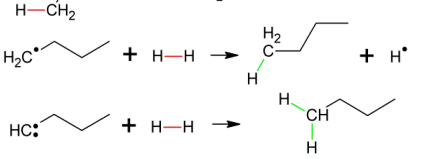
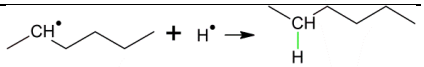
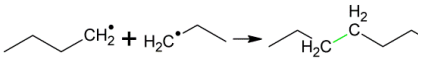
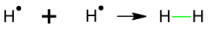
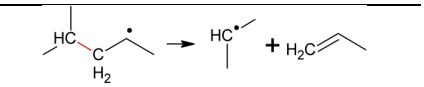
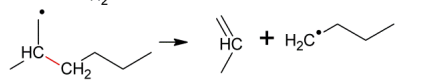
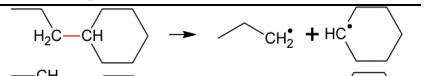
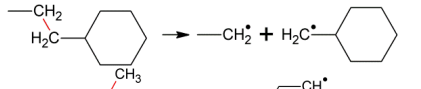
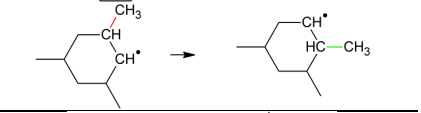
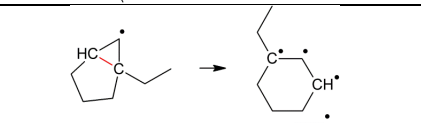
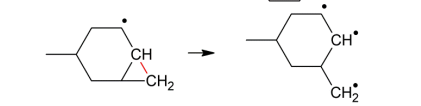
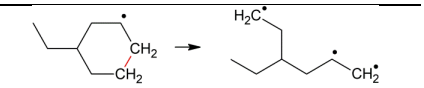
**Table S2**. Reactions classes of hydrocarbon pyrolysis defined for automatic reaction classification of ReaxFF MD simulations[7, 9]

| RxC | RxC name | Reaction instances |
|---|---|---|
| 1 | C-C bond homolysis |  |
| 0 | H-H bond homolysis |  |
| 2 | $\beta$-scission |  |
| 3 | $\alpha$-scission |  |
| 5 | Intra-molecular chain isomerization |  |
| 4 | Intra-molecular H-shift |  |
| 6 | H detachment |  |
| 7 | $H_2$ formation via dehydrogenation |  |
| 9 | Inter-molecular H-abstraction by C |  |
| 8 | H-abstraction by H |  |
| 10 | H-abstraction of $H_2$ by C |  |
| 11 | H radical addition to C |  |
| 12 | Recombination of C radicals |  |
| 13 | Combination of H radicals |  |
| 14 | Isopropyl detachment |  |
| 15 | Detachment of isopropyl radical |  |
| 17 | $\alpha$-branched bond scission of C ring |  |
| 16 | $\beta$-branched bond scission of C ring |  |
| 35 | Branch shift of C ring |  |
| 27 | Polycyclic bridge cleavage into a large ring |  |
| 28 | Adjacent C-C ring bond cleavage of polycyclic bridge bond |  |
| 22 | $\beta$-ring opening of ring carbon radical |  |

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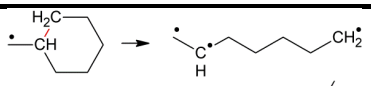
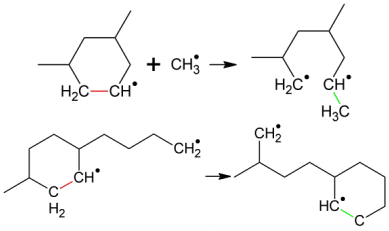
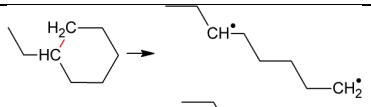
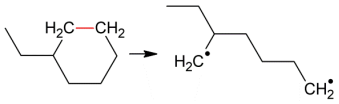
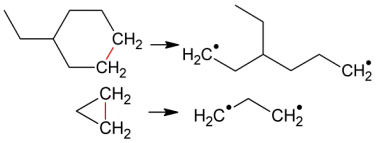
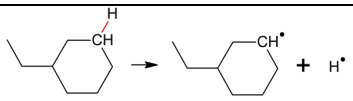
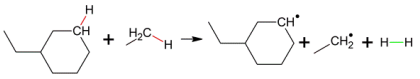
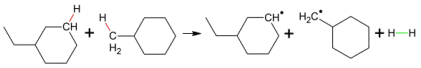
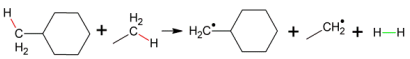
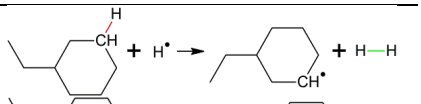
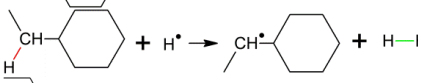
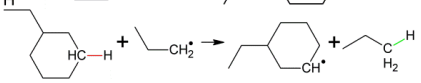
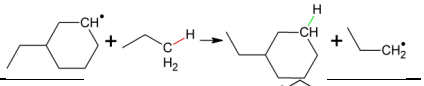
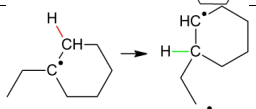
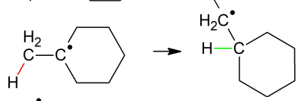
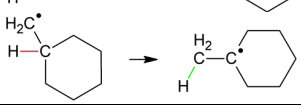
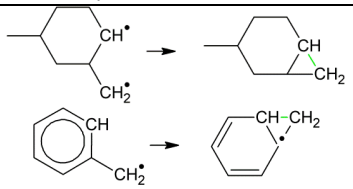
|---|---|---|
| 23 | $\beta$-ring opening of branched carbon radical |  |
| 21 | $\alpha$-ring opening of ring carbon radical |  |
| 18 | $\alpha$-ring bond scission of ring branch |  |
| 19 | $\beta$-ring bond scission of ring branch |  |
| 20 | Ring bond scission except for $\alpha$ and $\beta$ ring bond of ring branch |  |
| 29 | Ring dehydrogenation |  |
| 40 | $H_2$ formation via dehydrogenation of ring and acyclic fragment |  |
| 43 | $H_2$ formation via dehydrogenation of ring and α-C of ring branch |  |
| 26 | $H_2$ formation via dehydrogenation of α-C of ring branch and acyclic fragment |  |
| 24 | Cyclic H-abstraction by H |  |
| 25 | H-abstraction of α-C on ring branch by H |  |
| 32 | Cyclic H-abstraction by acyclic radical |  |
| 39 | Acyclic H-abstraction by ring radical |  |
| 37 | Intra-ring H-shift |  |
| 41 | Ring branch H-shift to ring |  |
| 42 | Ring H-shift to ring branch |  |
| 30 | Ring increment via branch linked to host ring |  |

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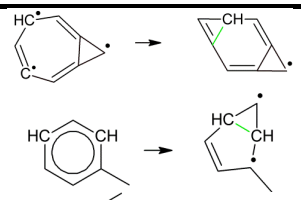
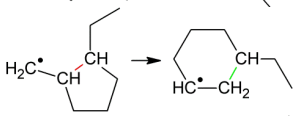
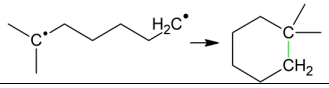
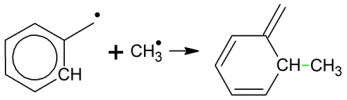
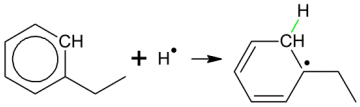
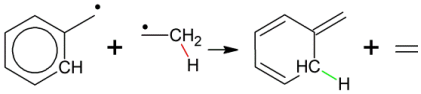
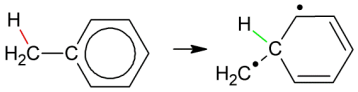
|---|---|---|
| 44 | Ring increment via intra-ring carbons connecting |  |
| 36 | Ring opening and recombination |  |
| 31 | Chain cyclization |  |
| 38 | Combination of aromatic carbon and C radical fragment |  |
| 34 | Combination of aromatic carbon and H |  |
| 33 | H-abstraction by aromatic carbon |  |
| 45 | H-shift from branched-chain to host aromatic ring |  |

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