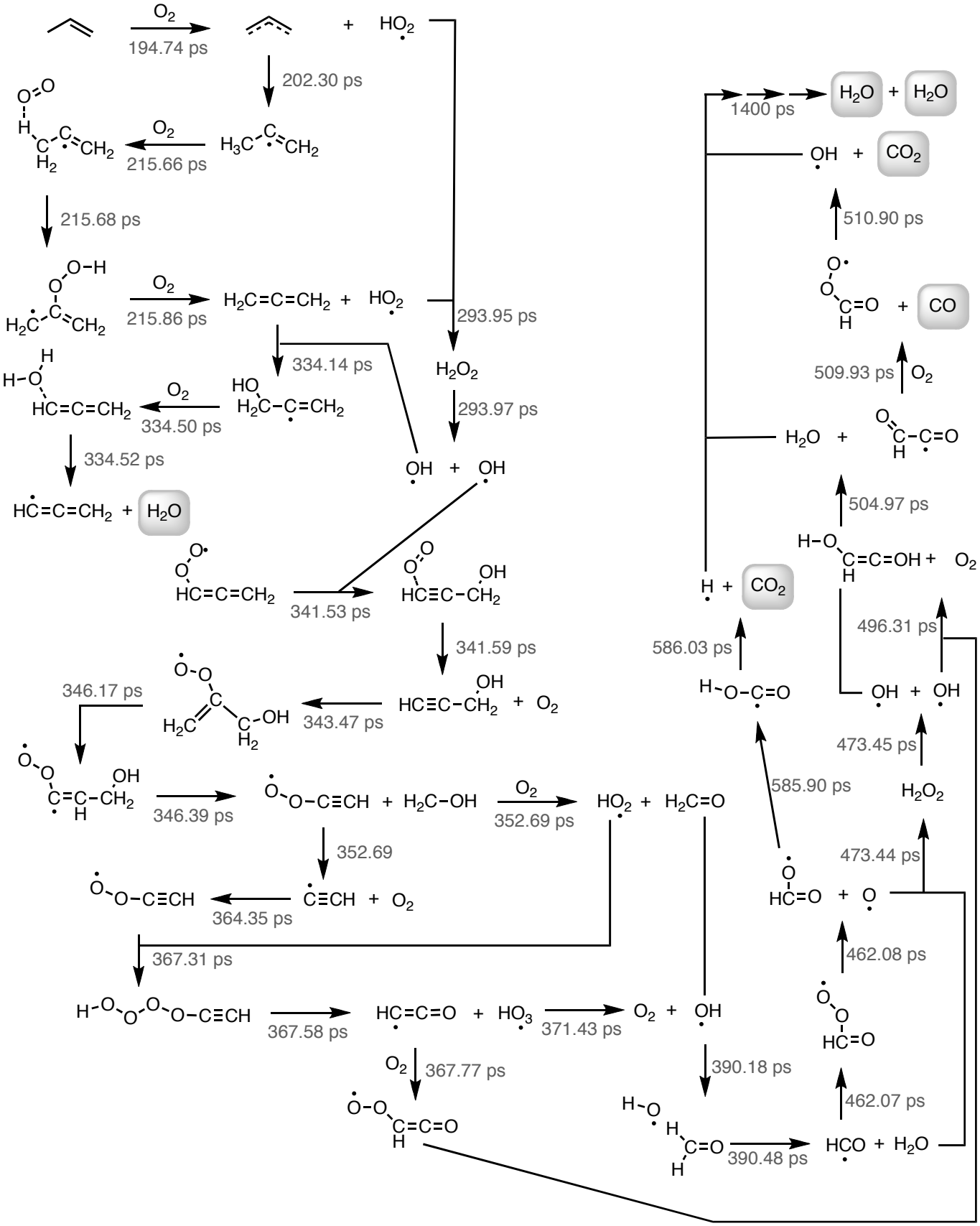
Supporting information for the manuscript "A ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation" by Chenoweth, van Duin and Goddard

Scheme A. Propene oxidation pathways observed during ReaxFF NVT-MD simulations.