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Shock-induced chemistry in simple organic molecules

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Interrogating chemical reactions behind a shock front is immensely difficult, and as a result, the details of shock-induced chemistry remain poorly understood. Shock compression creates transient distorted structures from which molecular reactions initiate. Previous works have reported that dimerizations, polymerizations, ring-opening and decomposition reactions occur under shock compression, depending on molecular structure. Certainly for explosives, exothermic decomposition reactions ultimately drive self-supported detonation. Questions regarding the thresholds for incipient reaction for different chemical functional groups, the nature of first and subsequent reaction steps, and the influence of shock input conditions on reaction kinetics remain to be answered. Evidence of reaction can be discerned from discontinuities in the mechanical variables for reactions with a change in density along the reaction coordinate, similar to first-order phase transformations. Here, we have applied in-situ electromagnetic gauging at multiple Lagrangian positions to elucidate the evolution of multiple-wave structures associated with shock-induced reactions. We have applied in-situ gauging, in concert with reactive molecular dynamic simulations, to investigate shock-reactivity of several simple functional groups: carbon-carbon double (-C=C-) and triple bonds, and nitriles (e.g. phenylacetylene and acrylonitrile), and aromatic ring structures (benzene), all building blocks for explosives. From measurements of the reactive flow, we have obtained detailed information about the temporal evolution of the waves, and global kinetics associated with transformation(s) between partially- and fully-reacted states. Near the reactive threshold, evolution in particle velocities point to reaction timescales on the order of several hundred nanoseconds. We have defined the reactive cusp Hugoniot states, and established the relative order of group reactivity under single shock conditions. These observations will be compared with reactions from the solid phase under static high pressure/temperature conditions, with a description of crystalline phase, and identification of polymerized products by in-situ x-ray diffraction and spectroscopic methods.