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Shock-driven chemistry and reactive wave dynamics in benzene

STEPHEN SHEFFIELD, DANA DATTELBAUM, JOSHUA COE, Los Alamos National Laboratory, LOS ALAMOS NATIONAL LABORATORY TEAM — Benzene is a stable organic chemistry molecule because of its electronic structure – aromatic stability is derived from its delocalized, π-bonded, 6-membered planar ring structure. Benzene principal shock Hugoniot states have been reported previously by several groups, at both high and low pressures. Cusps (or discontinuities) in the shock Hugoniot provide evidence that chemical reactions take place under shock-wave compression of benzene at input pressure conditions above 12 GPa. In other shock-driven experiments, spectral changes have been observed near this cusp condition, indicating that the cusp is associated with shock-driven chemical reaction(s). In this work, a series of gas-gun-driven plate impact experiments were performed to measure and quantify the details associated with shock-driven reactive flow in benzene. Using embedded electromagnetic gauges (with up to 10 Lagrangian gauge positions in-material in a single experiment) multiple, evolving wave structures have been measured in benzene when the inputs were above 12 GPa, with the details changing as the input pressure was increased. Detailed insights into the volume changes associated with the chemical reaction(s), reaction rates, and estimates of the bulk moduli of reaction intermediates and products were obtained. Using this new experimental data (along with the older experimental data from others), the benzene reactant and product Hugoniot loci have been modeled by thermodynamically complete equations of state.

Dana Dattelbaum
Los Alamos National Laboratory

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