

Abstract Submitted  
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**Thermodynamic and chemical behavior of benzene under shock conditions** JEAN-BERNARD MAILLET, NICOLAS PINEAU, EMERIC BOURASSEAU, CEA-DAM — The thermodynamic and chemical behavior of benzene along its hugoniot curve is investigated using Molecular Dynamics simulations with reactive potentials. The simulated hugoniot curve is in good agreement with experimental data at low pressures. Moreover, the decomposition threshold is well reproduced. In the high pressure regime, reactive simulations show that benzene rapidly decomposes, but resulting pressures do not match experimental ones anymore. Simulations starting with diamond nanoparticles and hydrogen gas give good pressures along the hugoniot. These simulations seem to confirm the existence of carbon clusters with diamond structure in the decomposition products of benzene.

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