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Physical and Chemical Changes in Liquid Benzene Multiply Shock Compressed to 25 GPa¹

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The dynamic, high-pressure response of liquid benzene was examined using multiple-shock compression to peak pressures from 0.6 GPa to 25 GPa. The lower temperatures generated in multiple-shock compression experiments allowed for exploration of the benzene phase diagram in regions inaccessible to single-shock experiments. Time-resolved transmission spectroscopy, Raman spectroscopy, and imaging measurements were used to monitor physical and chemical changes on sub-microsecond time scales. The transmission and imaging measurements showed no changes in the benzene transparency to 13 GPa. Up to 20 GPa the Raman spectra showed pressure-induced shifting and broadening, but no changes that could be attributed to a physical or chemical change. These results show that benzene remains in the liquid state on the experimental time scales. At 24.5 GPa, the Raman modes become indistinguishable from an increasing background within 40 ns of the sample attaining peak pressure, indicating a chemical change. A thermodynamically consistent equation of state (EOS) was constructed to calculate changes in the benzene density, temperature, and energy. Using the thermodynamic data and an idealized molecular configuration model, intermolecular separations between benzene molecules was determined. These calculations show that at 24.5 GPa, sufficient energy and π -orbital overlap exists for intermolecular bonding. The Raman data, along with the thermodynamic and intermolecular separation calculations, suggests that liquid benzene rapidly polymerizes through cycloaddition reactions when multiply-shock compressed to 24.5 GPa.

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