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Polymerization in Substituted Acetylenes: A Comparison between Static, Medium-Strain Rate, and Shock Compression Studies. RAJA CHELLAPPA, DANA DATTELBAUM, NENAD VELISAVLJEVIC, Los Alamos National Laboratory, HANNS-PETER LIERMANN, Extreme Conditions Beamline, PETRA III, DESY — Fast timescale of reactions occurring during shock compression create significant diagnostics challenges to fully quantify the mechanisms involved. Static compression provides a complementary route to investigate the equilibrium phase space and metastable intermediates during high pressure chemistry. Intermediate strain rate compression (0.001/s or higher) with time-resolved probes is a novel way to extract reaction kinetics and underlying pathways. In this study, we present our results from high pressure in situ synchrotron x-ray diffraction (XRD) and infrared (IR) spectroscopy studies on substituted acetylenes: tert-butyl acetylene [TBA: $(\text{CH}_3)_3\text{C}\equiv\text{CH}$] and ethynyl trimethylsilane [ETMS: $(\text{CH}_3)_3\text{SiC}\equiv\text{CH}$]. We observed that the onset pressure of chemical reactions at room temperature ($\text{C}\equiv\text{C} \rightarrow \text{C}=\text{C}$ polymerization) in these compounds was typically higher in static compression (TBA: 11 GPa and ETMS: 26 GPa) when compared to shock input pressures (TBA: 6.1 GPa and ETMS: 6.6 GPa). Expectedly, thermal effects during heating drive the threshold pressure were close to shock conditions as observed during the high temperature measurements. Under compression at medium strain rate (1 GPa/s or higher), a clear progression of the chemical reaction was observed via time-resolved XRD patterns obtained at 0.5s intervals. It is noted that the reaction products were visually observed to be glassy and recovered to ambient conditions, remaining stable with no degradation.

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