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Pressure-induced Polymerization in Substituted Acetylenes¹

RAJA CHELLAPPA, DANA DATTELBAUM, STEPHEN SHEFFIELD, DAVID ROBBINS, Los Alamos National Laboratory — A fundamental understanding of shock-induced chemical reactions in organics is still lacking and there are limited studies devoted to determining reaction mechanisms, evolution of bonding, and effect of functional group substitutions. The fast timescale of reactions occurring during shock compression create significant experimental challenges (diagnostics) 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, although at a much slower timescale. In this study, we present our results from our ongoing high pressure *in situ* synchrotron x-ray diffraction and vibrational spectroscopy experiments on substituted acetylenes: tert-butyl acetylene [TBA: $(\text{CH}_3)_3\text{-C}\equiv\text{CH}$] and ethynyl trimethylsilane [ETMS: $(\text{CH}_3)_3\text{-Si}\equiv\text{CH}$]. We observed that the onset pressure of chemical reactions (at room temperature) in these compounds is significantly 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). The products were polymeric in nature, recovered to ambient conditions with little degradation and fully characterized using spectroscopy, calorimetry, and other techniques to identify reaction mechanisms.

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