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Shock-Induced Chemical Reactions of Polycyclic Aromatic Hydrocarbons MARK ELERT, U. S. Naval Academy, SERGEY ZYBIN, California Institute of Technology, SHANNON REVELL, U. S. Naval Academy, CARTER WHITE, Naval Research Laboratory — Polycyclic aromatic hydrocarbons (PAHs) have been found in the atmospheres of Jupiter and Titan, and also in meteorites, interplanetary dust, and circumstellar graphite grains. The ubiquity of these complex organic structures and their stability under extreme conditions make them a significant factor in discussions of brebiotic chemistry in the solar system. To study the shock-induced chemistry of PAHs under conditions appropriate for astrophysical impacts, molecular dynamics simulations have been carried out for solid naphthalene and anthracene using a reactive empirical potential. The major reaction channels for these two closely related compounds were found to be substantially different. Product distributions were also found to depend strongly on the orientation of the PAH crystal relative to the shock propagation direction.

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