

Shock reaction of benzene up to 28.5GPa – Statistical approach

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Benzene is the simplest aromatic hydrocarbon with sigma bonds and delocalized pi electrons in the hexagonal ring. Benzene molecule is found in carbaceous chondrites and is believed to be ubiquitous in interstellar medium. From Murchison and other CM2 meteorites, the C₆ to C₂₂ free aromatic compounds are detected by GC-MS and suggestive of contribution from interstellar organic compounds and internal reactants of such compounds in carbaceous chondrites. We especially consider impact-shock-induced chemical reactions and their mechanisms in carbaceous chondrites. The shock wave experiments of benzene provide us fundamental information on reaction mechanisms of shock waves generated by the body impacts on the earth and in the space.

Shock experiments were conducted based on the Mimura's procedure (Mimura et al., 2003, Mimura and Nishida 2016 in this conference), liquid benzene was enclosed in a reactor and impacted by a projectile accelerated with a vertical powder gun. The calculated shock pressures and temperatures were 5.9-28.5 GPa and 380-1020K. The shocked samples were extracted by CH₂Cl₂. The products extracted from the shocked samples included insoluble (soot like materials) and soluble materials. Soluble materials in the shocked samples were analyzed with GC-MS. The data of shock pressures, shock temperatures, concentrations and molecular weight of detected molecules were applied to multicomponent statistical methods (factor, cluster and discriminant analysis).

The application of Hierarchical Cluster Analysis, based on all possible combination of classification method, showed three main group of detected molecules, The First group comprises molecules of polycyclic aromatic hydrocarbon (PAHs) and the second of methyl- and phenyl-derivatized PAHs. By the application of Discriminant Analysis, it was shown that bond cleavage reaction is the most significant variables in the discriminant function. Therefore, the production mechanism of shock-induced compounds should be considered to occur dominantly cycloaddition reaction.