
High-pressure high-temperature study of solid benzene

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Abstract

Benzene is one of the basic compounds in organic chemistry, the building unit of aromatic compounds, that are believed to be the most abundant organic molecules in the Universe (Ehrenfreund and Charnley, 2000; Tielens, 2008) possibly due to electron delocalization over their carbon skeleton, which makes them remarkably stable (Ehrenfreund and Charnley, 2000). The formation of aromatic hydrocarbons in space is usually associated with irradiation-driven polymerization of smaller hydrocarbons (Joblin and Tielens, 2011). Large aromatic hydrocarbons have a huge influence on the heating of cosmic gas and the degree of interstellar space ionization (Tielens, 2008). Moreover, aromatic hydrocarbons as well as amines and amino acids were found in meteorites (Becker et al., 1997; Oro et al., 1971). Carbonaceous chondrites containing aromatic hydrocarbons in their matrix could serve as a source of extraterrestrial organic prebiotic material during the period of heavy bombardment of the inner Solar System 3.8–4.5 billion years ago (Anders, 1989; Chyba and Sagan, 1992; Chyba et al., 1990). We have refined crystal structure and defined melting and decomposition parameters of benzene at 1.5–8.2 GPa and 298–923 K using multianvil apparatus and *in situ* neutron and X-ray diffraction. Our data show the minor temperature effect on the compression behavior of deuterated benzene at 7.8–8.2 GPa. At 3.5–4.0 GPa we observed the deviation of D atoms from ring plane with rising temperature caused by the displacement of benzene molecules and decrease of intermolecular van der Waals bond of π -conjugated carbon skeleton and the deuterium atom of adjacent molecule. Benzene decomposition was defined at 1.5–8.2 GPa between 773–923 K. The benzene decomposition products consist of carbonaceous material. Triple point between solid, fluid and decomposed state of benzene was defined at \sim 3.5 GPa and \sim 773 K. Phase diagrams of benzene, naphthalene, pyrene and coronene show consistent shift of triple point between fluid, solid and decomposed state to lower pressures. The equalities of carbonization parameters for aromatic compounds at pressures $>$ 4 GPa are related to the identity of molecular packing at these conditions.

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