

High-pressure study of coronene: phase transitions, oligomerization, decomposition and thermal expansion

Artem Chanyshev¹, *Konstantin Litasov¹, Anton Shatskiy¹, Yoshihiro Furukawa², Anna Likhacheva¹, Takashi Yoshino³, Yuji Higo⁴, Eiji Ohtani²

1. V.S. Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk, Russia, 2. Graduate School of Science, Tohoku University, Sendai, Japan, 3. Institute for Study of the Earth's Interior, Okayama University, Misasa, Tottori, Japan, 4. SPring-8, Japan Synchrotron Radiation Research Institute, Kouto, Hyogo, Japan

Coronene $C_{24}H_{12}$ is a polycyclic aromatic hydrocarbon (PAH) consisting of six benzene rings. PAHs 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). Coronene was found in hydrothermal (Echigo et al., 2007) and metamorphic rocks (Sawada et al., 2008) as well as in meteorites (e.g. Oro et al., 1971). Moreover, PAHs have been identified as inclusions in garnet, olivine, and diamond from mantle xenoliths in kimberlite pipes (e.g. Garanin et al., 2011; Kulakova et al., 1982). At 300 K and ambient pressure coronene possesses the space group $P2_1/a$ (Fawcett and Trotter, 1966). Two high-pressure phase transitions of coronene at 1.5 and 12.2 GPa were determined by Jennings et al. (2010). High-pressure phases were identified as monoclinic (1.5 P 12.2 GPa) and orthorhombic (P 12.2 GPa) crystal structures with space groups of $P2/m$ and $Pmmm$, respectively (Zhao et al., 2013).

Here we performed high-pressure experiments using multi-anvil apparatus and DAC. We observed phase transition ($P2_1/a$ - $P2/m$) between 0 and 0.9 GPa. Compressibility parameters of coronene phase $P2/m$ were defined in the pressure range of 0.9-8.1 GPa at 300 K as $K_0 = 13.0(3)$ GPa, $K_0' = 7$ at $V_0 = 795.5 \text{ \AA}^3$ using Vinet EOS (Vinet et al., 1987); the thermal expansion coefficient was found to be low at 2.0-7.5 GPa and 473-873 K (about 10^{-5} K^{-1}). The same low thermal expansion coefficient at $P > 3$ GPa was defined previously for naphthalene $C_{10}H_8$ (Likhacheva et al., 2014).

Coronene decomposition was determined in the pressure range of 2.0-15.5 GPa between 900-1000 K. Coronene decomposition products consist of nanocrystalline graphite, amorphous carbon and diamond with trans-polyacetylene lying along the grain boundaries. At lower temperatures (500-773 K) we observed significant oligomerization of coronene by MALDI measurements. Coronene oligomer formation occurs via PAH dehydrogenation and successive fusion of the initial hydrocarbon molecules through C-C bond formation. Based on our results and previous experimental study at ambient pressure (Talyzin et al., 2011) we have identified PT diagram of coronene phase transitions, oligomerization and decomposition parameters to 16 GPa and 1000 K (Fig. 1). Defined coronene phase diagram is extremely important for understanding the planet accretion by carbonaceous chondrites.

Figure 1. PT-diagram of coronene with phase transitions, oligomerization and decomposition parameters. Shaded area is a coronene oligomerization field.

Keywords: aromatic hydrocarbons, carbon cycle, planetary interiors

