

Oligomerization and carbonization of polycyclic aromatic hydrocarbons at pressures to 16 GPa

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We have examined the stabilities of different polycyclic aromatic hydrocarbons (PAHs) at pressures up to 16 GPa and temperatures to 1273 K. Experiments were performed using a large-volume multi-anvil apparatus. Quenched products were analyzed by matrix-assisted laser desorption/ionization (MALDI) and Raman spectroscopy. The MALDI measurements revealed the considerable oligomerization of PAHs at 7 GPa and 773 to 873 K and insignificant PAH oligomerization at 16 GPa and 300 K. At 7 GPa and 773 K, oligomers with atomic masses up to 3400 Da and higher were found, while only a small number of dimers of the starting PAHs were detected at 16 GPa and 300 K. PAH decomposition at 7 GPa occurred from 873 to 973 K, and the decomposition products consisted of nanocrystalline graphite. We also obtained solid-liquid-(C+H₂) triple points by in situ X-ray diffraction and X-ray radiography and found that they are located at relatively low pressures of 1-2 GPa for naphthalene, acenaphthene, pyrene, and coronene. Previously determined melting lines to 4-5 GPa were thus subjected for revision. The determined decomposition temperatures of the PAHs (873-973 K) are much lower than Earth's geotherms and the subduction slab P-T profiles at 6-7 GPa; therefore, PAH inclusions in mantle-derived minerals, which can be crystallized at 6 to 7 GPa and 1600 to 1700 K, should be secondary phases and could be formed by the successive polycondensation of simple hydrocarbon molecules under natural catalysts during eruption processes at sub-ambient pressures and temperatures. We also rebutted the high-temperature stability of PAHs suggested by previous shock compression experiments and theoretical predictions. However, metastable formation of PAHs in shock experiments at high PT-conditions may still be possible.

Keywords: high pressure, polycyclic aromatic hydrocarbons, carbon, oligomerization