

Abstract Submitted
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Synchrotron x-ray diffraction and infrared spectroscopy studies of C₆₀H₁₈ under high pressure BINGBING LIU — *In situ* high-pressure angle dispersive synchrotron X-ray diffraction and high-pressure mid-IR spectrum measurements of C₆₀H₁₈ were carried out up to 32 GPa and 10.2 GPa, respectively. Our diffraction data indicated the fcc structure of C₆₀H₁₈ was stable up to 32 GPa. The bulk modulus B₀ was determined to be 21±1.16 GPa, about 40% higher than that of C₆₀. The C-H vibrations still existed up to 10.2 GPa and the vibration frequencies decreased with increasing pressure. IR active vibrational frequencies and their corresponding eigenvectors of C₆₀H₁₈ were simulated by DMOL₃. The effects of hydrogen in the fullerene molecular cage on the stability of structure under high pressure were discussed.

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