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First principle investigation of iron pentacarbonyl energetic solid at high pressure KIEN NGUYEN CONG, BRAD STEELE, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida — Polymeric phase of carbon mono-oxide (p-CO), an extended non-molecular solid, is extremely energetic, and therefore represents a new class of low-Z energetic materials. Recently, iron penta-carbonyl $Fe(CO)_5$ has been experimentally investigated as a p-CO precursor: the presence of transition metal ions is believed to stabilize p-CO at ambient conditions. Since p-CO forms at high pressures, it becomes important to investigate the high-pressure behavior of $Fe(CO)_5$ as well. In this work, first-principles evolutionary structure search method is used to predict the crystal phases of $Fe(CO)_5$ at high pressure. Known experimental structure of phase I is confirmed. Moreover, previously unknown structure of phase II is predicted. The Raman spectra, calculated as a function of pressure, were used to demonstrate that the phase III, predicted by a recent experiment, is identical to phase II.

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