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Modeling the structure of croconic and squeric acids under pressure. ISKANDER G. BATYREV, US Army Rsch Lab - Aberdeen — Quantum mechanical simulations of modifications of structure of croconic and squeric acids under pressure up to 55 GPa indicate formation of a high-pressure extended network phase. Density functional theory plane wave calculations were performed to investigate the effects of isotropic and anisotropic compression on the structural transformation of croconic acid and elucidate the details of the transition. The onset of pressure-induced polymerization of croconic acid was observed near 12 GPa. Complete polymerization was noted at pressures near 25 GPa. The simulations revealed a hysteresis upon decompression in the pressure-volume curve as well as the O-H bond lengths; based upon the maximum pressure of confinement, the hysteresis was observed to shift. Calculated X-ray diffraction patterns and vibrational spectra of the high pressure acids crystals are in a reasonable agreement with previously published experimental diffraction and vibrational spectra. Strong H bonds were also found to result in the pressure-induced formation of an extended network in squeric acid, suggesting that the found phenomenon is common for oxocarbon acids.

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