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**Modeling of a random network of extended CO solids** I.G. BATYREV, WILLIAM D. MATTSON, BETSY M. RICE, US Army Research Laboratory — This presentation will describe first principles explorations of a random network of polymeric carbon monoxide (poly-CO), a high energy density material. Starting with 128 and 432-atom unit cells of a CO molecular solid in the disordered delta phase we performed atom relaxation and conjugate gradient cell optimization at different pressures. We found that during the compression of the delta phase in the range of 10-15 GPa, random networks consisting mainly of 4 and 5 member rings with O atoms in the cage of the rings, carbonyl units and few CO molecules form. The optimized structure has triclinic and orthorhombic distortions of the initial cubic structure of less than 3%. Vibrational frequencies of the random structures were calculated for comparison with FTIR and Raman spectroscopy experimental data. Additionally, the electron localization function and Bader analysis are used for understanding of stability and sensitivity of the extended CO structures.

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