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Stable and Metastable Mixed Polymeric Carbon, Nitrogen, and Oxygen Compounds at High Pressures BRAD STEELE, IVAN OLEYNIK, University of South Florida — Polymeric $C_xN_yO_z$ compounds are promising candidates for novel high energy density materials. Both nitrogen and carbon monoxide transform into polymeric high energy density materials at high pressures: over 100 GPa for nitrogen and just over a few GPa for polymeric carbon monoxide (p-CO). The recovery of polymeric nitrogen at ambient conditions remains problematic while p-CO is found to decompose at ambient conditions. In spite of the potential usefulness of $C_xN_yO_z$ compounds, very little is known about their high pressure chemistry. In this work, extensive first principles variable-composition evolutionary structure prediction calculations are performed to predict the mixed $C_xN_yO_z$ phase diagram at pressures up to 100 GPa. The search reveals the polymeric C_2N_2O structure in the space group $Cmc2_1$, which is a known structure of Si_2N_2O, to be stable at just 10 GPa. We also predict several metastable mixed $(CO)_x$-$(N_2)_y$ structures energetically favorable compared to p-CO and N_2. Several materials are predicted to have an energy density comparable to p-CO at ambient conditions. Predicted structures are characterized by their Raman spectra and equations of state.

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