

Abstract Submitted
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High Pressure Structures and Equations of State of HIO3 and HIO3O8¹ JOSEPH ZAUG, ELISSAIOS STAVROU, Lawrence Livermore National Laboratory, BRIAN LITTLE, AFRL/RWM, SORIN BASTEA, JONATHAN CROWHURST, Lawrence Livermore National Laboratory, CHEMICAL ENERGY COLLABORATION — Knowledge of high-pressure thermodynamic properties of iodine containing oxides and acids is important toward improving the accuracy of semi-empirical predictions of extreme condition explosive and combustive chemistry of iodine containing formulations. Here we report on the synthesis of explosive chemical products HIO3 and HIO3O8 and on the structures and isotropic equations of state up to 35 and 45 GPa respectively. EOS model parameters are provided including parametrized exponential-6 interatomic potential values used to conduct thermochemical calculations of iodine containing reactants.

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