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High Pressure Structures and Equations of State of HIO3 and HI3O8[1] JOSEPH ZAUG, ELISSAIOS STAVROU, Lawrence Livermore National Labortaotry, BRIAN LITTLE, Air Force Research Laboratory - RWM, SORIN BASTEA, JONATHAN CROWHURST, Lawrence Livermore National Labortaotry — 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 HI3O8 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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