Exploration of the Structure of the High Temperature Phase of the Hexagonal RMnO$_3$ System

T WU, T. A. TYSON, H. ZHANG, T. YU, New Jersey Inst. Tech., K. PAGE, Oak Ridge National Laboratory, S. GHOSE, Brookhaven National Laboratory — Temperature dependent structural studies of the high temperature phase of hexagonal RMnO$_3$ systems have been conducted. Both long range and local structural probes have been utilized. Discussions of the appropriate space groups and local distortions relevant to length scale will be given. Ab initio MD simulations are used to interpret the observations. This work is supported by DOE Grant DE-FG02–07ER46402.