

Novel Extended Phases of Molecular Triatomics

YOO C-S., IOTA V., PARK J., CYNN H.

Lawrence Livermore National Laboratory, Livermore, California 94551

Application of high pressure significantly alters the interatomic distance and thus the nature of intermolecular interaction, chemical bonding, molecular configuration, crystal structure, and stability of solid. With modern advances in high-pressure technologies, it is feasible to achieve a large (often up to a several-fold) compression of lattice, at which condition material can be easily forced into a new physical and chemical configuration. The high-pressure thus offers enhanced opportunities to discover new phases, both stable and metastable ones, and to tune exotic properties in a wide-range of atomistic length scale, substantially greater than (often being several orders of) those achieved by other thermal (varying temperatures) and chemical (varying composition or making alloys) means.

There are numerous theoretical and experimental results demonstrating that simple molecular solids transform into nonmolecular phases at high pressures and temperatures, ranging from monatomic molecular solids such as sulfur, phosphorous and carbon to diatomic molecular solids such as nitrogen, carbon monoxide and iodine, to triatomic molecules such as ice, carbon dioxide and carbon disulfide, and to polyatomics such as methane and cyanogen, and aromatic compounds. In this paper, we will focus on the pressure-induced phase transitions observed in a few molecular triatomics: first reviewing the transformations in two isoelectronic linear triatomics, carbon dioxide and nitrous dioxide, and then discussing about their outstanding issues and periodic analogies to carbon disulfide and silicone dioxide.

This work was performed under the auspices of the U.S. DOE by the Univ. of Calif., LLNL under contract No. W-7405-Eng-48. The authors acknowledge invaluable uses of beamtimes at the ESRF and the APS which made the present study possible. We also recognized the experimental contributions from other collaborators including M. Nicol, H. Kolhmann, S. Carlson, T. LeBihan, M. Mohammad, and D. Hausermann.