Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Extended-Solid Phases of Carbon Dioxide at High Pressures[1]
VALENTIN IOTA, ZSOLT JENEI, JAE-HYUN KLEPEIS, Lawrence Livermore National Laboratory, CHOONG-SHIK YOO, Washington State University, Pullman, WILLIAM EVANS, Lawrence Livermore National Laboratory — At high pressures and temperatures, CO_2 transforms to a series of solid polymorphs with differing crystal structures, intermolecular interactions and chemical bonding. Among them are a number of covalent (extended) solid phases, with crystal structures analogous to SiO_2 polymorphs. Above 40GPa and 1500K CO_2 transforms to phase V, a network of corner sharing CO_4 tetrahedra – structurally similar to SiO_2 tridymite. At room temperatures, CO_2 forms *a-carbonia,* an amorphous extended-solid phase similar to silica glass. Recently, we reported another phase, with a structure resembling that of SiO_2 stishovite, formed by compressing associated phase II above 50GPa. Here, we present a systematic picture of the structural and bonding diagram of carbon dioxide, focusing on the relationship between its molecular and extended phases at high pressures and temperatures.

[1]This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Valentin Iota
Lawrence Livermore National Laboratory

Date submitted: 27 Nov 2007 Electronic form version 1.4