

Abstract Submitted  
for the SHOCK11 Meeting of  
The American Physical Society

**High-pressure phase diagrams of liquid CO<sub>2</sub> and N<sub>2</sub>**<sup>1</sup> BRIAN BOATES, STANIMIR BONEV, Lawrence Livermore National Laboratory — The phase diagrams of liquid CO<sub>2</sub> and N<sub>2</sub> have been investigated using first- principles theory. Both materials exhibit transitions to conducting liquids at high temperatures ( $T$ ) and relatively modest pressures ( $P$ ). Furthermore, both liquids undergo polymerization phase transitions at pressures comparable to their solid counterparts. The liquid phase diagrams have been divided into several regimes through a detailed analysis of changes in bonding, as well as structural and electronic properties for pressures and temperatures up to 200 GPa and 10 000 K, respectively. Similarities and differences between the high- $P$  and  $T$  behavior of these fluids will be discussed. Calculations of the Hugoniot are in excellent agreement with available experimental data.

<sup>1</sup>Work supported by NSERC, LLNL, and the Killam Trusts. Prepared by LLNL under Contract DE-AC52-07NA27344.

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Date submitted: 08 Feb 2011

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