

Abstract Submitted
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Phase transitions in dense nitrogen and carbon dioxide liquids¹

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— The high-pressure phase diagrams of liquid nitrogen and carbon dioxide have been investigated using first-principles theory. Both liquids undergo rare first-order molecular-polymerization phase transitions at pressures comparable to their solid counterparts. Furthermore, both materials dissociate into metallic atomic fluids at high temperatures. The liquid regimes of their phase diagrams have been divided into several regions based on detailed analyses of changes in both structural and electronic properties for pressures and temperatures up to 200 GPa and 10,000 K, respectively. A comparison of the two liquid phase diagrams will be discussed to illustrate similarities and differences. Calculations of the shock Hugoniot are in excellent agreement with available experimental data.

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