

Abstract Submitted
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Molecular structures of CO₂ and N₂O under pressure¹ STANIMIR A. BONEV, BRENDAN OSBERG, Department of Physics, Dalhousie University, Canada — Carbon dioxide and nitrous oxide are investigated at pressures up to 50 GPa and 1000 K using *ab initio* methods. In this pressure-temperature range, both materials have a number of stable molecular structures. We demonstrate that the constituent molecules in these structures do not undergo significant changes and that the proposed phases are consistent with experimental data. The differences found between the CO₂ and N₂O phase diagrams can be understood in terms of the polarity of the N₂O molecules.

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