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Phase Diagram of Nitrogen at High Pressures and Temperatures. Eugene Gregoryanz, Chrystele Sanloup, Alexander Goncharov, Russell Hemley, Ho-kwang Mao, School of Physics, Univ. of Edinburgh, Mayfield St., Edinburhg EH9 3JZ, UK.

The evolution of molecular solids under pressure constitutes an important problem in condensed matter physics. Under compression, delocalization of electronic shells and eventual molecular dissociation is expected, leading to the formation of a framework or closed packed structures. However, this process may not necessarily be simple and direct, because of large barriers of transformation between states with different types of bonding and molecular structures with various types of orientational order, including possible associated and charge transfer intermediate states.

We report the discovery of a new class of molecular phases of solid nitrogen at high pressures and temperatures by Raman scattering, infrared and optical absorption, and powder synchrotron x-ray diffraction. The most remarkable is a new phase theta which is characterized by strong intermolecular interactions and infrared vibron absorption and can be reached within the wide pressure range at temperatures above 550 K. A second phase iota is diatomic with orientationally equivalent molecules. Both phases can be quenched to room temperature and are observed over a wide P-T range from 20 to 100 GPa and 30 to 1000 K. The results suggest a major revision of the phase relations of nitrogen at high pressures and temperatures.