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Structural and Vibrational Properties of Nitrogen-Hydrogen Mixtures at High Pressure DYLAN SPAULDING, Harvard University, Cambridge, MA, 02138, GUNNAR WECK, PAUL LOUBEYRE, Commissariat a l'Energie Atomique, Bruyeres-le-Chatel, France, FREDERIC DATCHI, IMPMC, UPMC/Paris 6, Paris, France, PAUL DUMAS, Synchrotron SOLEIL, Gif-sur-Yvette, France, MICHAEL HANFLAND, European Synchrotron Radiation Facility, Grenoble, France — The chemistry and equations of state of simple molecular systems (e.g. N2, H2, H2O, CO2, CH4 etc.) in the dense fluid state are of extreme importance to planetary astrophysics and are model systems for understanding the effects of pressure on chemical bonding, reactivity in the solid solution and potentially new routes to pressure-induced metallization. Here, we present the first comprehensive study of the binary N2/H2 system in the diamond anvil cell using Raman spectroscopy, synchrotron infrared micro-spectroscopy and visual observation. We find a eutectic-type binary phase diagram with two stable high-pressure compounds which we identify as (N2)6(H2)7 (R-3m) and N2(H2)2 (Pm-3m) using single-crystal x-ray diffraction. The former has a novel rhombohedral structure in which groups of hydrogen molecules are contained by the nitrogen lattice. We discuss further infrared absorption studies on this compound, including evidence for a gradual transformation from van der Waals to ionic interactions with pressure. A phase transition to an ionic compound with the same stoichiometry is observed at 55 GPa. Compression of this compound was carried out up to 200 GPa to investigate possible metallization.

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