

Abstract Submitted
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Equation of State of Ammonia ROBERTA MULFORD, Los Alamos National Laboratory, SEBASTIEN HAMEL, DAMIAN SWIFT, Lawrence Livermore National Laboratory — Ammonia and water are critical components of extraterrestrial bodies, determining the density and physical properties of the Outer Planets, their moons and of extrasolar planets. Several EOS are presented for ammonia and for mixtures of ammonia, water, and methane and their properties discussed, and compared with quantum molecular dynamics predictions of the properties and evolving compositions of these mixtures as pressure and temperatures become extreme. The NH_4OH hydrate of ammonia is known to exist as a separate molecular species at pressures above about 5 GPa, and an effort is made to include reaction between NH_3 and H_2O in the description of effective EOS for mixtures. A thermodynamically complete quasiharmonic EOS for ammonia is constructed, taking into account the vibrational state splitting by molecular inversion, in determination of the heat capacity. The EOS obtained are intended for application in mass-radius relations which bound the possible interpretations of composition and structure for extraterrestrial bodies of unknown composition, in particular exoplanets.

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