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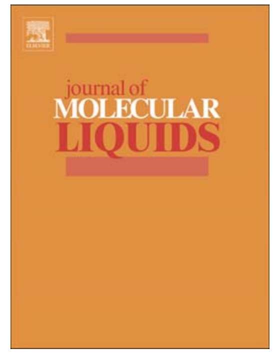


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# An Analytical Equation of State for Ammonia at High Temperatures and High Pressures

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**Abstract**
An analytical equation of state is presented for ammonia to describe its thermodynamic properties over wide ranges of temperatures and pressures up to 3000 K and 20 GPa, respectively. The equation of state contains well-defined parameters, two of which have been slightly adjusted around their global values based on a limited set of experimental data. The properties of ammonia predicted by the new equation of state are in very good agreement with the experimental data and the first-principles molecular dynamics simulation results over a broad range of temperatures and pressures. The new equation of state is expected to supplement molecular simulations at conditions where experimental data are not yet available.

**Keywords:** equation of state, ammonia, high temperature, high pressure

## 1 Introduction

Ammonia is abundantly found in the interiors of giant planets Uranus and Neptune [1]. Saturn, Jupiter, Titan and Enceladus also contain ammonia in various forms [2], [3], [4], [5], [6] . Previous investigations have shown that the presence of ammonia in these planets and moons might significantly affect their atmospheric composition and other observable properties [7], [8], [9]. A comprehensive understanding of these properties requires a detailed knowledge of the thermodynamic behavior of ammonia at different temperatures and pressures that are available in these planets and satellites. However, such temperature and pressure conditions are sometimes beyond the reach of available experimental techniques [10].

The phase diagram of ammonia has been the subject of various experimental and computational investigations [10], [11], [12], [13], [14]. Results of these investigations indicate that at temperatures below 3000 K ammonia has a stable fluid phase depending on the applied pressure, while at higher temperatures, it has a dissociated phase with a complex chemical behavior [10], [11], [12], [13], [14]. The thermodynamic properties of ammonia have been also investigated both experimentally and computationally [14], [15], [16], [17], [18]. However, the experimental data are limited to temperatures and pressures bellow 760 K and 1 GPa, respectively [15], [19]. Accordingly, our knowledge about the properties of ammonia at higher temperatures

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