

## Spectroscopy and Dissociation Energy of Ammonia Dimers and Trimers

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### Abstract

Infrared-action spectroscopy of small ammonia clusters obtained by detecting ammonia fragments from vibrational predissociation provides an estimate of the dissociation energy of the trimer. The product detection uses resonance enhanced multiphoton ionization (REMPI) of individual rovibrational states of ammonia identified by simulations using a consistent set of ground-electronic-state spectroscopic constants in the PGOPHER program. Comparison of the infrared-action spectra to a less congested spectrum measured in He droplets (Slipchenko *et al.*, *J. Phys. Chem. A*, **111**, 7460 (2007)) identifies the contributions from the dimer and the trimer. The relative intensities of the dimer and trimer features in the infrared-action spectra depend on the amount of energy available for breaking the hydrogen bonds in the cluster, a quantity that depends on the energy content of the detected fragment. Infrared-action spectra for ammonia fragments with large amounts of internal energy have almost no trimer component because there is not enough energy available to break two bonds in the cyclic trimer. By contrast, infrared-action spectra for fragments with low amounts of internal energy have a substantial trimer component. Analyzing the trimer contribution quantitatively shows that production of a monomer from the trimer requires energy in the range of 1700 to 1800  $\text{cm}^{-1}$ , a range that is consistent with several theoretical estimates.

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