

## MLS Scientific Publication

Scientific Themes: Atmospheric Chemistry, Submillimeter Spectroscopy.

**Rotational Spectrum of cis-cis HOONO** Brian J. Drouin, Juliane L. Fry, and Charles E. Miller, *Journal of Chemical Physics* Volume 120, Issue 12, 22 March 2004.

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### Summary

There now exists an abundance of convincing spectroscopic evidence supporting a significant HOONO channel in the gas phase reaction of OH + NO<sub>2</sub>. However, the lack of rotational resolved spectra in any of these studies has hampered efforts to provide an unambiguous assignment of the observed spectral features or to quantify the relative yields of cis-cis and trans-perp HOONO produced under different experimental conditions.

The pure rotational spectrum of cis-cis peroxyxynitrous acid, HOONO, has been observed for the first time. Over 220 transitions, sampling states up to  $J' = 67$  and  $K'_a = 31$ , have been fitted with an RMS uncertainty of 48.4 kHz. The experimentally determined rotational constants agree well with *ab initio* values for the cis-cis conformer, a five-membered ring formed by intramolecular hydrogen bonding. The small, positive inertial defect,  $\Delta = 0.075667(60)$  amu  $\text{\AA}^2$ , and lack of any observable torsional splittings in the spectrum indicate that cis-cis HOONO exists in a well-defined planar structure at room temperature.