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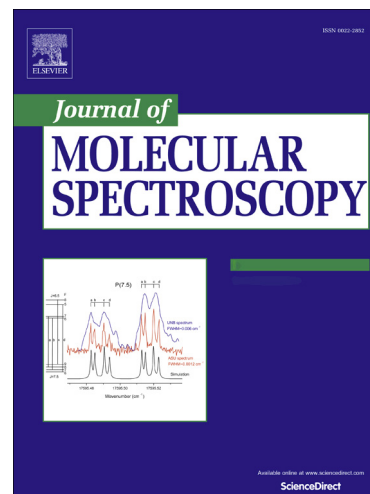
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Reevaluation of matrix-isolation infrared spectra of the isotopologues of *trans*-diazene and attempts to prepare *cis*-diazene by photoisomerization

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ABSTRACT

IR spectra of *trans*-diazene (diimide, HN=NH) have been recorded in nitrogen and argon matrices at 20 K. An IR spectrum of a mixture of *trans*-diazene-*d*₁ and -*d*₂ in a nitrogen matrix has also been recorded. The method for preparing pure *trans*-diazene has been clarified. Revised assignments are reported for these spectra. A definitive experimental assignment of the wavenumbers of normal modes the three hydrogen/deuterium isotopologues is given. Attempts were made to photoisomerize matrix-isolated *trans*-diazene into the elusive *cis* isomer. No bands for the *cis* isomer were found.

Keywords: *cis*- and *trans*-diazene, infrared, matrix isolation, calculated infrared intensities

1. Introduction

Though an elusive substance, *cis*-diazene (or diimide, HN=NH) is of great importance. *cis*-Diazene is a key intermediate in the reduction of atmospheric nitrogen to ammonia, where *cis*-diazene is complexed to the nitrogenase enzyme in an intermediate step in the mechanism [1,2]. *cis*-Diazene is also regarded as a fleeting intermediate in the stereospecific reduction of CC and NN multiple bonds with hydrogen [3,4].

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