STRUCTURES OF TWO ISOMERS OF NITROUS OXIDE TETRAMER FROM THEIR INFRARED SPECTRA

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Weakly bound complexes provide a convenient starting point for a detailed understanding of different pathways that can be taken between the gas and condensed phases of matter. In this regard, it is of considerable interest to determine the number of isomers for a cluster size and if and how geometrical choices made in the early stages of condensation influence the growth of larger clusters. Although it is expected that the number of isomers grows rapidly with cluster size, in many cases only a single isomer is observed experimentally.
High resolution spectroscopy has provided information on structural and vibrational dynamics of a large number of binary and ternary complexes formed from related linear triatomic molecules such as CO_2, N_2O, OCS and CS_2. But, there are much fewer detailed experimental studies which provide structures for the important cluster sizes in the range of $4 \sim 10$ monomers.
Here we report the structural determination of two isomers of nitrous oxide tetramer from their infrared spectra in the ν_1 fundamental region ($\sim$ 2230 cm^{-1}). Two bands are observed and analyzed, corresponding to two distinct isomers of the complex. A perpendicular band centered at 2232.209 cm^{-1} has been assigned to an isomer with S_4 symmetry (a subgroup of D_{2d} group). This is a rare symmetry group, but provides all the necessary ingredients. It allows for a tilt of the monomers from the symmetry axis of the complex as well as a twist. The experimentally determined structure has the monomers more or less perpendicular to the symmetry axis. A second band centered at 2237.424 cm^{-1} was assigned to a structure close to a perfect barrel-shaped tetramer with D_{2d} symmetry. This is a prolate symmetric top which gives parallel bands for the pure isotopomers and a c-type band for the mixed isotopomer containing three $^{15}N_2O$ monomers. This isomer is the same species as that observed by R.E. Miller and L. Pederson. [a]

[a] R. E. Miller and L. Pederson, Chem. Phys. Lett. 275, 307 (1997).