FIRST INFRARED SPECTRA OF NITROUS OXIDE PENTAMER

M. REZAEI, J. NOROOZ OLIAEE, N. MOAZZEN-AHMADI, *Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, AB T2N 1N4, Canada*; A.R.W. McKELLAR, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON K1A 0R6, Canada*.

High resolution spectra have previously been studied for N_2O dimers (two isomers), trimers (one isomer), and tetramers (two isomers). Here, we assign two new bands to the N_2O pentamer. The bands are observed in the region of the N_2O ν_1 fundamental using a tunable laser to probe a pulsed supersonic slit jet expansion. They are centered at 2233.9 and 2236.4 cm^{-1} for $^{14}N_2O$, and at 2164.4 and 2166.8 cm^{-1} for $^{15}N_2O$. Attribution to the pentamer is based on comparison of the observed rotational constants with theoretical ones from calculated cluster structures based on two rather different N_2O pair potentials. The first potential function is from a recent high level *ab initio* study.[a] The second potential is a relatively simple empirical one, based partly on fitting to bulk properties.[b] The likely pentamer structure is a completely unsymmetric one. It can be visualized starting with a highly symmetric oblate tetramer[c] which is attacked by a fifth monomer, locating itself at a favorable distance and breaking the symmetry. Interestingly, analysis of the two bands yields very similar but not quite identical ground state parameters. We believe that they are due to distinct isomers having this same basic structure but differing in the orientation direction of one N_2O monomer.

[a] R. Dawes, X.-G. Wang, A.W. Jasper, and T. Carrington, Jr., *J. Chem. Phys.* **133**, 134304 (2010).
[b] B. Kutcha, R.D. Etters, and R. LeSar, *J. Chem. Phys.* **97**, 5662 (1992).
[c] J.N. Oliaee, M. Dehghany, N. Moazzen-Ahmadi, and A.R.W. McKellar, *J. Chem. Phys.* **134**, 074310 (2011).