EIGENSTATE RESOLVED INFRARED SPECTRUM OF THE C-H STRETCHING FIRST OVERTONE REGION OF *s*-TETRAZINE.

G. PIETRAPERZIA[a], P. ENGELS[b], A. CALLEGARI, H. K. SRIVASTAVA, K. K. LEHMANN and G. SCOLES, *Department of Chemistry, Princeton University, Princeton NJ, 08544-1009*.

The infrared spectrum of *s*-tetrazine, $C_2H_2N_4$, was recorded in the C-H stretching first overtone region, using a build-up cavity coupled molecular beam laser spectrometer with optothermal detection. Among the well-known monocyclic azines, *s*-tetrazine is the least stable and thus of great interest to chemists. While the $S_1 \leftarrow S_0$ spectrum and subsequent concerted triple dissociation has been thoroughly studied, the vibrational overtone spectrum in the near-infrared region has not been previously reported. The molecule is an asymmetric rotor, of symmetry D_{2h}, whose ground state rotational constants are known from electronic spectroscopy data.
In the present study, the spectrum of *s*-tetrazine has been measured in the wavenumber region 6072-6078 cm^{-1}, with a resolution of 5 MHz and a beam temperature of $\sim$ 5 K. The spectrum shows a density of transitions as high as 500 lines/cm^{-1}. The calculated harmonic density of states at this frequency is 300 states/cm^{-1}, on average 1/8 of which have the right b_{1u} symmetry to interact with the bright state. A first estimate of the IVR lifetime for the vibrational mode investigated is 200 ps. This value can be compared with the lifetime of C-H stretching overtones in similar molecules previously investigated by us, which is about the same for pyrrole but ten times shorter for benzene. The analysis of the data is in progress and the results will be reported at the meeting.

[a] Visiting from LENS, Università degli Studi di Firenze, Largo Enrico Fermi 2, 50125 Firenze, Italia
[b] Visiting from the University of Bonn, Institut für Angewandte Physik, Wegelerstr. 8, 53115 Bonn, Germany