

JET SPECTROSCOPY OF THE H-F OUT-OF-PLANE LIBRATIONAL FUNDAMENTAL BAND OF HYDROGEN FLUORIDE PENTAMER IN THE 741 cm^{-1} REGION

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Using our pulsed slit-jet, infrared diode laser spectrometer, we have observed a rotationally-resolved parallel band centered at 741 cm^{-1} in a molecular beam formed by expanding a mixture of 4% HF in helium through a 200 μm x 12 cm slit with a backing pressure of ca. 1000 Torr. A set of excited and ground state spectroscopic constants were fit simultaneously to a data set of 75 transitions using a symmetric top, rigid rotor Hamiltonian. The fit constants are $\nu_0 = 740.9696(7) \text{ cm}^{-1}$, $B' = 0.07507(5) \text{ cm}^{-1}$, $(C' - B') - (C'' - B'') = 0.0014(1) \text{ cm}^{-1}$, and $B'' = 0.07570(5) \text{ cm}^{-1}$. Recently, we have reported the observation of two librational bands of HF tetramer in the 710 to 775 cm^{-1} region: one band is a perpendicular band centered at 752 cm^{-1} and the other band is a parallel band centered at 714 cm^{-1} . The ground state B value of the tetramer was found to be 0.132081(1) cm^{-1} . For hydrogen fluoride tetramer and pentamer, theory predicts (Maerker, et al.)^a planar, oblate symmetric top structures at their global minima with B_e values of 0.136 and 0.0767 cm^{-1} for (HF)₄ (C_{4h} symmetry) and for (HF)₅ (C_{5h} symmetry), respectively. We have assigned the 741 cm^{-1} band as the (A'') HF out-of-plane librational fundamental of the pentamer, the 714 cm^{-1} band as the (A_u) HF out-of-plane librational fundamental of the tetramer, and the 752 cm^{-1} band as the (E_u) HF in-plane librational fundamental of the tetramer.

^aC. Maerker, P. R. Schlyer, K. R. Liedl, T. -K. Ha, M. Quack, M. A. Suhm, *J. Comp. Chem.* 18 1695 (1997).