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

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Using our pulsed slit-jet, infrared diode laser spectrometer, we have observed a rotationally-resolved parallel band centered at $741\ \mathrm{cm}^{-1}$in a molecular beam formed by expanding a mixture of 4% HF in helium through a $200\ \mu$m 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 ν_0 = $740.9696(7)\ \mathrm{cm}^{-1}$, B' = $0.07507(5)\ \mathrm{cm}^{-1}$, $(C' - B') - (C'' - B'')$ = $0.0014(1)\ \mathrm{cm}^{-1}$, and B'' = $0.07570(5)\ \mathrm{cm}^{-1}$. Recently, we have reported the observation of two librational bands of HF tetramer in the 710 to $775\ \mathrm{cm}^{-1}$region: one band is a perpendicular band centered at $752\ \mathrm{cm}^{-1}$and the other band is a parallel band centered at $714\ \mathrm{cm}^{-1}$. The ground state B value of the tetramer was found to be $0.132081(1)\ \mathrm{cm}^{-1}$. 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 $\mathrm{cm}^{-1}$for $(HF)_4$ (C_{4h} symmetry) and for $(HF)_5$ (C_{5h} symmetry), respectively. We have assigned the $741\ \mathrm{cm}^{-1}$band as the (A'') HF out-of-plane librational fundamental of the pentamer, the $714\ \mathrm{cm}^{-1}$band as the (A_u) HF out-of-plane librational fundamental of the tetramer, and the $752\ \mathrm{cm}^{-1}$band as the (E_u) HF in-plane librational fundamental of the tetramer.

[a] C. Maerker, P. R. Schlyer, K. R. Liedl, T. -K. Ha, M. Quack, M. A. Suhm, J. Comp. Chem. 18 1695 (1997).