THE DIRECT OBSERVATION AND ANALYSIS OF THE JET COOLED ROTATION-TUNNELING TRANSITIONS $K = 0 \leftarrow 0$ OF HBr DIMER

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The $K = 0 \leftarrow 0$ rotation-tunneling transitions of HBr dimer centered at 450 GHz has been observed for the first time using the TAMU fast scan sub-millimeter wave spectrometer[a] with coaxially configured pulsed jet. Approximately 1200 completely resolved hyperfine components of the R and P branches with J=0 to 10 in the three isotopomers $H^{79}Br$:$H^{81}Br$, $H^{79}Br$:$H^{79}Br$ and $H^{81}Br$:$H^{81}Br$ were measured with an accuracy of about 5 kHz. The measured frequencies were fitted to a rms deviation of less than 12 kHz with a standard Hamiltonian which included the rotational (B and D_J) and quadrupole terms ($\chi_{aa}(\mathrm{Br}_1), \chi_{aa}(\mathrm{Br}_2), D_\chi(\mathrm{Br}_1)$ and $D_\chi(\mathrm{Br}_2)$) in the upper and lower states and the tunneling frequency ν_o. The accuracy of ν_o is improved from MHz to 1 kHz, and all the molecular parameters of the upper tunneling state are now determined with microwave accuracy also. The improved set of parameters for $K = 0 \leftarrow 0$ rotation-tunneling transitions of HBr dimer was extremely useful in the confirmation of the assignment of the observed broken symmetry infrared transitions associated with both ν_1 and ν_2 band origins. The parameters from microwave, infrared and the current study will be compared and used to determine structural and other molecular parameters for the dimer. The application of this data for generation of a morphed potential for the hydrogen bromide dimer will also be discussed.

[a] McElmurry, B. A.; Lucchese, R. R.; Bevan, J. W.; Leonov, I. I.; Belov, S. P.; Legon, A. C. J Chem Phys 2003, 119, 10687.