MICROWAVE SPECTRUM OF THE H₂S DIMER: OBSERVATION OF K_a=1 LINES

ARIJIT DAS, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India; PANKAJ MANDAL, Department of Chemistry, Indian Institute of Science Education and Research, Pune, Maharshtra, India; FRANK J LOVAS, Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD, USA; CHRIS MEDCRAFT, School of Chemistry, Newcastle University, Newcastle-upon-Tyne, United Kingdom; ELANGANNAN ARUNAN, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India.

Large amplitude tunneling motions in $(H_2S)_2$ complicate the analysis of its microwave spectrum. The previous rotational spectrum of $(H_2S)_2$ was observed using the Balle-Flygare pulsed nozzle FT microwave spectrometers at NIST and IISc. For most isotopomers of $(H_2S)_2$ a two state pattern of a-type K_a =0 transitions had been observed and were interpreted to arise from $E_1^{+/-}$ and $E_2^{+/-}$ states of the six tunneling states expected for $(H_2S)_2$. K_a =0 lines gave us only the distance between the acceptor and donor S atoms. a b c . The (B+C)/2 for E_1 and E_2 states were found to be 1749.3091(8) MHz and 1748.1090(8) MHz respectively. In this work, we have observed the K_a =1 microwave transitions which enable us to determine finer structural details of the dimer. The observation of the K_a =1 lines indicate that $(H_2S)_2$ is not spherical in nature, their interactions do have some anisotropy. Preliminary assignment of K_a =1 lines for the E_1 state results in B=1752.859 MHz and C=1745.780 MHz. We also report a new progression of lines which probably belongs to the parent isotopomers.

^aF. J. Lovas, P. K. Mandal and E. Arunan, unpublished work

^bP. K. Mandal Ph.D. Dissertation, Indian Institute of Science, (2005)

^cF. J. Lovas, R. D. Suenram, and L. H. Coudert. 43rd Int.Symp. on Molecular Spectroscopy. (1988)