ROTATIONAL SPECTRA AND STRUCTURE OF PHENYLACETYLENE-H_2S COMPLEX

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Rotational Spectra of phenylacetylene-H_2S, phenylacetylene-HDS, phenylacetylene-D_2S, phenylacetylene-$H_2^{34}S$, $C_8H_5D - H_2S$ have been measured. The spectra were recorded using a Balle-Flygare type PNFT Microwave spectrometer[1]. Helium was used as a carrier gas for these measurements. Both 'a' and 'b' dipole transitions have been observed. For the parent isotopomer, all the transitions are split into two. The rotational spectra of phenylacetylene-HDS indicate that the splitting is due to the interchange of equivalent hydrogens of H_2S unit in the complex. The measured rotational constants of the parent species are $A = 1206.551(7)MHz$, $B = 1134.152(6)MHz$, $C = 732.192(6)MHz$ for the stronger series and $A = 1206.732(7)MHz$, $B = 1134.056(6)MHz$, $C = 732.141(8)MHz$ for the weaker series. The constants derived from the experiments confirm a structure where H_2S is placed perpendicular to the plane of the phenylacetylene molecule. This study reveals that the binding of H_2O and H_2S to the phenylacetylene molecule is very different. Microwave spectroscopic investigations confirmed that H_2O prefers to be in plane of the phenylacetylene, donating one of its hydrogen to the acetylenic π cloud while the oxygen of H_2O is involved in a secondary interaction forming C-H—O hydrogen bond with the ring hydrogen ortho to the acetylenic group[2].

1. Arunan et al.*Current Science*,82(2002)533.

2. TA04,*63rd International Symposium on Molecular Spectroscopy*,Columbus, June 16-20, 2008.