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-$H_3^4S$, $C_6H_5D - H_2S$ 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 $\pi$ 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].

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