ROTATIONAL SPECTRA AND STRUCTURE OF PHENYLACETYLENE-WATER COMPLEX

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Rotational Spectra of phenylacetylene-water complex and its HDO and D_2O isotopomers have been measured. The spectra resemble an asymmetric top with $\kappa = -0.73$ for the parent isotopomer. Both 'a' and 'b' dipole transitions have been observed. All the transitions are split into two resulting from a possible internal rotation of H_2O in the complex. The measured rotational constants are $A = 2672.0931(31)MHz$, $B = 996.3581(8)MHz$, $C = 731.7056(4)MHz$ for the stronger series and $A = 2673.1331(44)MHz$, $B = 996.3926(10)MHz$, $C = 731.5737(6)MHz$ for the weaker series. Spectra for HDO isotopomer agree with a structure where water is in the plane of phenylacetylene by donating one of its hydrogen to the acetylene π cloud and the oxygen is involved in a secondary interaction forming C-H—O hydrogen bond with the ring hydrogen ortho to the acetylenic group. The experiments for D_2O isotopomer are in progress. The structure agrees with the one proposed from Fluorescence Dip Infrared Spectroscopy studies [1].

1. G. N. Patwari and co-workers, *Private Communication.*