ROTATIONAL SPECTROSCOPIC AND THEORETICAL INVESTIGATIONS ON BENZENE-ETHYLENE COMPLEX

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Theoretical studies and condensed phase experimental studies point towards a π stacked structure for benzene dimer, for which experimental evidence has not been found yet. This structure has no dipole moment and hence microwave spectroscopy can not be used. Benzene and ethylene can dimerise to give π stacked complex which will have a net dipole moment. Rotational spectroscopic technique can be used to detect this π stacked structure, if present, in the gas phase. Depending upon the nature of interaction, in addition to the π stacked structure, other geometries are also possible where either benzene or ethylene can act as hydrogen bond donor. Theoretical investigations led to five different structures including the π stacked one. Pulsed Nozzle Fourier Transform Microwave Spectrometer has been used to study the rotational spectrum of the benzene-ethylene complex, with helium as the carrier gas. A total of 24 'a' dipole transitions were observed. Out of these 24 transitions, 20 lines were fitted to the structure with C_2H_4 as the hydrogen bond donor. In the observed transitions the $K = 0$ lines show doubling. The line centres of the $K = 0$ doublets were used along with $K = 1$ transitions for the fitting. The fitted rotational constants are, $A = 5.4(1)GHz$, $B = 1221.879(3)MHz$, $C = 1206.794(4)MHz$. Search and assignments for $C_6H_6 - C_2D_4$ and $C_6D_6 - C_2H_4$ complexes are in progress.