CORIOLIS INTERACTIONS IN BENZENE-WATER AND RELATED COMPLEXES

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Microwave spectra of benzene-water and related complexes[a] have been fit in the past using a free internal rotor model, which was first proposed for the $CF_3H - NH_3$ complex[b]. Not all the lines observed experimentally could be fit using excited state torsional quantum number as an additional quantum state for the observed microwave transitions. Some of the lines give an RMS deviation of several hundred kHz if included in the fit. A detailed study of the literature revealed that a very similar spectral pattern was observed for the vibrationally excited state ($V_6 = 1$ or $V_8 = 1$) of the CF_3NC molecule, consisting of a relatively compact central group of lines flanked by two equidistant single lines[c]. We propose a Hamiltonian[d], including Coriolis interactions for an axially symmetric top molecule to fit the excited state spectra of benzene-water and related molecular complexes published so far by including all the omitted lines. We show that the new fit leads to RMS deviations within experimental accuracy. Details will be presented in the talk.

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