LARGE AMPLITUDE MOTIONS IN COUMARAN: A SPECTROSCOPIC AND THEORETICAL STUDY

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The structure of coumaran (2,3-dihydrobenzofuran) is characterized by a non-planar skeleton, due to the position of the most far apart carbon in the dihydrofuran ring. We have measured 133 a, b and c type lines of the rotational spectrum in the millimeter-wave region (59-78GHz), characterized by a doubling typical of an inversion motion such as the ring-puckering of the five-membered ring. By using a coupled Watson's Hamiltonian we found an energy splitting E= 93682.019(22) MHz; this value is quite in contrast with a previous far-infrared and Raman study[a] . In order to better interpret this large amplitude motion we performed also quantum chemical calculation (MP2 6-311++G** and B3LYP 6-311++G**) and used Meyer's flexible model.

[a]E. Bondoc, T. Klots, J. Laane, *J. Phys. Chem A* **104**, 275 (2000)