MULTI-DIMENSIONAL PROTON TUNNELING IN 2-METHYLMALONALDEHYDE

IWONA GULACZYK, MAREK KREGLEWSKI, *Faculty of Chemistry, Adam Mickiewicz University, Poznan, Poland*.

2-methylmalonaldehyde (2-MMA) has two large amplitude strongly coupled large amplitude vibrations (LAVs), internal rotation of the methyl group and proton tunneling between two equivalent oxygen atoms, which results in a multiple splitting of the ground vibrational state. Since the symmetry group of 2-MMA is G_{12} isomorphic to a point group C_{6v}, each vibrational level of LAV is split into nondegenerate (A_1, A_2, B_1, B_2) and degenerate (E_1, E_2) substates. In the present paper a four-dimensional model for 2-MMA is discussed where the out-of-plane vibrations are treated together with LAVs. In the standard approach the out-of-plane vibrations are handled as non-degenerate. In the non-rigid picture both out-of plane vibrations can be treated as a degenerate mode strongly coupled to LAVs and are also split into nondegenerate and degenerate substates. This effect is shown numerically using a simple harmonic model for out-of-plane degenerate mode. The results show that the out-of-plane vibrations are split into several components and their vibrational excitation should create a system of several transitions belonging to different species of the G_{12} symmetry group.