ANALYSIS OF CO-STRECHING-TORSION-ROTATIONAL TRANSITIONS OF METHANOL

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In an attempt to account for couplings among vibration, torsion and rotation in methanol, a five-dimensional vibration-torsion-rotation Hamiltonian is constructed. The form of the Hamiltonian is derived from a reduction of Hamiltonian of methanol in which the CO-streching mode ν_8, the large-amplitude torsion mode ν_{12} and the three degrees of freedom corresponding to the overall rotation of the molecule are considered simultanously. This Hamiltonian is used to carry out an analysis of previously published data for methanol. Another aim of the work is to investigate if a reduced model Hamiltonian can be used for assignments of the transitions involving two or more vibrational modes in methanol. Related calculations of the vibration-torsion-rotation energy levels of methanol, based on a rigorous kinetic energy operator and potential function, will also be described.