SPECTRA OF THE FORMALDEHYDE MOLECULE IN THE RANGE 3800−5100 CM^{-1}

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A comprehensive study of vibration-rotation spectral patterns of the formaldehyde molecule will be reported. Vibrational energy levels of H_2CO were computed using variational nuclear motion calculations from *ab initio* and empirically optimized full 6-dimensional potential energy surfaces in the electronic ground state. *Ab initio* calculations were carried out using extended electronic structure coupled-cluster method accounting for the dynamic electron correlations including triple and quadruple excitations as well as relativistic and diagonal Born-Oppenheimer corrections[1]. Effective Hamiltonian and effective dipole transition moments for the rovibrational polyads were derived from the *ab initio* surfaces using high-order contact transformations (CT) [2,3]. The analyses of experimental spectra recorded at T=160−165 K and various pressures were performed for the region of the 3-rd vibrational polyad. The experimental setup was described in Ref.[4]. The line positions and intensities were obtained by nonlinear least-squares fits with the SpectraPlot software[5] and analyzed using the CT-models for the effective Hamiltonian and effective dipole transition moments. Fifteen new vibrational levels were derived from these analyses in a good agreement with calculations[1]. In the range 4500−4700 cm^{-1}, a line list with the quantum identification was produced. It can be useful for a global modelling of the formaldehyde spectra and for an improvement of the line parameters in the databases[6,7,8].

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