Simulation of the Raman spectrum of CO_2 through an algebraic approach

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An algebraic description of the vibrational energy levels of carbon dioxide (CO_2) in its ground electronic state based on the U(2) x U(3) x U(2) model has been carried out [1,2]. With this model, a set of 101 experimental vibrational energies were fitted with a root mean square deviation of 0.53 cm^{-1} [1,2]. To keep the connection with the phase space, the Hamiltonian was expanded in terms of symmetry coordinates, which in turn are transformed into the algebraic representation.

On the other hand, from the eigenstates provided by the U(2) x U(3) x U(2) model, the transition moments of the mean polarizability were computed with the aim of simulating theoretically the vibrational Raman spectrum of CO_2 in a flame obtained experimentally in Ref. [3]. The intensities at room temperature of six Q-branch transitions are used to fit the derivatives of the mean polarizability with respect to the symmetry coordinates and compared with previous experimental [4] and ab initio [5,6] values. From these derivatives, the intensities of the complete set of lines located in the range 1150-1500 cm^{-1} is calculated at 1750 K [7]. This work could be useful in the quantitative diagnostics of combustion flames [3].

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