ANALYTICAL EXPRESSIONS OF FREQUENCIES, DIPOLE STRENGTHS AND ROTATIONAL STRENGTHS FOR OVERTONE TRANSITIONS IN A DISSYMMETRIC HCCH FRAGMENT

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In a recent paper [a] we derived useful analytical expressions for frequencies, dipole strengths and rotational strengths for CH-stretching transitions $\Delta v = 1, 2, 3$ in a two degrees of freedom model of an HCCH fragment endowed with C2-symmetry. The model includes mechanical and electrical anharmonicities [b], which are dealt with by second order Van Vleck perturbation theory [c]; expressions are derived through a computer algebraic manipulator. This dynamical study has been pursued quite efficiently also by other authors [d] [e], with Hamiltonians written in second quantization formalism. Herein we report on an update of our approach, that includes ideas derived from refs. (d) and (e), and allows us to deal with CH-stretching overtones dipole and rotational strengths up to $\Delta v = 4$, for a more general fragment deprived of C2-symmetry. In the latter case a 1:1 resonance is noticed in addition to the 2:2 Darling-Dennison resonance.

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