

# ANALYTICAL DESCRIPTION OF FREQUENCIES, DIPOLE STRENGTHS AND ROTATIONAL STRENGTHS FOR FUNDAMENTAL AND OVERTONE CH-STRETCHING TRANSITIONS

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The normal mode to local mode transition has been described in the past by basic arguments centered on symmetry and on perturbative-type numerical quantum mechanical calculations<sup>ab</sup>. In this work we investigate the absorption and Vibrational Circular Dichroism (VCD) spectra for a two degrees of freedom model of an HCCH chiral fragment endowed with C<sub>2</sub>-symmetry, for the fundamental ( $\Delta v=1$ ) and first two overtone regions ( $\Delta v=2,3$ ). We include electrical anharmonicity<sup>c</sup> in addition to mechanical anharmonicity, and deal with them in the framework of the Van Vleck contact transformation theory<sup>de</sup>. By making use of an algebraic manipulator (Maple) we are able to derive useful analytical expressions for frequencies, dipole strengths and rotational strengths for  $\Delta v=1,2,3$ .

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