DOES THE CIRCULAR DICHROISM OF CH-STRETCHING OVERTONES HELP ONE TO DISTINGUISH BETWEEN NORMAL MODES AND LOCAL MODES?

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Several years ago we presented a number of Vibrational Circular Dichroism (VCD) spectra of natural compounds in the CH-stretching 2nd and 3rd overtone regions [a]. In that paper we pointed out that normal modes and local modes in chiral molecules can be distinguished by means of VCD spectra. The presence or absence of VCD rotational strengths was accounted for as deriving from mechanical coupling between bond electric dipole moments. Based on recently acquired VCD data [b] and on further theoretical analysis [c], we have found that also local modes can generate VCD spectra of characteristic aspect, due to the interaction of CH-oscillators with polarizable groups. A very short review of our data will be reported and rationalized in the present talk.

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[a] S. Abbate, G. Longhi, L. Ricard, C. Bertucci, C. Rosini, P. Salvadori, A. Moscowitz, J. A. C. S. 111, 836 (1989)
[b] E. Castiglioni, F. Lebon, G. Longhi, S. Abbate, Enantiomer, 7, 161 (2002)
[c] S. Abbate, R. Gangemi, G. Longhi, J. Chem. Phys, 117, 7575 (2002)