

A NEW CRITERION TO PROVIDE A LOCALITY/NORMALITY DEGREE AND ITS RELEVANCE IN SPECTROSCOPY: RAMAN SPECTRA OF ISOTOPOLOGUES OF CO<sub>2</sub>

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In contrast to the traditional analysis of molecules presenting local mode behavior, where the degree of locality is given through a function in terms of the Morse potential parameters, new criteria of local/normal (LN) degree suitable to be applied to any molecular system are proposed. The approach is based on the connection between the algebraic normal and the local mode representations. It is shown that both descriptions are equivalent as long as the polyad in the local representation is not conserved. The imposition of a local polyad conservation naturally provides a criterion to assign a LN degree in quantitative form. This approach assumes bosonic operators, where only the fundamental energies are involved. The correlation between the different parameters are studied as well as their connection with spectroscopic properties. The importance of this connection is exemplified by the Raman spectra of isotopologues of carbon dioxide.