On the influence of isotopic composition on vibrational bandshapes in liquids.

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The influence of isotopic composition of molecules on vibrational band contours in condensed phases is demonstrated. Simulated bandshapes and vibrational and rotational correlation functions for selected A_1 modes of recently studied symmetric top molecules of the $(CH_3)_3XY$ type (X = C, Si, Ge; Y = Cl, Br, CN, C=CH, C=CD) are presented. The problem of inhomogeneous broadening due to isotopic composition and other effects is discussed in more detail for isotropic Raman bands. Procedures enabling the evaluation of “true” bandshapes and related correlation functions are discussed. Finally, methods for numerical description of the overall band contour of such systems are given. Experinental results are also demonstrated to show the relevance of effects mentioned above.

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