

Effect of double or single bonding in C-H stretching signal propagation in organic molecules. A computational study

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© 2018 The objective of this study is to evaluate vibrational energy propagation of a C-H stretching signal on unsaturated organic molecules and the effect of saturation in a specific site of those molecules using ab-initio molecular dynamic relaxation simulations. The results show that the inclusion of saturation at a specific site at the double bonded organic chain blockade the protrusion of C-H stretching vibrational energy at this site. As the saturation involves the change from double to single bonding regime, the effect is possibly originated by the loss of electron resonance at this specific site.