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Vibrational analysis of [4-[(E)-phenylazo] phenyl]ethanol based on the comparison between the experimental and DFT calculated raman spectra

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Abstract

© 2014 by Pleiades Publishing, Ltd. In this work we assessed the performance of the density functional theory (DFT) approach through a comparison study with the experimental Raman spectrum obtained for [4-[(E)-phenylazo]phenyl]ethanol (ABOH) in the wave number range 900-1800 cm-1. The assignment of the ten most active vibrational modes is achieved using the hybrid B3LYP method with the 6-311++G(2d,2p) basis set. Two molecules of reference [N-ethy--4-[(E)-(4-nitrophenyl)azo]anilino]ethanol (Disperse Red 1, DR1) and 4-[(E)-(4-nitrophenyl) azo]aniline (Disperse Orange 3, DO3) are also investigated in order to consider this method in the calculation of the Raman intensities. The experimental Raman spectrum of DR1 is compared with those of the three stable configurations obtained at the B3LYP/6-311++G(2 d,2p) level.

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Keywords

Azo dye, DFT calculation, Raman spectra