Raman, infrared, SERS and theoretical study of 3-(1-phenylpropan-2-ylamino) propanenitrile, fenproporex

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Infrared, Raman and surface-enhanced Raman scattering (SERS) spectra of 3-(1-phenylpropan-2-ylamino)propanenitrile (fenproporex) have been recorded. Density functional theory (DFT) with the B3LYP functional was used for optimizations of ground state geometries and simulation of Raman and SERS vibrational spectra of this molecule. Bands of the vibrational spectra were assigned in detail. The comparison of SERS spectra obtained by using colloidal silver and gold nanoparticles with the corresponding Raman spectrum reveals enhancement and shifts in bands, suggesting a possible partial charge-transfer mechanism in the SERS effect. Information about the orientation of fenproporex on the nanometer-sized metal structures is also obtained.