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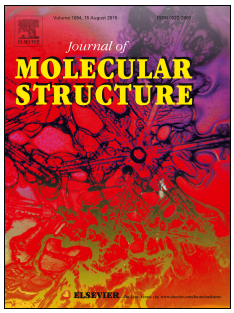

Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: A comparative study

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Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: a comparative study

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Abstract

A comparative electronic and spectroscopic analysis of 2,4,6-trichloroaniline (TCA) and 2,4,6-tribromoaniline (TBA) was carried out by theoretical and experimental techniques. The NH_2 inversion barrier in TCA and TBA molecules was predicted to be three times less than that in aniline and 2,4,6-trifluoroaniline. The size of the halogen substituents in the ortho positions is shown by density functional theory to play an important role in determining the electronic and structural properties of the amino group in the investigated haloaniline derivatives. A thorough interpretation of the infrared and Raman spectra has been performed on the basis of the observed and calculated infrared and Raman spectra as well as calculated potential energy distribution values. In addition, the SERS spectra for both trihaloanilines were successfully collected up to a concentration of 10^{-6} M using aged hydroxylamine-reduced silver colloid as an active substrate for TCA and TBA. SERS intensities of several peaks were found to linearly change with concentration allowing quantitative analyses of TCA and TBA. A relatively stronger interaction in the case of TBA–silver colloids is predicted compared to the TCA analogue.

Keywords: Trihaloanilines; Infrared and Raman spectra; Density functional theory (DFT); Surface-enhanced Raman scattering (SERS).