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The IR and RAMAN spectra of polyaniline adsorbed on the glass surface; comparison of experimental, empirical force field, and quantum chemical results.

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Abstract

Vibrational spectra of the oligomeric models of polyaniline (PANI) were explored by quantum chemical and molecular mechanical tools. First, calibration calculations were performed on aniline sample where several computational models were compared with measured IR and Raman spectra. Based on this 'calibration', the ωB97XD/6-31G(d,p) level was used for optimization and spectra determination of powder polymer and PANI deposited on the glass surface. From the individual models of PANI it was found that spectral shape converge relatively fast with the length of oligomeric chain and octamers can be considered as the structures, which recover most of the spectral properties – both shape and intensities of individual peaks. As suggested by Stejskal, vibrational spectra provided by saturated chains consisting purely from aniline building blocks do not correlate with experimental values. However, the increasing amount of quinonic structures improves the agreement of computed spectra with experimental one substantially. The best correspondence occurs for the quinone:aniline ratio 1:3. This conclusion also follows from the fitted Raman spectrum calculated for the set of decameric structures – saturated and oxidized to three subsequent states (0, 2+, 4+, and 6+) where expansion coefficient of the 4+ state, which corresponds to two quinonic units clearly dominate.

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