

Home > Russian Journal of Physical Chemistry B > Article

# Synthesis, Characterization, and Computational Insights Into the Conductive Poly(*p*-aminophenol)

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## Abstract


In this work, poly(*p*-aminophenol), a conductive polymer, was synthesized via chemical polymerization from the monomer of *p*-aminophenol in a basic aqueous medium using ammonium persulfate as the initiator. The polymer's properties were assessed using ultraviolet-visible spectroscopy, fourier transform infrared, thermogravimetric analysis, scanning electron microscope, and X-ray diffraction methods. The fourier transform infrared results show a peak such as the robust signal at 3126 cm<sup>-1</sup>, corresponding to O–H vibrations associated with phenoxide ion existence in the polymer. The presence of N–H stretching vibration of an aromatic amine was affirmed by the peak at 2989 cm<sup>-1</sup>. The presence of a strong, broad peak at 2θ of 17.52° indicated amorphous behavior in poly(*p*-aminophenol). The weight loss was shown at 87, 276 and 517°C due to moisture removal, anion removal, and the degradation of polymer. Scanning electron microscopy showed sphere-like particles in poly(*p*-aminophenol) surface morphology. The electronic properties of poly(*p*-aminophenol) were investigated using quantum chemical calculations at the density functional theory level of theory. Density functional theory calculations were performed using two functionals, namely B3LYP and wB97XD, in combination with the 6-311+G(2d, p) basis set. These calculations aimed to determine various quantum chemical parameters, conduct natural bond orbital analysis, assess topological parameters, investigate nonlinear optical properties, and evaluate thermal properties. This approach balanced computational efficiency and accuracy to investigate reactivity, stability, charge transfer, optical properties, and thermal behavior. The calculations revealed significant changes in the reactivity and stability of the studied compound as it transitioned from the non-protonated to the protonated state, analyzed in both the gas phase and various aqueous environments. Furthermore, the presence of strong hydrogen bonds and limited nonlinear optical potential suggest the material may be suitable for applications beyond nonlinear optics. Additionally, the calculations explored static thermodynamic properties, including heat capacity, entropy, and enthalpy, highlighting their temperature-dependent behaviors. Poly(*p*-aminophenol) has excellent thermal stability and robust hydrogen bonding. However, its low nonlinear optical potential indicates its usefulness for uses other than nonlinear optics.

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