Molecular modeling of polyaniline macromolecules and physic-chemical properties of composites on their basis

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Polyaniline (PANI) is an electrically conductive polymer as a promising material, you can use for a variety of electronic devices. In practice, polymer-polymer composites (PPC) are often used from macromolecules of ladies and film-forming polymers as: polyvinyl alcohol (PVA), polymethacrylic acid (PMAA), etc. The results of a quantum-chemical study of PPC based on PANI are present in our work. Quantum-chemical calculations were performed using the MOPAC2016 programming method PM7 and the Winmostar graphical interface.

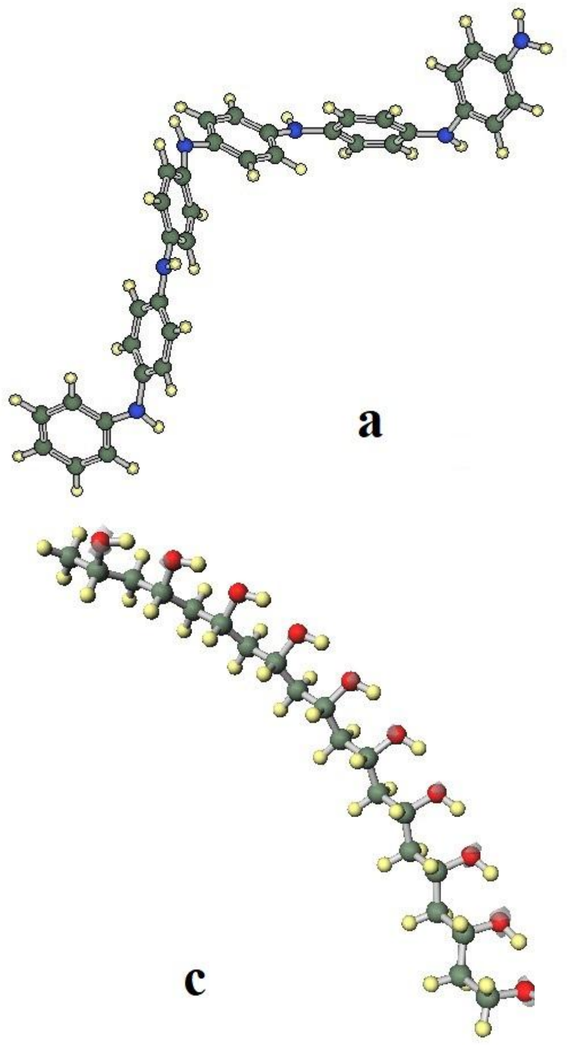

Figure 1. Conformers of macromolecules: PANI: **a** – compressed spiral; **b** – rigid rod; PVA (**c**); PMAA (**d**)

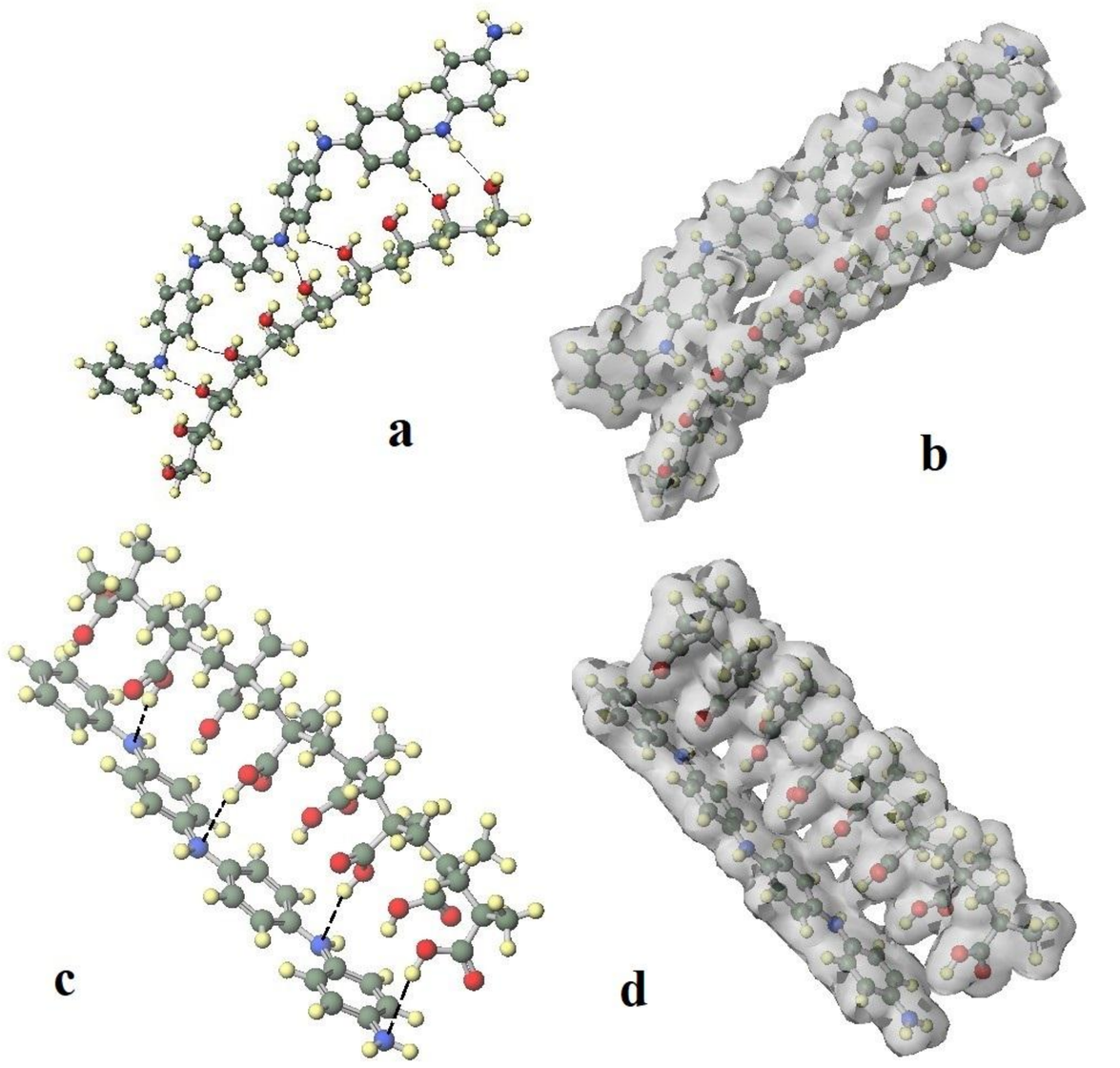

Figure 2. PPC models: PVA – PANI with H-bonds (**a**) and their electron density surface (**b**); PMAA – PANI with H-bonds (**c**) and their electron density surface (**d**)

Quantum–chemical calculation of thermodynamic parameters (enthalpy, entropy, and heat capacity) of individual PANI, PMAA and PVA macromolecules (Figure 1) and their comparison with the thermodynamics of the PANI-PVA and PANI-PMAA intermolecular complexes (Figure 2) also indicates a strong interaction between polymers. X-ray studies by powder diffraction confirm the conclusions about the interaction between the macromolecules of PANI - PVA and PANI - PMAA (Figures 3 and 4).

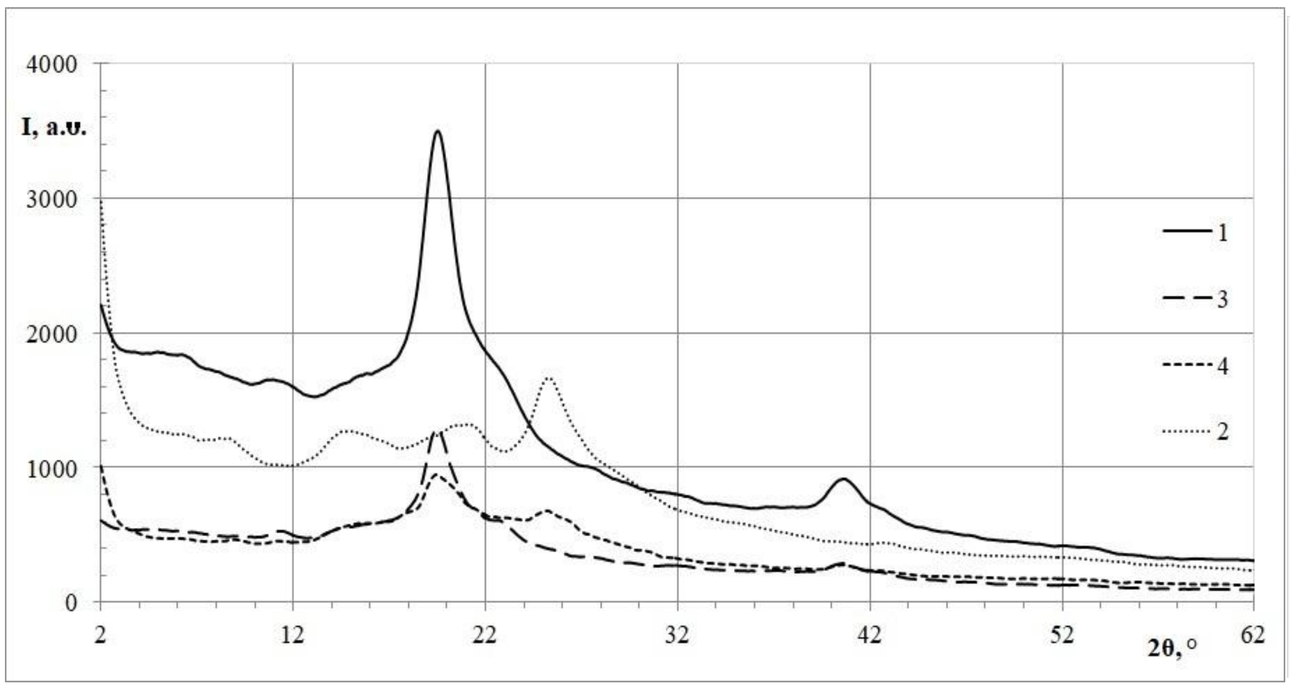

Figure 3. XRD pattern of PVA (1), PANI (2) and PPC with 20 %mass. PANI (3) and 70 %mass. PANI (4)

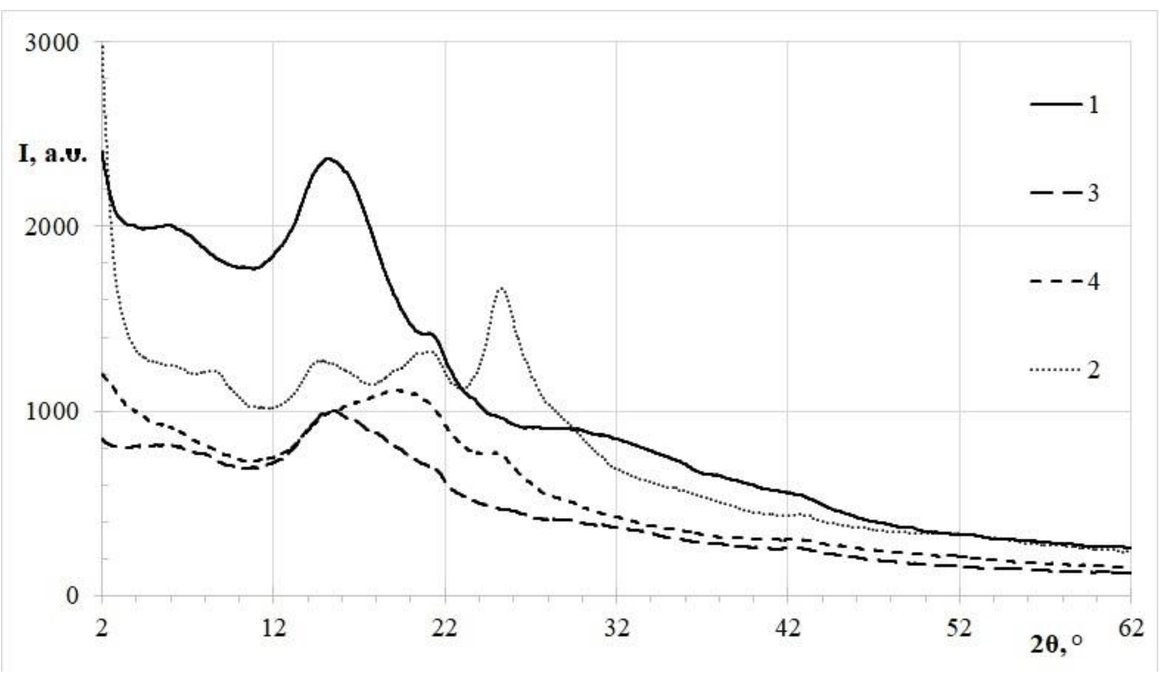

Figure 4. XRD pattern of PMAA (1), PANI (2) and PPC with 20 %mass. PANI (3) and 70 %mass. PANI (4)