MOLECULAR MODELING OF INTERACTION BETWEEN MACROMOLECULES OF POLYVINYL ALCOHOL AND POLYANILINE

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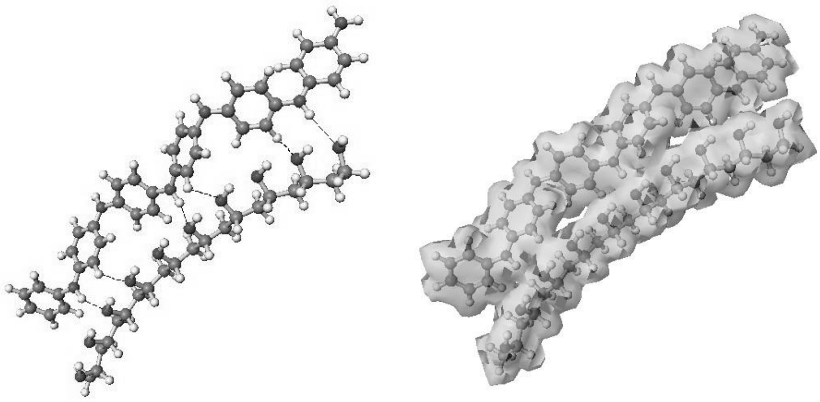
Quantum-chemical modeling of macromolecules of polyvinyl alcohol (PVA), emeraldine salt of polyaniline (PANI) and its composite (PPC) were performed using the semi-empirical PM7 method taking into account the dielectric constant of water (EPS=78.4) as a solvent using the MOPAC2016 program and the Winmostar graphical interface. Thermodynamic calculations of the models were performed using the key parameter THERMO (290,330,10).

An X-ray examination of the original polymers and composites with different PANI content was performed. It is shown that intermolecular hydrogen bonds of different strength are formed between PVA and PANI macromolecules, which affect the physic-chemical properties of the obtained composites.

Quantum chemical calculations indicate that PANI macromolecules can assume different conformational states. Depending on the size of the dihedral angle, the PANI molecule can form a spiral structure (folded or unfolded spiral) or a rigid rod. It should be noted that during the formation of PPC due to intermolecular interaction may change the conformation of PVA and PANI.

The calculated values of the heat of formation ($\Delta_f H^o$) for the composite are smaller than the sum of the corresponding values of the fragments of the studied polymers. The decrease in $\Delta_f H^o$ energy is associated with the formation of hydrogen bonds between the fragments of PVA and PANI. The difference between the corresponding values of $\Delta_f H^o$ is about 78 kJ/mol, which corresponds to the formation of 4–6 intermolecular hydrogen bonds of the fragments N-H…O and C-H…O (Figure). A further confirmation of the formation of hydrogen bonds in the composite between PVA and PANI molecules can be a decrease in the numerical values of entropy. The decrease in entropy is 382.6–388.1 J/mol·K.



a b

Fig. PPC model with 10 fragments of PVA and 6 fragments of PANI with H-bonds (a). The electron density surface of the PPC (b)