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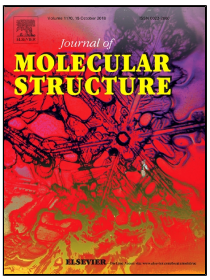

Preparation and spectroscopic properties, density functional theory calculations and nonlinear optical properties of Poly (acrylic acid-co-acrylamide)-graft-Polyaniline

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Preparation and spectroscopic properties, density functional theory calculations and nonlinear optical properties of Poly (acrylic acid-co-acrylamide)-graft-Polyaniline

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Abstract

Poly (acrylic acid-co-acrylamide)-graft-Polyaniline was synthesized via chemical oxidation polymerization using ammonium persulphate as initiator at 40 ^{0}C under N_2 atmosphere. The prepared poly (acrylic acid-co-acrylamide)-graft-Polyaniline was characterized by different analytical tools. The apparent activation energy of grafting reaction was calculated and found to be 48.7753kJ/mol. Also, ΔH*and ΔS* as thermodynamic parameters for activation were calculated which equal to 46.4300 k J/mol. and -14.0379 J/mol. K respectively. The optimized structures of the graft (one, two and three units or (monomer, dimer and trimer) were theoretically investigated at the B3LYP/6-311G level. The geometry of the graft are non-planar as indicated from the values of dihedral angles. The global properties of hardness, global softness and electronegativity were calculated. The calculated small energy gap between highest occupied and lowest unoccupied molecular orbital energies shows that charge transfer occurs within the graft compound. The molecular electrostatic potential for the graft was investigated. The obtained total static dipole moment, mean polarizability, anisotropy of polarizability and mean first-order hyperpolarizability (<β>) were compared with those of urea as a reference material. The results for <β> showed that the graft is excellent candidates as nonlinear optical materials.

Key Words: kinetic studies, polarizability, hyperpolarizability,DFT calculations

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