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Quantum-chemical description and experimental proof of microstructure heterogeneity of maleic anhydride copolymers

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Abstract

The microstructure heterogeneity of vinyl chloride-maleic anhydride copolymer is formed spontaneously as a result of tautomerization of the initial repeating units into enol (*en*) and dienol (*den*) tautomers. The *en* and *den* units include molecular ensembles with new reactivity which makes it possible to develop a method for their delicate chemical probing with nucleophilic reagents having similar ensembles such as $NaNO_2$, NaN_3, and DMF. Non-empirical quantum-chemical modeling of the structure and energy of the tautomers enabled us to estimate the microstructure heterogeneity of the macromolecules *a priori* and allowed to analyze the electron density distribution of the highest occupied molecular orbitals and the lowest unsaturated molecular orbitals in the charge-transfer complexes. The calculations were validated by extensive experimental evidence. The microstructure heterogeneity of the vinyl chloride-maleic anhydride copolymer was investigated and presence of the *en* and *den* tautomers in its units was also supported by the calculations.