Nanocomposites and nanomaterials

Quantum-chemical simulation of interactons in the systems of silica-anaesthetic, silica-polymer and polymer-anaesthetic

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Model conceptions of interactions between silica-anaesthetic, silica-polymer and polymer-anaesthetic are of great importance when creating application forms of anaesthetics. The developed method of approach will permit the prognosticating of adjusting educe of preparations in the dependent on chemical nature of components. being a part of composite material. Artecaine is widely used in anaesthesia practice. The including it in the composition of application preparations will permit decrease their toxic influence to patients with high sensitiveness.

The goal of present work was to develope model conceptions for listed above interactions between components consisted in the composition of applications composite preparation. Calculations of electronic structure were fuefield by methods of quantum chemistry (PM7,program MOPAC 2012) with establishment of limit values of molecular orbitals E_{HUMO} and E_{LUMO} for hydroxilated(SiO2)64(H2O)32 and methylated(SiO2)64(H2O)18(CH3)14 silicas, also for similar fuleren structure silicas (SiO2)60(H2O)50 and (SiO2)60, and dextrane C166O65H166. The values of adsorption energy for surfaces of these silicas were determinated

$$E_{ad}=E(surface+articaine)-E(surface)-E(articaine).$$

Their decreasing in the line of surfaces

hydroxylated<dehydroxylated< methelated

were obtained. It was established that interactions under consideraction occurred without transferring of electrons density($\rho\approx0,03$) i.e. at the expense of dispersive and Van der Vaalse forces. So the intensity of artecaine keeping may be adjusted by changing the relation between hydrophilic and hydrophobic components in the system.