Quantum Chemical Simulation of Relaxation and Thermally Stimulated Processes: a Vibration Excitation-relaxation Stochastic Optimization

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A new method for theoretical examination of thermal inter-conversions via the space structure vibration excitation-relaxation stochastic optimization method has been proposed. The software to perform implementation of the methodology has been developed and tested on a silica $27SiO_2$ cluster. A set of thermodynamically probable space structures of amorphous silica particles and temperatures of their inter-conversions has been simulated. The simulated space structures have been verified by comparison of calculated inelastic neutron scattering spectra of different highly dispersed silicas with experimental ones.

Key words: Quantum Chemistry; Semi-empirical Method; Silica; Thermo-chemical Processes; PM3.