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

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Z. Naturforsch. \textbf{60a}, 797 – 804 (2005); received June 8, 2005

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\textsubscript{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.

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