



Ageing effects in supercooled silica: a molecular dynamics investigation

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Titre Ageing effects in supercooled silica: a molecular dynamics investigation

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The two-, three- and four-body effective collision induced scattering spectral line shapes are calculated for dense gaseous krypton using the pairwise additivity (PA) approximation and different polarizability models. These spectra and several interaction induced spectra calculated at various densities are compared with the experimental measurements of Barocchi et al. [1988, Europhys. Lett., 5, 607]. The potential effect on the spectrum is found to be weak. The results obtained with the Meinander et al. [1986, J. chem. Phys., 84, 3005] empirical polarizability model and molecular dynamics fit well the experimental two- and three-body spectral shapes. The irreducible contribution to the spectral shape is evaluated using the dipole induced dipole irreducible polarizability [Buckingham, A. D., and Hands, I. D., 1991, Chem. Phys. Lett., 185, 544]. This contribution is found to be relatively weak for the anisotropic spectra in the frequency and density range studied, explaining the good agreement between the pairwise approximation calculations and the experimental data. The spectra radiated by the quasi-molecules Kr₂, Kr₃, and Kr₄ (the total spectrum within the PA approximation) are also simulated.

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Liens

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