Dielectric relaxation and molecular conformational energy of some arylazo benzothiazine derivatives.

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Streszczenie

We carry out semi-empirical calculations on some arylazo benzothiazine derivatives to obtain the energy barriers for internal rotation and dipole moments, using the PM3 Hamiltonian. By means of the correlation function method and some probabilistic procedures we describe then the dielectric relaxation of these molecules and we try to explain what the contribution of different relaxation modes is in the process of relaxation. Moreover, we account for the consequences of the nonrigidity of the molecules in dielectric response.

Słowa kluczowe

Dielectric relaxation, Dielectric absorption, Semi-empirical calculation, Relaxation mode

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