Israel Journal of Chemistry 2003 vol.43 N3-4, pages 363-371

## Relation between macroscopic and microscopic dielectric relaxation times in water dynamics

Arkhipov V., Agmon N.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

## Abstract

A simplified derivation for the ratio of macroscopic to microscopic relaxation times of polar liquids is based on the Mori-Zwanzig projection-operator technique, with added statistical assumptions. We obtain several useful forms for the lifetime ratio, which we apply to the dynamics of liquid water. Our theoretical single-molecule relaxation times agree with the second Debye relaxation times as measured by frequency-domain dielectric spectroscopy of water and alcohols. From the theory, fast relaxation modes couple to the Debye relaxation time,  $\tau D$ , through very large water clusters, and their temperature dependence is similar to that of  $\tau D$ . Slower modes are localized to smaller water clusters and exhibit weaker temperature dependence. This is exemplified by the lifetime ratios measured by time-domain dielectric spectroscopy and optical Kerr effect spectroscopy, respectively.

http://dx.doi.org/10.1560/5WKJ-WJ9F-Q0DR-WPFH