

标题: Dielectric Behaviors of Typical Benzene Monosubstitutes, Bromobenzene and Benzonitrile

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来源出版物: JOURNAL OF PHYSICAL CHEMISTRY B 卷: 116 期: 41 页: 12605-12613

DOI: 10.1021/jp308037n 出版年: OCT 18 2012

在 Web of Science 中的被引频次: 0

被引频次合计: 0

引用的参考文献数: 44

摘要: The dielectric behaviors of typical benzene monosubstitutes, bromobenzene (Br-Bz) and benzonitrile (NC-Bz), were investigated up to 3 THz in the pure liquid state over a temperature range from 10 to 60 degrees C to understand differences in molecular motions of these simple, planar molecules bearing rather different electric dipole moments: 1.72 and 4.48 D for Br-Bz and NC-Bz in gaseous state, respectively. Temperature dependence of spin-lattice relaxation time (T-1) for C-13 NMR and viscosities for these liquids were also determined to obtain information for molecular motions. Moreover, depolarized Rayleigh scattering (DRS) experiments were carried out for both liquids at 20 degrees C to determine frequency dependencies of optical susceptibilities up to 8 THz directly relating to rotational motions of their molecular planes. Most Br-Bz molecules rotate freely over a temperature range examined, showing a Kirkwood correlation factor close to  $g(K)$  similar to 1.0 at dielectric Debye-type relaxation times (ca. 18 ps at 20 degrees C) essentially identical to microscopic (dielectric) relaxation times evaluated from T-1 C-13 NMR data. A small amount of Br-Bz molecules forms dimeric intermolecular associations in an antiparallel configuration of dipole moments. On the other hand, NC-Bz molecules form stable dimers in the antiparallel dipole configuration at a population much higher than that of Br-Bz because of a markedly greater dipole moment than that of Br-Bz. A major dielectric relaxation mechanism for NC-Bz found at ca. 70 ps at 20 degrees C results from the dissociation process of dimers with a lifetime longer than a rotational relaxation time, observable as a minor dielectric relaxation mechanism at ca. 12 ps at 20 degrees C, of individual monomeric NC-Bz molecules without the formation of dimers. The formation of stable dimers in an antiparallel configuration is responsible for the observed small  $g(K)$  values, ca. 0.5, and disagreement between major (or minor) dielectric relaxation times and microscopic dielectric relaxation times over the entire temperature range examined.

入藏号: WOS:000309902400025

语种: English

文献类型: Article

KeyWords Plus: ANISOTROPIC MOLECULAR-REORIENTATION; CARBON-TETRACHLORIDE; NONPOLAR LIQUIDS; LIGHT-SCATTERING; DIPOLE-MOMENTS; POLAR LIQUIDS; RELAXATION; ASSOCIATION; CONSTANTS; C-13

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出版商: AMER CHEMICAL SOC

出版商地址: 1155 16TH ST, NW, WASHINGTON, DC 20036 USA

Web of Science 类别: Chemistry, Physical

研究方向: Chemistry

IDS 号: 021RG

ISSN: 1520-6106

29 字符的来源出版物名称缩写: J PHYS CHEM B

ISO 来源出版物缩写: J. Phys. Chem. B

来源出版物页码计数: 9