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标题: Dielectric Behavior of Some Small Ketones as Ideal Polar Molecules
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来源出版物: JOURNAL OF PHYSICAL CHEMISTRY A 卷: 116 期: 19 页: 4735-4744
DOI: 10.1021/jp301520f 出版年: MAY 17 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: 34
摘要: The dielectric behaviors of some small symmetric ketone molecules, including acetone, 3-pentanone, cyclopentanone, 4-heptanone, and cyclohexanone, were investigated as a function of temperature (T) over a wide frequency range from 50 MHz (3.14 x 10(8) s(-1), in angular frequency) to 3 THz (1.88 x 10(13) s(-1)). The temperature dependencies of the rotational diffusion times (tau(r)) determined using O-17 NMR spin-lattice relaxation time (T-1) measurements and viscosities of the ketones were also examined. The obtained temperature dependencies of the parameters for the ketones were compared with those of ideal polar molecules, which obey the Stokes-Einstein-Debye (SED) relationship without the formation of intermolecular dimeric associations and without orientational correlations between dipoles (molecular axes), that is, free rotation. Kirkwood correlation factors (g(K)) of only acetone and 3-pentanone were close to unity over a wide temperature range, whereas those of other ketones were obviously less than unity. These results revealed that no correlations exist between the rotational motions of dipoles in acetone and 3-pentanone, as expected in ideal polar molecules. However, other ketones exhibited orientational correlations in their dipoles because of dipole-dipole interactions via antiparallel configurations. Furthermore, because acetone and 3-pentanone satisfied the SED relationship and because their microscopic dielectric relaxation times (tau(mu)), which were calculated from the determined dielectric relaxation times (tau(D)) via the relationship tau(mu), = tau(D)g(K)(-1), were identical to 3 tau(r), and were proportional to V eta(k(B)T)(-1) over the wide temperature range examined, where V, k(B), and eta represent the effective molecular volume, Boltzmann's constant, and the viscosity of the liquid molecules, respectively, these two ketone molecules behave as ideal polar molecules. In addition, other ketones not significantly larger than acetone and 3-pentanone in molecular size likely form dimeric intermolecular associations with antiparallel cyclic configurations, which demonstrates the g(k) values less than unity.
入藏号: WOS:000304073200007
语种: English
文献类型: Article
KeyWords Plus: O HYDROGEN-BONDS; CARBON-TETRACHLORIDE; COMPLEX PERMITTIVITY; ALIPHATIC-KETONES; DIPOLE-MOMENTS; CYCLIC-KETONES; LIQUIDS; ACETONE; RELAXATION; SPECTROSCOPY
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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 分类: Chemistry, Physical; Physics, Atomic, Molecular & Chemical
学科类别: Chemistry; Physics
IDS 号: 942TS
ISSN: 1089-5639
29 字符的来源出版物名称缩写: J PHYS CHEM A
ISO 来源出版物缩写: J. Phys. Chem. A
来源出版物页码计数: 10