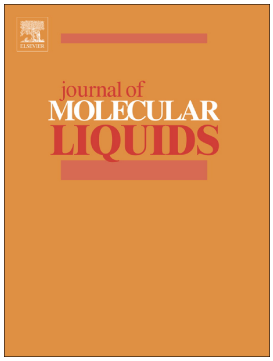

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Shiyue Wu, XiaoqingYang, Lanshuo Li, Yang Yin, Kama Huang

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Modification of Bruggeman's Formula for Binary Liquid Mixtures with Hydrogen Bonds

Shiyue Wu, XiaoqingYang*, Lanshuo Li, Yang Yin and Kama Huang
College of Electronics and Information Engineering, Sichuan University, Chengdu 610064, P.R. China.
***Correspondence to [yyxxqq_mail@163.com]**

Abstract The measured permittivity of binary liquid mixture with hydrogen bonds is larger than that of any component at some proportions or at some frequencies, which is not accurately consistent with Bruggeman's formula. Mathematical analysis about this phenomenon was made and compared with experimental data, the results indicates that there is a limitation of Bruggeman's formula about liquid mixture. Furthermore, a correction term was introduced by Debye relation model about binary liquid mixture with 1 hydrogen acceptor and donator. The numerical results obtained from modified Bruggeman's formula agrees approximately with experimental results.

Keywords permittivity; Bruggeman's formula; binary liquid mixtures; hydrogen bonds; modification; Debye relation model

1. INTRODUCTION

In recent years, microwave heating has been widely used to promote organic chemical reactions because of its characters of efficiency and fast heating[1-5]. Many chemists believe that microwave-assisted acceleration of reaction is nothing but the consequence of thermal effect by microwave irradiation[6]. However, there are reports which also demonstrate the existence of "non-thermal" effect [7-10] that is independent of temperature. According to those reports, non-thermal effect is always strongly related to hydrogen bonds[7-13]. Therefore, the study on the permittivity of mixture solution with hydrogen bonds has great significance.

X.Q. Yang and K.M. Huang etc.[14] studied the dielectric properties of Dimethyl Sulfoxide (DMSO)-H_2O mixtures, the result shows that the imaginary part of the solution permittivity was larger than each component at 2.45 GHz. And their work indicates that the classical Bruggeman's formula must be modified in order to calculate the complex permittivity. Then, many studies[15-20] on the dielectric properties of mixtures with hydrogen bonds were made. L.J. Yang[21] etc. investigated the dielectric properties of DMSO-H_2O by molecular dynamics (MD) simulation, and Debye-like model was found suitable in this mixture. MD simulation[16-24] can get some dielectric properties form intermolecular interaction, which explains the basic theory about interaction of microwave and materials.

T. P. Iglesias[25] etc. studied the excess relative permittivity of liquid mixtures by three separate contributions, namely from the volume change upon mixing, the permittivity contrast and molecular interactions. They obtained new, symmetric equations for predicting the relative permittivity of binary mixtures. Their