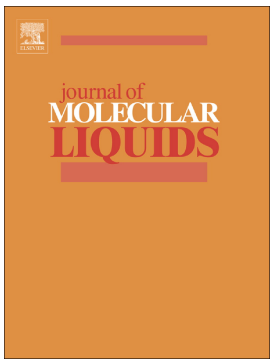

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PII: S0167-7322(17)34273-3
DOI: https://doi.org/10.1016/j.molliq.2017.12.064
Reference: MOLLIQ 8360

To appear in: *Journal of Molecular Liquids*

Received date: 13 September 2017
Revised date: 5 December 2017
Accepted date: 7 December 2017

Please cite this article as: N.K. Karthick, G. Arivazhagan, P.P. Kannan, A. Mahendraprabu, A.C. Kumbharkhane, S.S. Shaikh, Y.S. Joshi , Hydrogen bond interactions in the binary solutions of ethyl acetate with nitrobenzene: Spectroscopic, theoretical and dielectric studies. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), https://doi.org/10.1016/j.molliq.2017.12.064

Hydrogen bond interactions in the binary solutions of Ethyl Acetate with Nitrobenzene: Spectroscopic, theoretical and dielectric studies

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Abstract

FTIR spectroscopic studies have been carried out on pure ethyl acetate (EA), nitrobenzene (NBZ) and their equimolar binary solution. Theoretical calculations have been performed to validate the results of the FTIR spectral studies. Through the calculations, it is found that dimers of cyclic geometry with the hydrogen bonds between the methyl/methylene hydrogen and ester linkage oxygen (oxygen that is bonded with carbon through the single bond) can prevail in neat EA. These dimers , being highly unstable, dissociate into monomers in the binary solution and participate in the formation of 1:1 and 1:2 (EA : NBZ) systems. The 1:2 system is found to be more stable than the NBZ and EA dimers and the 1:1 system. The EA-NBZ solutions of entire composition range have been subjected to dielectric relaxation studies at 298 K using Time Domain Reflectometry (TDR) in the frequency range 10 MHz to 30 GHz. The results obtained have been interpreted with the aid of the findings of FTIR studies and DFT calculations.

Keywords: dissociation, heterointeraction, dimer, dielectric constant, relaxation time.

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