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Hydrogen bond interactions in the binary solutions of formamide with methanol: FTIR spectroscopic and theoretical studies

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Abstract

FTIR spectroscopic studies on the binary solutions of formamide with methanol reveal the presence of "free" $O-H$ in methanol. These "free" $O-H$ groups are found in methanol tetramers which is confirmed from the DFT calculations. DFT calculations on the formamide dimers of five different geometries encompassing one or more of the $N-H\cdots O$, $C-H\cdots O$ and $N-H\cdots N$ hydrogen bonds tell that $N-H\cdots N$ bonds are the strongest. Dissociation of the $N-H\cdots N$ bonds of formamide in the binary solutions with methanol has a major impact on the NH_2 symmetric stretching mode of formamide in the FTIR spectra. In these solutions the formation of 1:4 (formamide : methanol), 1:5 and 2:4 complexes are possible. These complexes are more stable than the formamide dimers, methanol tetramer and pentamer investigated in the present work. Methanol methyl group plays no role in the either the self-association or heterointeraction with formamide.

Keywords: dimer, homointeraction, heterointeraction, hydrogen bond, dissociation.

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