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journal homepage: www.elsevier.com/locate/saaA study of van der Waals complexes of 1,2-dichloroethane in paraffin oil by FTIR spectroscopy and *ab initio* calculations

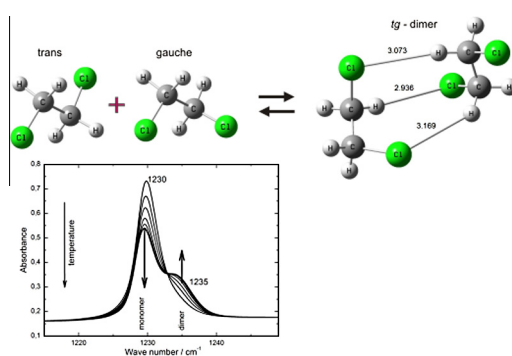
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HIGHLIGHTS

- Weak interactions of 1,2-dichloroethane in paraffin oil were studied.
- Conformers of 1,2-dichloroethane are involved in the complexation, forming *tg*-dimer.
- Structure of *tg*-dimer were determined from the DFT calculations.
- The complexation enthalpy was determined from FTIR spectra.

GRAPHICAL ABSTRACT



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ABSTRACT

Weak molecular interactions of 1,2-dichloroethane dissolved in paraffin oil were investigated by FTIR spectroscopy. Occurrence of isosbestic points in the spectra along with the factor analysis showed that DCE···DCE dimers are formed in solutions at DCE concentrations between 7 and 15 vol.%. It was found that both *trans* and *gauche* conformers are involved in the complexation, forming a *tg*-dimer. From the spectra collected at 200–222 K, the complexation enthalpy was determined: -4.2 ± 0.4 kcal mol⁻¹. The equilibrium geometry of *tg*-dimer and the vibrational frequencies were determined from the density functional calculations performed at B3LYP/6-311++G(d,p) and 6-31G(d,p) levels. The C–C bonds of the two molecules involved in *tg*-dimers were found to be oriented nearly perpendicular to each other. The complexation energy calculated using 6-31G(d,p) and 6-311++G(d,p) basis sets was found to be -1.59 and -1.52 kcal mol⁻¹, respectively.

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Introduction

Molecular complexes have been attracting considerable attention due to the fact that intermolecular interactions play a crucial role in reaction and dissolution kinetics, adsorption thermodynamics [1,2], self-organization of molecules, and formation of supramolecular systems with non-typical physical and chemical properties [3]. Also it is known that intermolecular, in particular dispersive, forces govern major physical phenomena in solids [4].

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It has been reported that non-classical hydrogen bonds such as C–H···X (X = N, O, Cl, etc.) significantly influence stability of metal complexes and the extension of the complex networks [5]. Such bonds need to be accounted for in engineering of crystals [6,7] and biomolecular systems [8]. C–H···X bonds stabilize molecular conformation [9] which affects biological activity [10]. Such bonds are observed in synthetic receptors where they play an important role binding halogenated guests [11].

Significant progress in theoretical analyses of weak molecular interactions along with development of new experimental approaches in this area is due to works of different research groups, including the one headed by prof van der Veken [12–17].