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Thermodynamic of dissolution and hydrogen bond of the pyrrole, *N*-methylpyrrole with proton acceptors

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ABSTRACT

Enthalpies of dissolution of pyrrole, *N*-methylpyrrole in proton acceptor solvents and proton acceptors in the medium of pyrrole, *N*-methylpyrrole were measured. The enthalpies of hydrogen bond of pyrrole, *N*-methylpyrrole with proton acceptors were calculated from experimental data of solution enthalpy of amines with organic compounds. The hydrogen bond enthalpies of proton acceptors with *N*- methylpyrrole are equal to zero unlike with pyrrole. The hydrogen bond enthalpies of proton acceptors (B) in pyrrole are significantly lower than the enthalpies of hydrogen bonding of systems of pyrrole-base in the complexes 1:1 due to reorganization effects of pyrrole as solvent. The cooperative effects in multi-particle complexes of pyrrole with bases are negligible.

1. Introduction

Pyrrole and its derivatives are important molecules because they are widespread in the flora and fauna. Pyrrole and its derivatives are structural fragments of synthetic peptides which stability is realized through the formation of hydrogen bonds (HB) [1]. These compounds are involved in molecular recognition [2–4], determine the properties of polymers [5–7], are used as catalysts [8] and antibiotics [9] since they are responsible for the selectivity and affinity [10], are part of polyamides which anticancer properties are realized by means of hydrogen bonding with DNA system [11,12]. Pyrrole is capable to exhibit the properties of acidic and basic properties due to having a N—H group and π – electron system correspondingly. Hydrogen bonding between these active centers determine a self-association of pyrrole molecules [13–17] and a formation the complexes with another organic molecules [18–24]. Estimation of energy parameters and strength of hydrogen bonds of pyrrole and its derivates assist in understanding the nature and mechanism of different processes and solution effects in supramolecular systems.

Hydrogen bonds of pyrrole and its derivates in the complexes with organic molecules were studied by different structure methods: IR-spectroscopy [13–16,23–26], UV- spectroscopy [23,26], NMR-spectroscopy [27,28], Raman spectroscopy [16,29]. Energy parameters of hydrogen bond of pyrrole with organic molecules were determined by computational chemistry [13,14,22,25,26]. Hydrogen bonds of pyrrole with organic molecules were studied by structural methods in inert solvent, matrix of inert gas or proton acceptor solvents [13–16,23,25]. It should be noted, that only in several works [30–35] hydrogen bonds of pyrrole with organic molecules are investigated by thermodynamic solvation method. Enthalpies of specific interaction of pyrrole in proton donors and proton acceptors obtained by «pure-base» method [30] are close to enthalpies of specific interaction in the complexes pyrrole with proton acceptors [36]. However, an influence of proton acceptors structure on a strength of hydrogen bonds in complexes of pyrrole-base is not enough studied [30]. The question remains what happens when one dissolve proton acceptor in environment of associated amine such as pyrrole. Influence of reorganization effect of pyrrole and of cooperative effects in multi-particle complexes of pyrrole with bases on enthalpies of specific interaction in the environment of pyrrole was not investigated.

In the present work solution enthalpies of pyrrole, *N*-methylpyrrole in proton acceptor solvents and proton acceptors in the medium of pyrrole, *N*-methylpyrrole were measured. The enthalpies of specific interaction of pyrrole, *N*-methylpyrrole with bases were calculated using the solution enthalpies of amines in proton acceptors and vice versa. Relationship between enthalpies

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