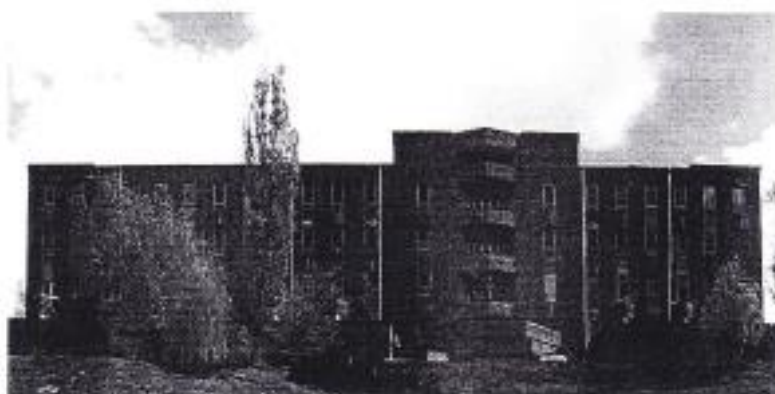


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EXPERIMENTAL AND THEORETICAL STUDIES ON COMPETITIVE INTERACTIONS IN GALLIC ACID - WATER SYSTEM

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Gallic acid (GA) and its derivatives, which belong to the class of natural hydrolysable polyphenolic compounds and are found in different plants and fruits (grape, pomegranate, tea, coffee), represent great interest due to their high biological activity (antimicrobial, antioxidant, antifungal) and formation of complexes with biomolecules, especially with proteins.

The reactivity of these compounds in aqueous solutions depends on the competitive intermolecular interactions. We present the results of experimental (2D, 3D fluorescence spectroscopy, densitometry) and quantum - chemical calculations on competitive interactions in GA - water system at 296.15, 301.15 and 306.15K in the concentration range of GA $5.88 \cdot 10^{-4} - 5.88 \cdot 10^{-2} \text{ mol l}^{-1}$.

On the basis of the fluorescence intensity dependence on GA concentration (Fig.1), density (ρ) and apparent molar volume (V_a) values of GA in aqueous solutions (see table 1) at different temperatures, it is shown that the preference of competitive interactions of monomolecular GA (self-association GA-GA and hydration GA - H₂O) and associated form of GA (GA - GA - H₂O) depends not only on the concentration but on temperature rise as well.

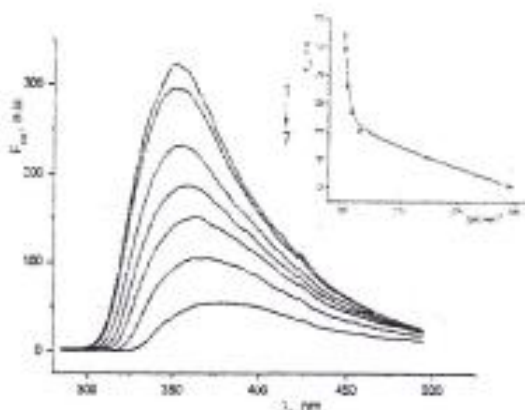


Fig.1. Fluorescence spectra of GA in aqueous solutions: GA=1 – $5.88 \cdot 10^{-4}$; 2 – $7.32 \cdot 10^{-4}$; 3 – $1.47 \cdot 10^{-3}$; 4 – $2.94 \cdot 10^{-3}$; 5 – $5.88 \cdot 10^{-3}$; 6 – $4.5 \cdot 10^{-2}$; 7 – $5.88 \cdot 10^{-2} \text{ mol l}^{-1}$; $t=306.15\text{K}$.

Table 1

The densities and apparent molar volumes of GA in aqueous solutions

$\rho, \text{g cm}^{-3} (\pm 0.00002)$			
GA, mol.l ⁻¹	296.15 T, K	301.15 T, K	306.15 T, K
5.88	1.00143	1.00010	0.99852
2.94	0.99973	0.99874	0.99687
0.588	0.99797	0.99668	0.99514
0.294	0.99777	0.99648	0.99493
0.0588	0.99764	0.99633	0.99478
${}_0V, \text{cm}^3 \text{mol}^{-1} (\pm 0.002)$			
5.88	169.812	170.034	170.307
2.94	170.095	170.312	170.579
0.588	170.394	170.615	170.872
0.294	170.425	170.646	170.901

The structure, charges and the energy values of intermolecular interactions of stable GA dimer and GA - water complexes (Fig.2) in gas phase and in aqueous media ($\epsilon_{\text{H}_2\text{O}} = 78.36$) were estimated. Solvent effects were modeled using the Onsager reaction field method. All the

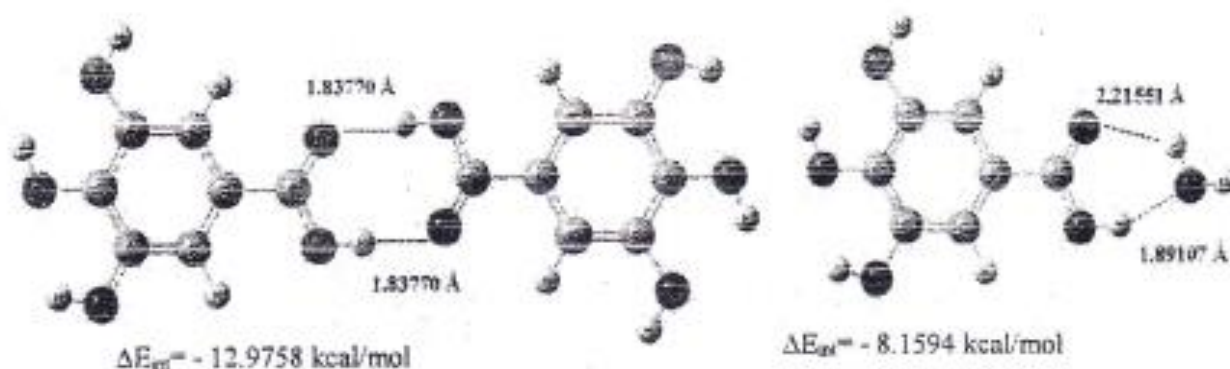


Fig. 2. Structures of stable GA dimer and GA-water complexes.

quantum chemical calculations were performed using *ab initio* RHF/6-311+G* basis set by GAUSSIAN 03 program package. It has been found that in the presence of the solvent (water) more stable is GA dimer ($\Delta E_{\text{int}} = -12.9758 \text{ kcal/mol}$) than GA/H₂O complex ($\Delta E_{\text{int}} = -8.1594 \text{ kcal/mol}$), though the presence of this complex can not be precluded in the solvent.