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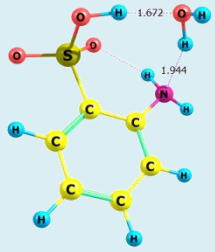
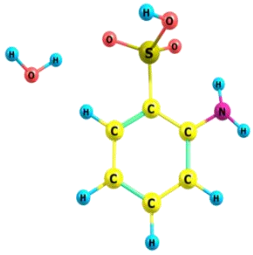
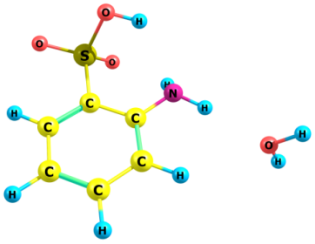
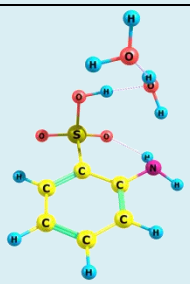
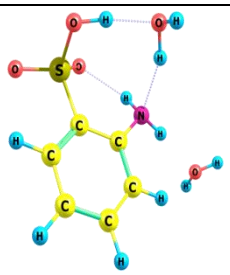
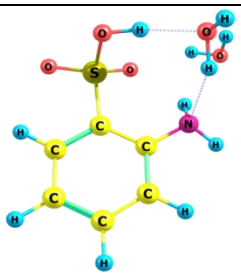
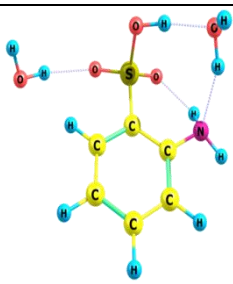
PREDICTION OF PROTON-DONOR PROPERTIES OF AROMATIC SULFONIC ACIDS AMINOSILANE

Aromatic sulfonic acids, due to their relatively high acidity, are promising compounds for modifying proton-exchange membranes of fuel cells of chemical current sources. To modify proton-exchange membranes, it is necessary to understand the regularities of changes in the proton-conducting capacity in the rows of sulfonic acids. To do this, it is advisable to use theoretical methods and various models of deprotonation. Since the presence of water in the membrane plays an important role in proton exchange processes, models should take this into account.

In the course of calculations, water molecules were added to 2-ABSA sequentially. By adding a single water molecule to the most energy-efficient 2-ABSC conformer, three different structures of the 2-ABSA complex were obtained: $1H_2O$. In the most energetically advantageous complex, the water molecule is located between $–SO_3H$ and-NH_2 groups, thus forming two intermolecular hydrogen bonds O-H...O (r = 1.672 Å) and O–H...N (r = 1.944 Å).

Modeling of 2-ABSA:$2H_2O$ complexes was carried out on the basis of the most energy-efficient 2-ABC complex:1 H_2O. As a result, 4 variants of the geometric structure of 2-ABSA:$2H_2O$ were obtained. A complex with minimal energy corresponds to a structure in which the second water molecule forms an intermolecular hydrogen bond with the first water molecule.

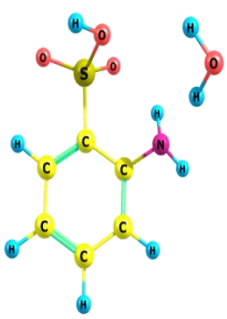
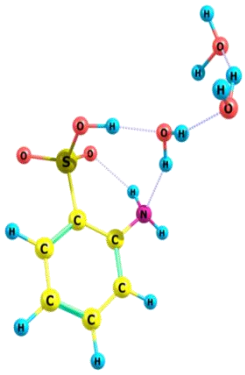
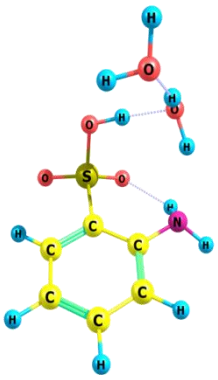
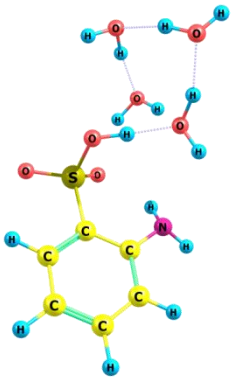
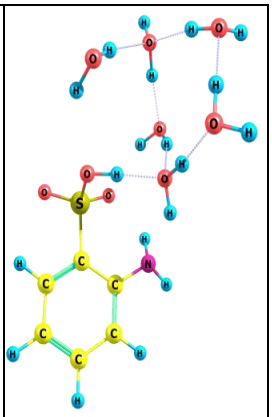
2-ABSA hydrate complexes: nH_2O

			
ΔE=0 kcal/mol	ΔE=7.28 kcal/mol	ΔE=6.98 ккал/моль	
			

ΔE=0 kcal/mol	ΔE=1.64 kcal/mol	ΔE=0.32 kcal/mol	ΔE=1.62 kcal/mol

Similarly, the most energy-efficient structures of the previous step were used for the 2-ABSA:3H_2O and 2-ABSA:4H_2O complexes.

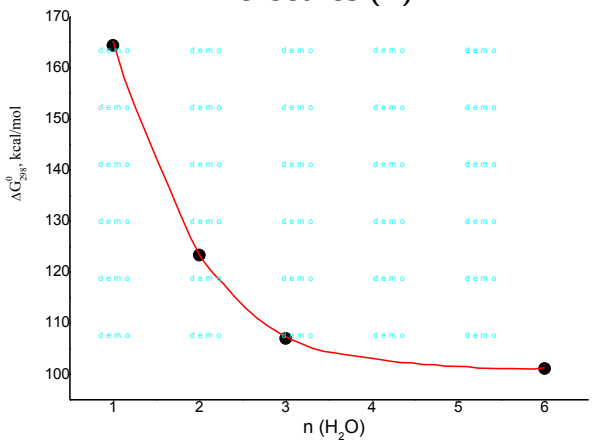
The geometric structure of hydrated complexes of 2-ABSA:nH_2O

				
2-ABSA:1H_2O	2-ABSA:2H_2O	2-ABSA:3H_2O	2-ABSA:4H_2O	2-ABSA:6H_2O

Deprotonation energies of 2-ABSA in hydrate complexes

nH_2O	**ΔG^0_{298}, kcal/mol**
n=1	164.4
n=2	123.34
n=3	107.01
n=6	101.13

Dependence of the deprotonation energy of 2-ABSA:nH_2O complexes on the number of water molecules (n)



Various variants of the structure of complexes were obtained, among which complexes with minimal energy have a structure characterized by the formation of hydrogen bonds between water molecules. Thus, each subsequent water molecule forms hydrogen bonds with other water molecules located in the complex, this is the most energy-efficient way. The deprotonation energies of 2-ABSA in each of the studied complexes were calculated. The resulting relationship between the number of water molecules in the complex and the Gibbs deprotonation energy is not linear, but exponential. The figure shows that for n = 3 and for n = 6, the values of ΔG^0_{298} are almost identical.