QUANTUM-CHEMICAL MODELING OF INTERMOLECULAR HYDROGEN BONDING BETWEEN NEUTRAL MOLECULES

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Semiempirical quantum mechanical PM7 method is successful for molecular energies reproducing, molecular structures replicating, and chemical reactions interpreting. Twenty neutral complexes were optimized by PM7 method with the help of Molecular Orbital PACkage MOPAC. Results of the PM7 calculations and experimental data are presented on the table.

Complex	D	A	r(D-A), Å	Charge transfer	Heats of association, kcal/ mol	
					PM7	Exp.
H_2O - H_2O	H_2O	H_2O	2.79	-0.009	-7,01	-4.4 - -5.4
$(H_2O)_3$	H_2O	H_2O	2.63	-0.006	-6,07	
$(H_2O)_4$	H_2O	H_2O	2.56	-0.009	-4,58	
$(H_2O)_5$	H_2O	H_2O	2.56	-0.009	-7,67	
$(H_2O)_6$	H_2O	H_2O	2.55	-0.009	-7,51	
H_2O - CH_3OH	H_2O	CH_3OH	2.77	-0.022	-5,00	-3.2 - 7.3
H_2O - HCOOH	H_2O	HCOOH	2.74	-0.011	-9,67	
H_2O - CH_3COOH	H_2O	CH_3COOH	2.74	-0.010	-8,41	
H_2O - C_6H_5COOH	H_2O	C_6H_5COOH	2.74	-0.009	-10,2	
H_2O - CH_2O	H_2O	CH_2O	2.74	-0.024	-3,78	
H_2O - NH_3	H_2O	NH_3	2.74	-0.004	-6,41	-4.4

It was found that for water dimer the length of hydrogen bond is 1.825 Å and the energy of hydrogen bond is 7.01 kcal mol^{-1}. Structures of water trimer, tetramer and pentamer were calculated to evaluate the relationship between hydrogen bond strength and charge transfer. The structure of water pentamer was taken similar to the ice structure in calculations. It was assumed that the pentamer symmetrical configuration helps more efficient charge transfer between molecules in the complex. It was established that hydrogen bond energies and geometric characteristics of hydrogen bond are close in value for water-methanol complex and methanol dimer. It was noted that methanol dimer has the weakest hydrogen bond, then followed the water methanol complex and the methanol water complex. These results, as well as results for water dimer, indicate that water molecule compared to methanol is the best donor as well as acceptor.