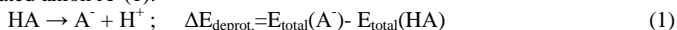


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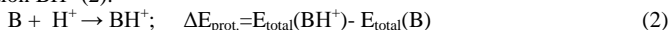
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Molecule of glycine is capable for dual protolytic ability: it is demonstrate properties of acid by *splitting off a proton* from the carboxyl group and base properties by connecting a proton to the amino group. Besides glycine demonstrates a tendency to form dimers due to the presence of carboxyl and amino functional groups in structural unit. It was interesting to observe the alterations of acid-base properties in dimeric molecules changing protolytic ability of glycine by applying quantum chemical methods.

It was shown earlier [1], that the acid strength can be characterized by deprotonation energy  $\Delta E_{\text{deprot}}$  estimated by quantum chemical methods as the difference between total energy of the acid HA and its deprotonated anion  $A^-$  (1):



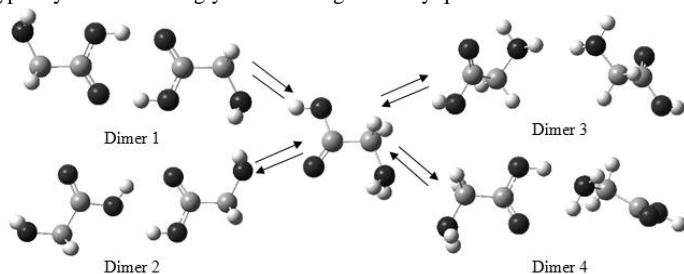
And the base strength [2] can be characterized by the proton affinity or protonation energy  $\Delta E_{\text{prot}}$  estimated by quantum chemical methods as the difference between total energy of the base B and its protonated cation  $BH^+$  (2):



At the same time, a low deprotonation energy corresponds with a more easy proton transfer and with a greater strength of the acid. On the other hand, a large protonation energy corresponds with a more strong base.

Based on the foregoing deprotonation energy and proton affinity of glycine and its dimers were estimated by *ab initio* UHF 6-31G method taking into account the solvent (water) within the CPCM model using Gaussian-2009 program.

Four types cyclic dimers of glycine were registered by quantum-chemical method:



Calculated data are presented below:

Structure	$E_{\text{total}}$ , A.U.	$E_{\text{total}}(A^-)$ , A.U.	$\Delta E_{\text{deprot.}}$ , A.U.	$E_{\text{total}}(BH^+)$ , A.U.	$\Delta E_{\text{prot.}}$ , A.U.
Monomer	-282,71189	-282,23498	0,47692	-283,16366	0,45176
Dimer 1	-565,44073	-564,96993	0,47080	-565,89313	0,45239
Dimer 2	-565,43391	-564,97101	0,46290	-565,88550	0,45158
Dimer 3	-565,42527	-564,95130	0,47397	-565,89212	0,46684
Dimer 4	-565,43473	-564,96427	0,47047	-565,89218	0,45743

Presented data shows, that deprotonation energy in dimers is reduced (i.e. the acid strength increased) and protonation energy is increased (i.e. basicity increased). Hence the acid-base properties in dimers of glycine are enhanced.

1. Pustolaikina I.A. et al. *Bulletin of Karaganda University. Chemistry*, 2011, **3(63)**: 3-8.
2. Pustolaikina I.A. et al. *Chemical Journal of Kazakhstan*, 2012, **38**: 109-113.