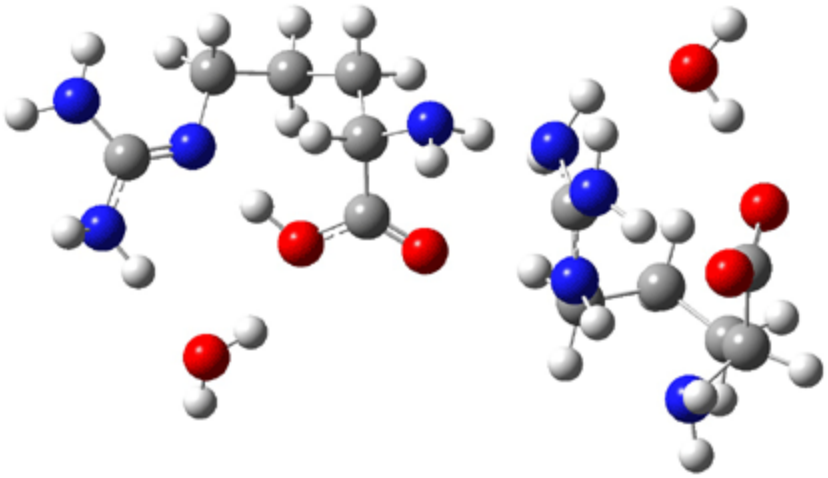
ARGININE: WATER CLUSTER

The gas phase structure of the amino acids is in their canonical or neutral form, while their aqueous solution phase structure is zwitterionic. An interesting question is how many water molecules are needed to make the zwitterionic structure more energetically favorable than the neutral form. For glycine, it appears that seven water molecules are needed to make the zwitterion the favorable tautomer.[1,2]

Arginine, on the other hand, appears to require only one water molecule to make the zwitterion lower in energy than the neutral form.[3] The B3LYP/6-311++G** structures of the lowest energy neutral (**1N**) and zwitterion (**1Z**) cluster with one water are shown in Figure 1. The zwitterion is 1.68 kcal mol^{-1} lower in energy. What makes this zwitterion so favorable is that the protonation occurs on the guanidine group, not on the amine group. The guanidine group is more basic than the amine. Further, the water can accept a proton from both nitrogens of the guanidine and donate a proton to the carboxylate group.



1N (1.68)

1Z (0.0)

Figure 1. B3LYP/6-311++G** structures and relative energies (kcal mol^{-1}) of the lowest energy arginine neutral (**1N**) and zwitterion (**1Z**) cluster with one water.[3]

Source: http://comporgchem.com/blog/?p=104