

# Role of Solvent in Aqueous Glycine Condensation

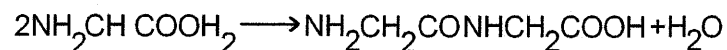
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We report an improved *ab initio* mechanism for aqueous glycine condensation



which details catalytic effects of solvent molecules. The MP2/6-31G\* model chemistry is used to calculate structures and energies of stationary points on the reaction coordinate diagram. Carbonyl oxygen on a hydrated nucleophilic reactant pair complex (RPC) attacks a proton of a reactive water molecule, with the aid of a terminal amine zwitterion-water complex ( $W_{\text{az}}$ ). This enables a reactive water oxygen atom to remove a proton from the nucleophilic nitrogen of the RPC, with activation from a third solvent molecule and a terminal carboxylate-water complex. The result is a hemiacetal-like intermediate (hemi). The  $W_{\text{az}}$  accepts the proton from one of the hemi oxygen atoms ( $O_{\text{h1}}$ ), while releasing one of its protons to the nucleophilic attraction of the second hemi oxygen atom ( $O_{\text{h2}}$ ). The  $O_{\text{h2}}$  thus becomes product water as its covalent bond to the electrophilic C of hemi breaks in response to C  $sp^2$  hybridization with  $O_{\text{h1}}$ . A minimum of four solvent molecules participate substantively in the mechanism. We report structures and energies of tetrahydrated RPC, hemi, products, and a side reaction intermediate, and discuss the reaction coordinate diagram.