

Quantum?Chemical modeling of catecholamine storage including continuum solvent effects

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A model for catecholamine storage in vesicles is analyzed within the SCRF?CNDO/2 approach including continuum solvent effects. The model considers the approach of cationic norepinephrine (NE) to a positively charged guanidinium moiety. Ion?pair formation is found for the whole range of dielectric constants. Even though stable states of H?bonded partners are found for large dielectric constants, this process is ruled out to occur because it involves too high energies. It appears that the medium's polarity is determinant in lowering the energy barrier between the ion?pair complex and the separated partners. Thus, as the medium dielectric constant increases, the equilibrium between the two states is enhanced. Copyright © 1991 John Wiley & Sons, Inc.