Theoretical Study of Cisplatin Interactions with Glycine in Gas-phase and Implicit Water Solution – COSMO.

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Interactions of hydrated cisplatin complexes with glycine were explored. The square-planar cis-$[Pt(NH_3)_2(H_2O)X]^+$ complexes (where X=Cl, OH and H_2O) were chosen as models for mono- and dihydrated reactants. Theoretical calculations using DFT techniques with B3LYP functional were performed. Both gas-phase and polarizable continuum model (in COSMO version) were employed for the reaction energies and bonding energies determinations in approach of isolated molecules as well as supermolecular complexes. The formations of monodentate complexes by replacing aqua-ligand with N and O atoms of the amino acid represent exothermic processes. The formation of chelate structures is an exothermic reaction for dihydrated form of reactants.