

Non-empirical quantum chemical studies on electron transfer reactions in *trans*- and *cis*-diamminedichloroplatinum(II) complexes.

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Streszczenie

The search was made for theoretical confirmation of hypothesis that mechanism of cisplatin cytotoxicity is based on dissociative electron transfer (ET) processes. Applying quantum chemical calculations based on supermolecular approach, the reactions mimicking presumed steps of cisplatin activation were evaluated. The electronic structure of model systems: *cis*- and *trans*platin with free electrons, hydrated electrons, and water, was studied by using density functional (DFT) within the Huzinaga basis set and GAUSSIAN-09 package. The respective energy was evaluated with the use of B3LYP density hybrid functional. The calculations were performed for gas phase and water solution; the solvent effects were studied by using the polarizable continuum model. Analysis of the energetic and structural parameters of cisplatin vs. *trans*platin behavior in the model systems leads to conclusion: there are two possible ways of cisplatin biotransformation, hydrolysis and hydrated electron impact, dependent on the medium redox state.

Słowa kluczowe

Cisplatin and *trans*platin, DFT, Electron transfer (ET), Hydrated electron impact, Hydrolysis, Quantum chemical studies

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