



Non-empirical quantum chemical studies on hydration of *trans*- and *cis*-[Pt(NH₃)₂Cl₂]. Possible role of relativistic effects.

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Streszczenie

The motivation to this work results from the recognition of cis-diamminedichloroplatinum(II) (cisplatin) hydration processes as essential for the fate of this drug in host organism. Applying quantum chemical calculations, there were evaluated the first stages of water molecule impact on platinum complexes: cisplatin and its trans isomer. Non-empirical quantum chemical calculations have been performed for reactions of cis and trans-diamminedichloroplatinum(II) (transplatin) with the water molecule, assuming the associative mode of reactions running with the addition of a fifth ligand to a square planar d⁸ complex and formation of a trigonal-bipyramidal structure of the transition state. For the obtained structures of reactants, transition states, and products, the thermodynamic characteristics (energies and Gibbs free energies) were estimated. Energetics for the ligand exchange reactions were estimated both in gas phase and water solution by using the PCM model. The hydration reactions under consideration are principally endothermic except of the solvated transplatin. Basing on our ab initio ZORA calculations, the possible role of relativistic effects in the reaction mechanism is pointed out as well. Obtained results may throw some light on processes which determine the interchange of pro-drug (cisplatin) into activated drug (aqua-form) and implicate their significance in designing of anticancer, Pt-containing chemotherapeutics.

Słowa kluczowe

cisplatin, transplatin, interactions with water molecule, quantum mechanical calculation, relativistic ZORA calculations