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Isotopic Effects on the Hydrolysis of anticancer drug titanocene dichloride: A DFT study

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Anticancer activity of titanocene dichloride (namely bis(cyclopentadienly)titanocene dichloride, Cp_2TiCl_2, Cp = η^5-(C_5H_5)) has been discovered in the ١٩٨٠s, and since then it has attracted continuous attention in the experimental literature [١-٧]. In this work, hydrolysis of the anticancer drug titanocene dichloride complex was illustrated using quantum mechanical method. BP٨٦ functional and basis sets of ٦-٣١١G(d,p) and Def٢-TZVPPD for main group element and Ti atoms, respectively, were considered. Two typical reactions involved in the complex hydrolysis include the first and second hydrolysis processes:

First hydrolysis: $[Cp_2TiCl_2].H_2O$ (R١A) $\rightarrow$ $[Cp_2TiCl(OH_2)]Cl$ (PA١)

Second hydrolysis: $[Cp_2TiCl(OH_2)]^+$. H_2O (R٢A) $\rightarrow$ $\{[Cp_2Ti(OH_2)_2].Cl\}^+$ (PA٢)

It was tired to show how the thermodynamic, and kinetic parameters of titanocene dichloride hydrolysis were affected by the replacing of hydrogen atoms of Cp ligand with deuterium.

Keywords: Anticancer drug , Isotopic Effects, Hydrolysis, Titanocene dichloride

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