

It has been proven that platinum complexes are active in anticancer treatment as well as several other transition metals complexes. There is an effort in recent medicine to replace cisplatin complexes by drugs with smaller side effects. This work focuses on the reaction of 5'-dGMP (2'-deoxyguanosine-5'-monophosphate) and cGMP (cyclic 2'-deoxyguanosine-monophosphate) with a platinum complex $\text{Pt}^{\text{IV}}(\text{dach})\text{Cl}_4$ (dach=diaminocyclohexane). In these two cases the Pt(IV) complex is only reduced in the presence of 5'-dGMP. The first part of the explored mechanism is the substitution reaction where a coordinate-covalent bond between platinum and nitrogen N7 of guanine is formed. In the next step oxygen of phosphate group is transferred to the C8 site. Subsequently the Pt(IV) complex is reduced. The final products represent 8-oxo-GMP and $\text{Pt}^{\text{II}}(\text{dach})\text{Cl}_2$, which are active in anticancer treatment in comparison with the kinetically inert reactant. The substitution of a chloride anion ends the reaction path for cGMP forming $\text{Pt}^{\text{IV}}(\text{dach})\text{Cl}_3(\text{N7-cGMP})$ complex. The structures were optimized at the DFT level with B3LYP functional in the basis set 6-31G(d) and PCM/UA0 solvation model. The energy parameters were computed at the B3LYP/6-311++G(2df,2pd) level in the IEFPCM/sUAKS solvation model. Finally, the rate constants were determined and compared with experimental data.