

This work is focused on the reactions of diaqua-tetrakis(μ -acetylato)dirhodium(II,II) with guanine, that shows anti-cancer activities. Guanine can bond to the complex either by oxygen O6 or by nitrogen N7. We studied three possible versions of the system – one that is protonated on guanine, one protonated on the paddle-wheel and a neutral one. For all 6 reactions transition structures were found. For reactants, transition states and products we computed the values of electron density in the critical points of bonds, partial atom charges and the interaction energies of the system, guanine and water on the b3lyp/aug-cc-pvdz level. Pseudobasis and pseudopotentials were employed in the case of rhodium atom. For all the reactions thermodynamical properties were computed.