This work focuses on the study of interactions of the Diaqua-tetrakis(-acetylato)dirhodium(II,II) complex. This complex belongs to compounds of transition metals, which show activity in anticancer treatment. In this work, the interactions of this complex with ammonia and guanine are studied. The interactions with ammonia are represented by a replacement reaction of oxygen from acetyl ligand or aqua ligand. Another reaction is the replacement of water bonded to rhodium by guanine. Guanine can form a bond to rhodium with oxygen O6 or nitrogen N7. Optimization of the structures are made at the DFT level with 6-31G* basis set. For reactions with ammonia transition states were found. NPA charge analyses, thermodynamical and kinetical analyses were performed. All these analyses were done at the DFT level with aug-cc-pvdz basis set. To describe the electronic structure of rhodium atoms pseudopotentials and pseudobasis were used. All calculations were modeled in gas phase.