

In this thesis we make use of methods applied in quantum chemistry and molecular dynamics to interpret the results of the spectroscopy of two rhenium donor-acceptor complexes  $\text{ReCl}(\text{CO})_3$  (N,N'-4-((4-(diphenyl)phenyl)carbamoyl)-2,2'-bipyridine) and  $\text{ReCl}(\text{CO})_3$  (N,N'-5-((4-(diphenyl)phenyl)carbamoyl)-2,2'-bipyridine) after exciting them with a ultrashort laser pulse in the near UV range. Specifically we concentrate on the transition between the state with the character of  ${}^3\text{MLCT}/{}^3\text{IL}$  and  ${}^3\text{CS}$ , and why it is faster for the latter. The structures of the complexes in the ground state and the  ${}^3\text{MLCT}$  state were obtained from the classical and QM/MM MD simulations in dimethyl sulfoxide in the form of an explicit solvent. The geometrical parameters, electron density distribution and the electrostatic effect of the solvent were analysed from the acquired structures. Their influence on the rate of the electron transmission was estimated based on the value of the electronic coupling. It is shown that due to their size ( 25 meV for GS), the process of transition of the electron was mostly adiabatic. Determined electrostatic potentials show the crucial effect of the solvent during the stabilisation of the  ${}^3\text{CS}$  and  ${}^3\text{MLCT}$  states, where the changes in the potential are the largest in the area around bpy.