Work plan
(Coimbra, Portugal, February 28 – March 12)

Title: **Modeling the potential energy surfaces and their couplings for nonadiabatic systems.**

The aim of this STSM is to foster collaboration between the group of Prof. Antonio Varandas (University of Coimbra, Portugal) and the group of Prof. Stanka Jerosimić (University of Belgrade, Serbia). Prof. Varandas is MC member of MOLIM COST action.

So far, within the group at the Faculty of Physical Chemistry (University of Belgrade), the Applicant M. Milovanovic studied electronic and vibronic spectra of linear molecules with degenerate ground electronic states, taking into account spin-orbit and Renner-Teller effects (C_2P, C_2As, C_2Pb, $C_2H_2^+$, C_5^-, $C_4N_2^+$…). To modeling these spectra, one could use transformation of the adiabatic electronic wave functions into their diabatic counterparts. It should start with computations of the potential surfaces, and locating and computations of nonadiabatic matrix terms.

During the two weeks of the visit, M. Milovanovic should focus on three main issues: 1) obtaining accurate ab initio potential energy surfaces using scheme for extrapolating energies to the complete one-electron basis set limit; 2) modeling the nonadiabatic matrix terms and 3) using diabatization scheme developed by Prof. Varandas for potential surfaces of small molecules. Once an accurate results for potential energy surfaces and their couplings are obtained, they may be used to modeling the dynamics of chemical systems of interest. The aim of Applicant is to understand existing models and to find possible applications for new chemical species.

Dr Milan Milovanovic
University of Belgrade
Faculty of Physical Chemistry