QUANTUM COMPUTATIONS OF TETRATOMIC HALIDE-H_2O COMPLEXES

WORK PLAN OF THE STSM

We propose fully coupled quantum calculations of the vibrational energy levels of the X^-H_2O (X=halides) complexes using the WAVR4 codes. A schedule of the research activities is given below.

1^{st} week:

- Kinetic energy operator in an appropriate coordinate system (Radau-Jacobi) for any X^-H_2O tetratomic molecules.
- Evaluation of the reliability of available potential energy surfaces, e.g. *ab initio*-based ones.

2^{nd} week:

- Preliminary convergence tests of the basis sets for the lighest anion (F^-, Cl^-) systems .

3^{rd} week:

- Organization and analysis of the obtained data together with some concluding remarks on the underlying potential, and/or direction for further investigation on the proposed study.