SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CM1405 STSM reference number 38330
STSM title: Quantum computations of tetratomic Halide-H2O complexes
STSM start and end date: 07/08/2017 to 25/08/2017
Grantee name: Raúl Rodríguez Segundo

PURPOSE OF THE STSM:

The Short-Term Scientific Mission (STSM) of Raúl Rodríguez entitled "Quantum computations of tetratomic Halide-H 2 O complexes" took place from 07/08/2017 to 25/08/2017 in the group of Prof. Jonathan Tennyson at Departmentof Physics and Astronomy, UCL, London. The goal of the project is the study of the spectroscopy of tetratomic clusters formed by water halide ion complexes. The calculation of the corresponding vibrational energy levels involves the use of DVR3D and WAVR4 codes.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

1. We chose to work in Radau coordinate for DVR3D [1] and Jacobi for the WAVR4 software [2]. We adapted the potential energy surfaces for both coordinate systems. We chose to use the PESs from the Refs ([3-5])
2. First tests on the basis sets for the Cl − water system and optimization of the parameters in the Laguerre polyno-
mials basis set.
3. Analysis of the obtained data, modification and evaluation in the potential [6].

References

[1] Jonathan Tennyson, Maxim A. Kostin, Paolo Barletta, Gregory J. Harris, Oleg Polyansky, Jayesh Ramanlal, and Nikolai F. Zobov. DVR3D: A program suite for the calculation of rotation-vibration spectra of triatomic molecules. Computer Physics Communications, 163:85–116, 11 2004.
[2] Igor N. Kozin, Mark M. Law, Jonathan Tennyson, and Jeremy M. Hutson. New vibration–rotation code for tetraatomic molecules exhibiting wide-amplitude motion: WAVR4. Computer Physics Communications, 163(2):117 – 131, 2004.
[3] Jaime Rheinecker and Joel M. Bowman. The calculated infrared spectrum of Cl − H 2 O using a new full dimen-sional ab initio potential surface and dipole moment surface. The Journal of Chemical Physics, 125(13):133206, 2006.
[4] Janos Sarka, David Lauvergnat, Vincent Brites, Attila G. Csaszar, and Celine Leonard. Rovibrational energy lev-els of the F − (F 2 O) and F − (D 2 O) complexes. Phys. Chem. Chem. Phys., 18:17678–17690, 2016.
[5] Eugene Kamarchik, Daniele Toffoli, Ove Christiansen, and Joel M. Bowman. Ab initio potential energy and dipole moment surfaces of the F − (H 2 O) complex. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 119:59 – 62, 2014.
[6] Xiao-Gang Wang and Tucker Carrington Jr. Rovibrational levels and wavefunctions of Cl − H 2 O. The Journal of
Chemical Physics, 140(20):204306, 2014.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

Preliminary results on potential energy surfaces performance were obtained, as well as optimized parameters for the DVR basis sets to be used for different type of ion atoms. Further convergence tests are currently in progress.

FUTURE COLLABORATIONS (if applicable)

The present collaboration will continue with vibrational state calculations in Jacobi (in a first step), as well as including the more appropriated Jacobi-Radau coordinates in the WAVR4 code for ro-vibtational calculations of such systems.