Applicant Details
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STSM Details
Action Number: CM1405 – Molecules in motion (MOLIM)
STSM Title: Resonance Treatment for Formation of CO+ by Radiative Association
Select Grant Period: AGA-CM1405-4:2018-05-01 – 2019-03-19
Start Date: 2018-05-14
End Date: 2018-05-24
Duration: 11
Motivation and Workplan:
Martina Zámečníková is a PhD student dealing with radiative processes in diatomic systems [1-4]. Currently, she is working with prof. Magnus Gustafsson on formation of astrochemically significant CO+ by radiative association. Six different radiative association processes are involved in the project:

$A^2\Pi \rightarrow X^2\Sigma^+$ + photon,
$X^2\Sigma^+ \rightarrow A^2\Pi$ + photon,
$D^2\Pi \rightarrow X^2\Sigma^+$ + photon,
$D^2\Pi \rightarrow A^2\Pi$ + photon,
$C^2\Delta \rightarrow A^2\Pi$ + photon,
$1^2\Sigma^- \rightarrow A^2\Pi$ + photon.

The cross sections for them are being calculated semiclassically (SC) with the resonances contribution to be included by the Breit-Wigner (BW) theory [5]. These cross sections are compared with quantum perturbation theory (QMPT) calculations. The rate coefficients will be calculated from the SC+BW cross sections. While the SC calculations are done and the QMPT almost done, the BW calculations are unfinished. Because M. Zámečníková is using in this project all computer codes written in the group of prof. Gustafsson, it is very useful for her to have an opportunity to discuss problems that she has encountered in the BW calculations with prof. Gustafsson. Outcome of this STSM will be an aticle in which the support of the COST action CM1405 will be greatly appreciate as in all possible seminars or other presentations. This project is also a part of M. Zámečníková’s dissertiation thesis.

A workplan:
The first two days to solve problems for the $A^2\Pi \rightarrow X^2\Sigma^+$ + photon BW calculations.
The third day successfully calculate the resonance contribution to the $A^2\Pi \rightarrow X^2\Sigma^+$ + photon process.
The fourth and fifth day, use the BW theory on the opposite process $X^2\Sigma^+ \rightarrow A^2\Pi$ + photon and for the $1^2\Sigma^- \rightarrow A^2\Pi$ + photon process.
The sixth, seventh and eighth day, use the BW theory on the processes: $D^2\Pi \rightarrow X^2\Sigma^+$ + photon and $D^2\Pi \rightarrow A^2\Pi$ + photon.
In the end, use the BW theory for the $C^2\Delta \rightarrow A^2\Pi$ + photon.

For every process, the Einstein coefficients for the spontaneous emission by the LEVEL 8 programme need to be calculated, together with the positions and tunnelling widths of resonances. Then, the BW cross sections can be obtained.

[1] L. Augustovičová, M. Zámečníková, W. P. Kraemer, P. Soldán, Radiative association of He(2^3P) with lithium cations, Chem. Phys. 462 (2015) 65-70.
[2] M. Zámečníková, W. P. Kraemer, P. Soldán, Radiative association of He(2^3P) with lithium cations: $\Pi \rightarrow \Sigma$ processes, J. Quant. Spectrosc. Radiat. Transfer 191 (2017) 88-95.
[3] M. Zámečníková, P. Soldán, Radiative decay of HeLi+($b^3\Sigma$+), Chem. Phys. 500 (2018) 1-6.
[4] M. Zámečníková, W. P. Kraemer, P. Soldán, Radiative charge transfer between metastable helium and lithium cations, ApJ, in preparation.
[5] G. Nyman, M. Gustafsson, S. V. Antipov, Int. Rev. Phys. Chem. 34 (2015) 385-428.

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