

Training in data calculations for environmental applications: calculation of the rotational and vibrational cross sections for plasma modelling

Scientific field: Quantum physics, modelling, engineering sciences, numerical calculations

Key words: Ozone, ITER, ro-vibrational excitations, databases, electron-molecule collisions, Quantemol,

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Salary: 600 €/month

Period: from September 2023 for 6 months

In the study of the atmosphere of the Earth or the other planets and for the development of the thermonuclear reactor ITER (www.iter.org/fr/welcome) built to CADARACHE, the modelling plasma plays a key role. This modelling is based on atomic and molecular data. It consists in identifying all the elements (elements, molecules) composing the plasma as well as the collisional processes (electronic attachment, ionization, etc.) which occur in the latter. Nowadays, the International Atomic Energy Agency (IAEA), coordinator of the ITER project, develops and maintains a database for the modelling. However this basis is not complete and requires to be enriched in particular by data on collisions electrons-molecules.

As an example, to model the earth atmosphere and study the process of destruction of the ozone layer, it is necessary to have data on the processes of vibrational and rotational excitations of the molecules N_2 , O_2 , O_3 . Besides that, the construction of the divertor, the crucial element in the reactor ITER, requires to model the plasma and to identify its composition to determine its geometry. To model the plasma close to the divertor, it is necessary to have data on the cross sections of vibrational modes of molecules such as H_2^+ , H_2 , D_2 , D_2^+ , HD , HD^+ , T_2 , HT .

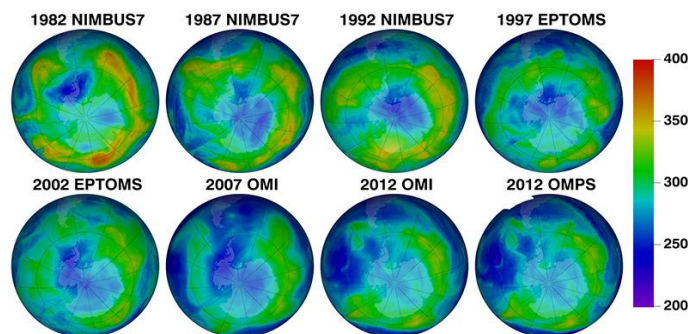


Figure 1: Depletion of the ozone layer since 1982.
NAS Aimage (<http://www.nasa.gov/>)

Research subject, work plan:

The aim of this project is to contribute to enrich the database of the IAEA by determining the cross sections for the rotational and vibrational excitations of the molecules N_2 , O_2 , O_3 . The approach will consist in using the R-matrix formalism via the *Quantemol* software. This method will allow



determining cross sections of collision processes which will be introduced into plasma codes to simulate the dynamics of destruction of the stratospheric ozone (see Fig.1).

The obtained results will be a part of a publication in a specialized scientific journal. These data will be also included in the atomic and molecular databases of the IAEA. A similar study on the rotational and vibrational excitations of molecules H_2^+ , H_2 , D_2 , D_2^+ , HD , HD^+ , T_2 , HT is planned. These works are to be considered with the candidate, depending on his interest and motivation. A PhD position is also planned after this internship.

Collaboration with the University of Central Florida with a possibility of stay is planned for this project

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