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# Theoretical line lists for planetological and astrophysical applications: the TheoReTS database

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## Abstract

Knowledge of intensities of rovibrational transitions of various molecules and theirs isotopic species in wide spectral and temperature ranges is essential for the modeling of optical properties of planetary atmospheres, brown dwarfs and for other astrophysical applications. Greenhouse gases are also of great interest. This demonstrates the necessity of having adequate and reliable molecular line lists. The TheoReTS (Theoretical Reims Tomsk Spectra) project [1] aims at providing complete and comprehensive theoretical lists of transitions based on accurate *ab initio* and variational calculations for a large variety of highly symmetric molecular species as $CH_4$, $PH_3$, $C_2H_4$, $SiH_4$, $CH_3F$, $GeH_4$ including all isotopologues. Predicted hot methane and ethylene line lists are also included. In case of very large high-temperature line lists, a data compression is implemented for fast interactive spectra simulations of a quasi-continual absorption due to big line density. Calculations on other molecular systems are available or currently in progress ($CH_3Cl$, $CH_3I$, $CF_4$, $H_2CO$, $SF_6$, $NF_3$, $C_2H_2$, $CHF_3$, *etc*.).
The information system provides the associated software for spectra simulation including absorption coefficient, absorption and emission cross-sections, transmittance and radiance. The simulations allow Lorentz, Gauss and Voigt line shapes. Rectangular, triangular, Lorentzian, Gaussian, sinc and sinc squared apparatus function can be used with user-defined specifications for broadening parameters and spectral resolution.
The system is freely accessible *via* internet on the two mirror sites: in Reims, France (http://theorets.univ-reims.fr) and in Tomsk, Russia (http://theorets.tsu.ru).
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## 1. Introduction

Radiative properties of molecules are of major importance in various domains of science and applications. Absorption/emission spectroscopy is an excellent diagnostic tool to control partial pressures of molecular species, their isotopic ratios and time evolution. Though many spectroscopic databases provide very accurate information on line parameters, the temperature and wavenumber coverage is often not sufficient to meet the requirements of new and future astrophysical targets. Moreover line-by-line assignment and fits of experimental spectra included in traditional databases are tedious and difficult tasks that can only progress slowly by considering one spectral interval after the other, in increasing order of energy. The temperature dependence of spectral features is crucial, but quantified experimental information at high temperature is generally missing. For high temperature, it is not feasible to obtain millions or even billions (at high T) of line parameters from laboratory observations alone: they must be provided only by theory based on ab initio calculations.

## 2. Philosophy of the information system

The complete modeling of absorption or emission spectra at a given temperature will require at least four quantities, namely, the line positions, the line intensities (Sif), the lower state energies (Ei) and the partition function. At this stage, three major theoretical ‘‘ingredients” are thus necessary: (i) An accurate intra-molecular potneital energy surface at a large range of vibrational displacements in order to compute the wavefunctions and to predict ro-

vibrational energy levels Ei and line positions. (ii) dipole moment surface components also defined in a large range of nuclear configurations are necessary for calculation of transition probabilities between upper and lower vibration–rotation states. (iii) Efficient quantum nuclear motion computational methods are necessary to achieve a good numerical convergence of calculations in a large basis set with a full account of molecular symmetry properties.

## 3. Illustrations

Many applications could benefit from theoretical predictions of molecular radiative properties even if ab initio predications do not yet provide a high-resolution accuracy for line positions. This could be useful for the radiative transfer modeling of planetary and terrestrial atmospheres, for opacity calculations in astrophysics and for searching the transparency windows in cases where experimental spectra at a required temperature, pressure or path length conditions are not available or not yet fully analyzed.

An example of the TheoReTS graphical user interface dedicated to XS calculations is shown below. The user is first invited to choose a molecular species, isotopologue if Fig1 and a wave number range from and to define the requested options/conditions for the calculations. A comparison is given in Fig2 between our calculation and the HITRAN2012
database

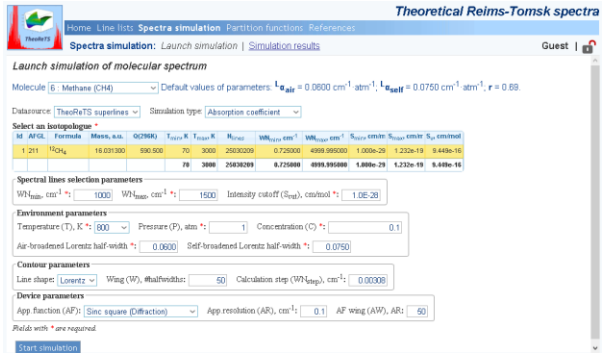


Fig1 : graphical user interface

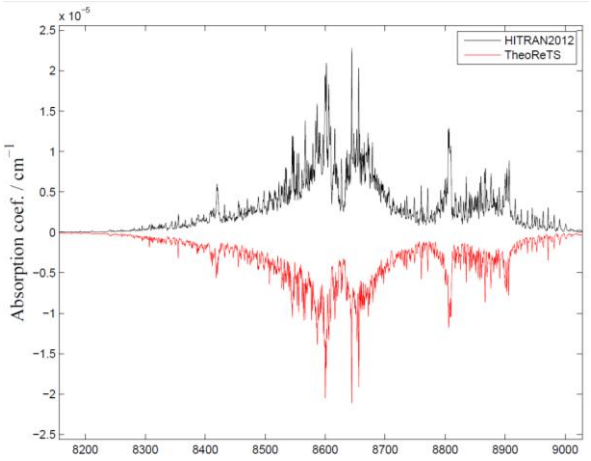


Fig2 : CH4 simulation at 296K

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## References

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