Photodissociation induced isotopic effects; theoretical calculations of UV absorption cross-sections and atmospheric model implementation.

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The study of light induced isotopic effects occurring in planetary atmospheres needs consider not only the isotopic effects on the light absorption properties of the molecule in question but also all possible light absorbing bodies that compete for the absorption of the same photons. The study of this sort of complex systems requires molecular data such as diffusion coefficients and reaction rate constants to calculate how physical and chemical change affects the modelled system. For the case of photochemical reactions, light absorption properties are required to estimate photo-dissociation rate constants and light conditions at different altitudes of a given atmosphere. We present the latest development of the Dianarm code which uses an R-Matrix expansion coupled to non-adiabatic transitions [1] in which the discreet absorption bands are calculated with their natural broadening in a Lorentz profile then Doppler and pressure broadening effects are computed separately and convoluted to the final absorption spectrum. This set of techniques allows us to produce absorption spectra suitable for different atmospheric conditions ranging low temperature-low pressure stratospheres to high temperature andhigh pressure systems such meddle atmospheres of hot Jupiters.

We also present our latest version of the KROME [2] model which implements a photochemical code with variable spectral resolution that allows to account for isotopic effects at different atmospheric conditions while optimizing the computational resources required for the calculation of photodissociation rate constants and light opacities.

[1] Danielache et al. (2014) J. Chem. Phys. 140, 044319.
[2] Grassi et al. (2014) Mon. Not. R. Astron. Soc.. 439 (3), 2181-2187.