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TITLE: Quantitatively probing water and its isotopomers: from theory to experiments; the contribution of a chemical and astrophysical European network 'Our Astrochemical History'

ABSTRACT BODY:

Abstract Body: In order to retrieve actual molecular abundances from astrophysical observations of molecular spectral lines, knowledge of the rotational levels excitation schemes is essential to go beyond Local Thermodynamical Equilibrium. These rates are almost always obtained from theoretical investigations, by computing classical or quantum dynamics of the interaction of molecules with these colliders (roueff2013).

Our laboratories have recently calculated a set of collision coefficients characterizing the efficiency of energy transfer between molecular hydrogen of helium and a large variety of interstellar molecules. One of the main goal has been water and its isotopomers, computing

rates for H₂O, HDO and D₂O in collision with H₂ (valiron2008,faure2012,daniel2011).

We felt it necessary to have a multidisciplinary approach: theoretical on the one hand, experimental on the second.

Indeed, excitation coefficient computation is a process involving many codes and approximations. Hence we compared our theoretical results to several experiments: spectroscopy of the H₂O-H₂ van der Waals complex (vanderavoird 2012), differential cross sections (yang 2010, 2011), pressure broadening (drouin 2012).

Thanks to these precise determinations, many water abundances could be quantitatively measured, like the HDO/H₂O ratio (coutens 2012).

While the excitation of water is by now well understood, much remains to be done for heavier molecules, paving the way to quantitative measures of complex organic molecules . A multi disciplinary approach is necessary, that keeps in mind the necessities of actual astrophysical observations. To do so, we describe the European COST network 'Our Astrochemical History' (<http://prague2015astrohistory.vscht.cz/>) , which brings together specialists of many areas of chemistry together with astronomy, in order to address this kind of problem. It focusses on the molecular evolution towards higher complexity and aim sat delivering new schemes for physical chemistry at large, like chemistry of transient species and photochemistry, in gas or on surfaces.

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