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EXOMOLHD: UPDATES ON PHOTODISSOCIATION OF SMALL MOLECULES.

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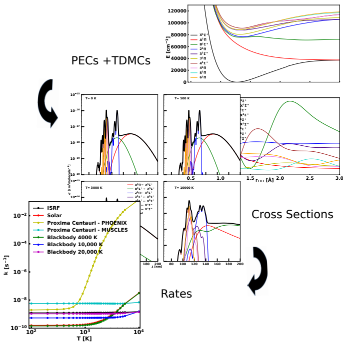

Photodissociation, the destruction of a molecule after absorbing one or more photons, is an important phenomenon to consider when studying the composition and dynamics of exoplanets' atmospheres, particularly in the presence of UV-rich stellar environments. The ExoMolHD project provides temperature-dependent photodissociation cross sections and rates for molecules found in these atmospheres as a necessary step for building a realistic model of planetary chemistry. The cross sections are calculated by solving the nuclear-motion Schrödinger equation as part of the ExoMol project using codes Duo, DVR3D, and Exocross[1], and EVEREST[2] using the methodology previously described[3]. Photodissociation rates are computed by integrating the cross section with model and real stellar field models representing different star types.

New tools and results for HF, HCl, and HCN are presented. Cross sections and rates for the diatomics are compared with previously available data[4], finding good agreement for the interstellar medium at low temperatures. Cross sections and rates exhibit a dramatic temperature dependence for temperatures above 1000 K. Our results for HCN are compared with the results obtained by previous works employing the time-dependent Schrödinger equation[5].

The new database structure and web interface are presented.

[1] Yurchenko et al *Comput Phys Commun* 2016 **202** 262; Tennyson et al *Comput Phys Commun* 2004 **163** 85; Yurchenko et al *A&A* 2018 **614** A131

[2] A. O. Mitrushchenkov *J. Chem. Phys.* 2012 **136** 024108

[3] Pezzella et al *Phys. Chem. Chem. Phys.* 2021 **23** 16390

[4] Heays et al *A&A* 2017 **602** A105

[5] Chenel et al *J. Chem. Phys.* 2016 **144** 144306; Aguado et al *Astrophys. J.* 2017 **838** 33

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