EXOMOLHD: RECENT PROGRESSES ON PHOTODISSOCIATION OF SMALL MOLECULES

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The destruction of hot molecules by photodissociation influences the composition and dynamics of exoplanets, particularly in the presence of a UV-rich stellar environments. We compute temperature-dependent photodissociation cross sections and rates for molecules found in these atmospheres, for building a more realistic model of the 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[a], using the methodology previously described[b]. Photodissociation rates are computed integrating the cross section with different stellar field models representing different star types.
New tools and results for HF, HCl and HCN. Cross sections and rates for the diatomics are compared with previously available data[c], finding a good agreement for the interstellar medium for low temperatures. Both cross sections and rates have 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[d].

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[a] Yurchenko *et al* Comput Phys Commun 2016 **202** 262–275; Tennyson *et al* Comput Phys Commun 2004 **163** 85-116; Yurchenko *et al* A&A 2018 **614** A131

[b] Pezzella *et al* Phys. Chem. Chem. Phys. 2021 **23** 16390–16400

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

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