https://doi.org/10.69646/aob241115

New molecular dataset for planet formation chemistry and modeling

Srećković, V.A.,[1] Pop, N.,[2] Vujčić, V.,[3] Dimitrijević, M.S.,[3] Christova, M.D.[4] and Mijić, Z.[1]

[1]Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade, Republic of Serbia
[2]Politehnica University of Timisoara, Timisoara, Romania
[3]Astronomical Observatory, Volgina 7, 11060 Belgrade 38, Serbia
[4]Department of Applied Physics, TU Sofia, Bulgaria
E-mail: vlada@ipb.ac.rs

Detailed astrochemical models are essential for interpreting observations of interstellar and circumstellar molecules because they allow important physical features of the gas and its evolutionary history to be derived (Williams and Cieza 2011). Advances in astrochemical models are linked to changes in astrochemical databases, as well as experimental and theoretical estimations of rate coefficients (see e.g. Öberg et al. 2021). The science community now need access to such molecular data, including preferred ones, for further modeling, and it is critical to our knowledge of the chemistry of planet formation. As a result, atomic and molecular datasets and databases (such as VAMDC) have become critical for constructing models and simulations (see Albert et al. 2021 and references therein). The analysis of the studied rates provides valuable information on the presence of species. As a result, it is critical to investigate not only radiative processes, but also concurrent processes involving molecular ions, such as dissociative recombination (Kamp et al., 2017). Our goal is to calculate, compare, and analyze cross sections and rate coefficients for molecular ions such as hydrogen and helium for a various model parameters.

Acknowledgments: This work was funded by the Institute of Physics Belgrade, University of Belgrade, through a grant by the Ministry of Science, Technological Development, and Innovations of the Republic of Serbia. We acknowledge the support the Science Fund of the Republic Serbia, Grant No. 3108/2021—NOVA2LIBS4fusion and COST Action CA22133 - The birth of solar systems (PLANETS).

References

Albert, D.; Antony, B.; Ba, Y.A.; Babikov, Y.L.; Bollard, P.; Boudon, V.; Delahaye, F.; Del Zanna, G.; Dimitrijević, M.S.; Drouin, B.J.; Dubernet, M.-L.;et al. A Decade with VAMDC: Results and Ambitions. Atoms 2020, 8, 76.

ALMA Partnership et al., 2015, ApJL, 808, L3

Kamp, I., Thi, W. F., Woitke, P., Rab, C., Bouma, S., & Menard, F. (2017). Consistent dust and gas models for protoplanetary disks-II. Chemical networks and rates. Astronomy & Astrophysics, 607, A41.

Öberg, K. I., Guzmán, V. V., Walsh, C., Aikawa, Y., Bergin, E. A., Law, C. J., ... & Zhang, K. (2021). Molecules with ALMA at Planet-forming Scales (MAPS). I. Program overview and highlights. The Astrophysical Journal Supplement Series, 257(1), 1.

Miyake, S., Gay, C. D., & Stancil, P. C. (2011). Rovibrationally resolved photodissociation of HeH+. The Astrophysical Journal, 735(1), 21.

Visser, R., Bruderer, S., Cazzoletti, P., Facchini, S., Heays, A. N., & van Dishoeck, E. F. (2018). Nitrogen isotope fractionation in protoplanetary disks. Astronomy & Astrophysics, 615, A75.

Walsh, C., Nomura, H., Millar, T. J., & Aikawa, Y. (2012). Chemical processes in protoplanetary disks. II. On the importance of photochemistry and X-ray ionization. The Astrophysical Journal, 747(2), 114.

Williams, Jonathan P., and Lucas A. Cieza. "Protoplanetary disks and their evolution." Annual Review of Astronomy and Astrophysics 49 (2011): 67-117.