Updates and New Sections of the CoLine Database

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Elevated temperatures and high fluxes of stellar radiation characteristic for exoplanet atmospheres lead to formation of molecules and molecular ions whose spectroscopic line-shape parameters are very poorly known or simply inexistent. Whereas extensive line lists of positions and intensities of isolated spectral transitions for "ordinary" atmospheric molecules are provided in several spectroscopic databases (e.g., HITRAN [1], GEISA [2], ExoMol [3], etc.), pressure-broadening line-shape parameters, identified as the most important need [4] for experimental and theoretical studies, remain practically unknown or completely missing.

This point has been addressed recently in the framework of the European-Research-Council-funded ExoMol-HD project via a new line-broadening section created in the ExoMol database [5]. Because of "exotic" molecules needed as optically active species and a wide range of required perturbers, we provided as a first step rotationally independent estimates of pressure line-broadening parameters with their temperature dependence for infrared/microwave transitions of 52 absorbers and 12 perturbers [6] with one-value "default values" included in the ExoMol and complete datasets collected in the specifically created for this purpose ColLine (Collisional Line broadening) database.

In the present work we consider the last updates and extensions of ColLine, focusing at robust theoretical approaches to calculations of rotationally-dependent line-shape parameters over wide temperature ranges. Such data will be essential for developing appropriate database structures, including opacities, k-tables and precomputed atmospheric models.

[1] I. E. Gordon et al., JQSRT 277, 107949 (2022)

[2] T. Delahaye et al., JMS 380, 111510 (2021)

[3] J. Tennyson et al., JQSRT 255, 107228 (2020)

[4] J.J. Fortney et al., arXiv:1905.07064 (2019)

[5] J. Tennyson et al., JQSRT 326, 109083 (2024)

[6] J. Buldyreva et al., ApJS 276, 23 (2025)