

ExoMol Extensions: ExoAtom and ExoPhoto — Spectroscopic Databases for Atomic and Molecular Photodissociation

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Recent advances in high-resolution spectroscopy and atmospheric modeling have created a growing demand for high-accuracy molecular and atomic data. Therefore, we developed two extensions to the ExoMol framework.

The first extension is ExoPhoto database (<https://exomol.com/data/data-types/photo/>) [1]. It extends the ExoMol database to provide high-accuracy, temperature-dependent photodissociation cross-section data at short ultraviolet wavelengths. ExoPhoto combines theoretical models from three computational databases (ExoMol, UGAMOP, and PhoMol) with experimental datasets from two research groups, covering a broad range of wavelengths and temperatures. Currently, ExoPhoto includes photodissociation data for 20 molecules: AlH, HCl, HF, MgH, OH, NaO, MgO, O₂, AlCl, AlF, CS, HeH⁺, CO, CO₂, H₂O, SO₂, C₂H₂, C₂H₄, H₂CO, and NH₃. It also provides detailed branching ratios and quantum yields for selected datasets. Data are organized in JSON-based files with a consistent naming convention, and cross sections are stored in .photo files for each molecule and temperature. Future developments will include additional photodissociation data and support for non-local thermodynamic equilibrium (non-LTE) conditions.

The second extension is ExoAtom database (<https://exomol.com/data/data-types/atom/>) [2]. It extends the ExoMol database by providing atomic line lists in the ExoMol format, derived from NIST and Kurucz databases. ExoAtom uses five main file types: 'all', 'def', 'states', 'trans', and 'pf'. The 'states' file lists energy levels with quantum numbers, uncertainties, and lifetimes; the 'trans' file records transition wavenumbers and Einstein A coefficients; the 'pf' file supplies partition functions over various temperatures. Future work will expand ExoAtom to include additional ionization stages.

[1] (*submitted*) Ni QH, Hill C, Yurchenko SN, Pezzella M, Fateev A, Qin Z, Venot O, Tennyson J. ExoPhoto: A database of temperature dependent photodissociation cross sections. RAS Techniques & Instruments (2025)

[2] (*preparation*) Ni QH, Wang R, Xie T, Zhang J, Hill C, Yurchenko S N, Tennyson J. ExoAtom: A Database of Atomic Spectra in ExoMol Format. RAS Techniques & Instruments (2025)