DUO: A GENERAL MULTI-STATE PROGRAM FOR SOLVING THE NUCLEAR MOTION SCHRÖDINGER EQUATION FOR DIATOMIC MOLECULES WITH ARBITRARY COUPLINGS

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DUO is a general, user-friendly program for computing rotational, rovibrational and rovibronic spectra of diatomic molecules.[1] DUO solves the Schrödinger equation for the general case of an arbitrary number and type of couplings between electronic states (typical for open-shell diatomics and excited states). Possible couplings include spin-orbit, angular momenta, spin-rotational and spin-spin.

DUO requires user-specified potential energy curves and, if relevant, dipole moment, coupling and correction curves. From these it computes energy levels, line positions and line intensities. DUO can refine potential energy and coupling curves to best reproduce reference data such as experimental energy levels or line positions. DUO is provided as a free-access Fortran 2003 program.[2] DUO has been used for many studies of diatomics including AlH, AlO, AlCl, C_2, CaH, CaO, HF, HCl, MgH, MgO, NaO, NO, NS, PO, PS, SH, SiN, SiH, SiO, SO, TiO, VO, as part of the ExoMol project.[3] In this presentation, we report recent DUO updates, including implementations of

- Non-adiabatic couplings;
- Hyperfine effects, such as hyperfine resolved spectra and refinement;
- Reduced radial density analysis;
- Treatment of continuum states;
- Pre-dissociation effects;
- Quadrupole and magnetic spectra;
- Photo-absorption cross-sections.

[1] S.N. Yurchenko, L. Lodi, J. Tennyson, and A.V. Stolyarov, Duo: A general program for calculating spectra of diatomic molecules, *Comput. Phys. Commun.*, **202**, 262 (2016)

[2] https://github.com/exomol/Duo/

[3] J. Tennyson and S.N. Yurchenko, ExoMol at 10, *Astron. Geophys.*, **62**, 6 (2021)

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