

COMPUTING SPECTRA OF OPEN-SHELL DIATOMIC MOLECULES WITH DUO

SERGEI N. YURCHENKO, *Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom*; JONATHAN TENNYSON, JAMES R. ASHFORD, HENG YING LI, ELIZAVETA PYATENKO, *Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom*; MAIRE N. GORMAN, *Department of Physics, Aberystwyth University, Aberystwyth, UK*.

DUO is a program designed to solve a coupled Schrödinger equation for the motion of nuclei of a given diatomic molecule characterized by an arbitrary set of electronic states.^a DUO is capable of both refining potential energy curves (by fitting data to experimental energies or transition frequencies) and producing line lists. Our most recent results of applying DUO to produce hot line lists for open-shell diatomic molecules include NO,^b SiH,^c PS and PO,^d C₂,^e SN and SH,^f and AlH.^g The published version of DUO only considers truly bound states. We are now working on extending DUO to treat quasi-bound or resonance states, or indeed the continuum itself, using the stabilization method.^h As an illustration, we present simulations of spectra of the quasi-bound system A ¹Π – X ¹Σ⁺ of AlH and of the continuum system A ¹Π – X ¹Σ⁺ and B ¹Σ⁺ – X ¹Σ⁺ of NaCl.

^aS.N. Yurchenko, L. Lodi, J. Tennyson, and A.V. Stolyarov, *Comput. Phys. Commun.* **202**, 262 (2016).

^bA. Wong, S. N. Yurchenko, P. Bernath, H. S. P. Mueller, S. McConkey, and J. Tennyson, *Mon. Not. R. Astron. Soc.* **470**, 882 (2017).

^cS. N. Yurchenko, F. Sinden, L. Lodi, C. Hill, M. N. Gorman, and J. Tennyson, *Mon. Not. R. Astron. Soc.* **473**, 5324 (2018)

^dL. Prajapat, P. Jagoda, L. Lodi, M. N. Gorman, S. N. Yurchenko, and J. Tennyson, *Mon. Not. R. Astron. Soc.* **472**, 3648 (2017).

^eS. N. Yurchenko, J. Tennyson, and et al, *Mon. Not. R. Astron. Soc.* in preparation (2018).

^fS. N. Yurchenko, W. Bond, M. N. Gorman, L. Lodi, L. K. McKemmish, W. Nunn, R. Shah, and J. Tennyson, *Mon. Not. R. Astron. Soc.* submitted (2018)

^gH. Williams, P. C. Leyland, L. Lodi, S. N. Yurchenko, and J. Tennyson, *Mon. Not. R. Astron. Soc.* in preparation (2018).

^hA.U. Hazi, H.S. Taylor, *Phys. Rev. A* **1**, 1109 (1970)