DVR3DUV: A SUITE FOR HIGH ACCURACY CALCULATIONS OF RO-VIBRONIC SPECTRA OF TRIATOMIC MOLECUlES

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We present a computer code (DVR3DUV) for calculations of high-accuracy ro-vibronic spectra of triatomic molecules. The current implementation is an extension to the DVR3D suite [1], which operates with the exact kinetic energy operator, a single potential energy surface and a single dipole moment surface (ro-vibrational transitions only). The main function of the new code is calculation of transition intensities between different electronic states in the rotational-vibrational resolution. As a case study, two electronic states of SO_2 molecule are considered. Ro-vibrational wavefunctions and energy levels for the ground $\tilde{X}^1A_1$ state of SO_2 are calculated using Ames PES [2], while energy levels and wavefunctions of the $\tilde{C}^1B_2$ state are calculated using *ab initio* PES (MRCI-F12-AVTZ). Transition intensities are computed using a) Franck-Condon approximation; b) *ab initio* dipole moment surface between the two electronic states. Results are compared to the latest theoretical and experimental works. Future applications of the DVR3DUV code will focus on highly accurate electronic spectra for atmospherically important species, such as ozone molecule.

[1] J. Tennyson, M A. Kostin, P. Barletta, G. J. Harris, O L. Polyansky, J. Ramanlal, N. F. Zobov, Computer Physics Communications 163 (2004) 85–116.

[2] X. Huang, D. W. Schwenke, T. J. Lee, J Chem Phys. 2014 ;140(11):11431