PARTRIDGE-SCHWENKE ROVIBRATIONAL ENERGY LEVELS FOR WATER: SPECTROSCOPIC ASSIGNMENT AND COMPARISON WITH EXPERIMENTAL ENERGY LEVELS

SERGEI A. TASHKUN, TATIANA A. PUTILOVA and SEMEN MIKHAILENKO, *Laboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics, 1, Akademicheskii Av., 634055 Tomsk, Russia*.

Unambiguous rovibrational spectroscopic assignment (v_1, v_2, v_3, J, K_a, K_c) up to J,K_a=30 of PS energy levels for the (000), (010), (100), (020) and (001) vibrational states of nine isotopic species ($H_2{}^{16}O$, $H_2{}^{18}O$, $H_2{}^{17}O$, $HD^{16}O$, $HD^{18}O$, $HD^{17}O$, $D_2{}^{16}O$, $D_2{}^{18}O$, $D_2{}^{17}O$) of the water molecule will be presented. PS levels were calculated with the help of an accurate isotope dependent potential energy surface by Partridge and Schwenke[a] and a large basis set. PS levels will be compared with experimental levels collected from the literature. Differences between PS and BT2[b] calculated levels for the $H_2{}^{16}O$ isotopic species will be also given and discussed.

[a]H. Partridge and D.W. Schwenke, *J. Chem. Phys.* 106(11), 4618-4639 (1997)
[b]R.J. Barber J. Tennyson, G.J. Harris and R.N. Tolchenov, *Mon. Not. R. Astron.* 368, 1087-1094 (2006)