ASSIGNMENT OF HOT WATER SPECTRA

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The oxyacetylene flame emission spectrum in the region 500 – 2000 cm^{-1} was analyzed using variational calculation linelist based on spectroscopically determined potential [1]. The spectrum was recorded in 2002 in Brussels with estimated temperature of the flame 3000 K, about the same as of sunspot spectrum in 770 – 1010 cm^{-1} region [2]. The flame spectrum is about 5 times less dense than the sunspot spectrum making it easier to assign. The assigned lines contains mostly pure rotational transitions in 10 lower lying vibrational states (frequencies up to about 1000 cm^{-1}) and transitions with ν_2 vibrational quantum number changing from n to n+1.

The first step in spectrum analysis was trivial assignment using experimentally determined energy levels [3]. The extensive previous work with hot water spectra allowed us to assign trivially about 70 % of 10500 experimental lines in the studied region. Further analysis lead to determining of about 600 new energy levels in the ground and bending vibrational states up to (080). The hot ν_2 bands (070) – (060) and (080) – (070) were assigned for the first time, leading to estimated values for band origins as 10086.7(1) cm^{-1} and 11253.9(2) cm^{-1}. In the ground vibrational state the maximum J number of the known energy level was raised from 35 to 42. Candidate transitions were confirmed, were possible, by presence of the appropriate combination difference transitions. Quite a lot of transitions involving levels with high J and K_a values were assigned by direct comparison with theoretical predictions as there was only one strong pure rotational transition with the level.

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[3]. J. Tennyson, N.F. Zobov, R. Williamson, O.L. Polyansky and P.F. Bernath, J. Phys. Chem. Ref. Data, 30, 735-831 (2001).