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Relaxation of vibrational levels H_2O (002, 101, 200): effect of new rate constants on the H_2O vibrational level populations and ro-vibrational spectra in the mesosphere and lower thermosphere

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In this work, we investigate the sensitivity of the H_2O vibrational level populations and ro-vibrational spectra in the mesosphere and lower thermosphere (MLT) to new values of rate constants for the collision-induced transitions from the upper vibrational levels of H_2O molecule. This study contributes to the development of the H_2O non-equilibrium radiation model used for water vapor altitude distribution retrieval from the MLT radiation measurements.

Our model accounts for 13 excited vibrational states up to energies 7445 cm $^{-1}$ (the upper levels are 002, 101, 200) [Feofilov et al., 2009]. The model takes into account 54 vibrational-translational (V-T) and vibrational-vibrational (V-V) energy exchange processes at collisions of H_2O with N_2 , O_2 and O. The 32 ro-vibrational transitions forming 1.4, 1.9, 2.7, 3.2, 4.7 and 6.3 μ m water vapor radiation bands are considered.

Currently, the rate constants of intermolecular transitions between vibrational levels at collisions with N_2 and O_2 are known only for the transitions (010-000) and (001,100-020). In our model of H_2O vibrational level kinetics [Feofilov et al., 2009], we assumed that for all collisional transitions, at which the bending mode quantum number, v_2 , increases by 2:

 $H_2O(v1,v2,v3) + M = H_2O(v1-1,v2+2,v3) + M$ $H_2O(v1,v2,v3) + M = H_2O(v1,v2+2,v3-1) + M (1)$

the rate constants are equal to that of the process $H_2O(001, 100) + M = H_2O(020) + M$.

Based on the analysis of currently available experimental and theoretical data, we have updated k, the rate constant of transitions (002, 101) \rightarrow 021 and (101, 200) \rightarrow 120, and estimated the effect of a new rate on the H₂O vibrational levels populations and limb radiation spectra. The "upper limit" of the effect was estimated using the same rate constant k for all processes of type (1), excluding process (001, 100) \rightarrow 020.

The H_2O vibrational levels populations and limb radiation spectra were calculated using the ALI-ARMS non-LTE code [Kutepov et al. 1998; Feofilov and Kutepov, 2012] for characteristic atmospheric conditions and compared with the populations and spectra obtained for "regular" rate constants used in [Feofilov et al., 2009].

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