Water dimer millimeter wave spectrum at atmospheric conditions: simple model for practical purposes

T. A. Odintsova[a], M. Yu. Tretyakov[a], and C. Leforestier[b]

[a] Institute of Applied Physics, Russian Academy of Sciences, 46 Ulyanova str. 603950, Nizhniy Novgorod, Russia, Tel.: +7(831)4164866, E-mail: odintsova@appl.sci-nnov.ru
[b] Institut Charles Gerhardt, CC 1501, Universite Montpellier II-CNRS, 34095 Montpellier, Cedex 05, France, Tel.: +33467143339, E-mail: Claude.Leforestier@univ-montp2.fr

Recent observation of the rotationally resolved millimeter wave spectrum of water dimer recorded in equilibrium water vapor at room temperature [1] unequivocally proved previous hypotheses that this exotic molecule is responsible for an essential fraction of the excess atmospheric absorption called the continuum. Usual spectroscopic approach is not suitable for extracting quantitative information about the dimer from experimental observations because of extreme complexity of its spectrum at atmospheric temperatures. In this work we report the model of the dimer millimeter-wave spectrum expressed by simple analytical functions, which can be easy fitted to observed spectra. The model employs i) general peculiarities of the dimer spectrum and its temperature dependence from the most accurate to date quantum chemistry calculations [2] and ii) results of experimental measurements of dimer rotational lines in a cold supersonic molecular beam [3]. Correspondence of the model to experimental recordings of water dimer spectra at atmospherically relevant temperatures is presented. Possibility of direct observation of the dimer rotational features in the atmosphere by remote sensing instruments is discussed on the basis of the model predictions. We believe that the model will permit to retrieve the dimer equilibrium constant and its temperature dependence from experimental recordings of the dimer spectrum in pure water vapor as well as in its mixtures with major atmospheric gases.

The work was partly supported by Russian Foundation for Basic Research.

[1] M. Yu. Tretyakov, E. A. Serov, M. A. Koshelev, V. V. Parshin, A. F. Krupnov, *Phys. Rev. Lett.* **2013**, *110*, 93001.
[2] Y. Scribano, C. Leforestier, *J. Chem. Phys* **2007**, *126*, 234301.
[3] G. T. Fraser, R.D. Suenram, L. H. Coudert, *J. Chem. Phys.* **1989**, *90(11)*, 6077-85.