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The water vapor self-continuum in the "terahertz gap" region (15-700 cm⁻¹): Experiment versus MT_CKD-3.5 model.

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Key words: Atmospheric continuum; THz gap; water vapor, MT_CKD model

Recently reviewed results of studies on the water vapor related continuum in the range of "terahertz gap" are compared with the current version of the MT_CKD model (v.3.5) instead of version 3.2, which was outdated at the time of submission. The MT_CKD-3.5 model reproduces the available experimental data in the range of 3.5-700 cm⁻¹ much better than its previous versions.

Recently published review of experimental studies of atmospheric continuum in the region 15–700 cm⁻¹ [1], hereafter referred to as Paper I, includes a comparison of experimental data on water vapor self-continuum cross-section (Fig. 1), its temperature exponent (Fig. 3), and spectral function (Fig. 4) with version 3.2 of the semi-empirical water continuum model MT_CKD [2]. It is the only model covering the entire infrared frequency range (0-20000 cm⁻¹), and it is most widely used for atmospheric applications, including radiative transfer and climate models. After the publication of Paper I one of the model developers, Dr. Eli Mlawer, noted that authors of the aforementioned review compare experimental data with an outdated (at the time of submission) version of the MT_CKD model, which may mislead readers and discredit the model quality. To avoid this, we present in the current note the comparison of experimental data with latest version of the MT_CKD model (v.3.5), which is presently relevant. Indeed, version 3.5 was released before the publication of Paper I and took into account the experimental data considered in Paper I. The updated MT_CKD-3.5 model is presented instead of v.3.2 in the renewed figures below.

The MT_CKD-3.5 model was updated [3] considering laboratory experimental data on the continuum cross-section and its temperature dependence in the range of the pure rotational band of the water molecule (3.5-1100 cm⁻¹) from our studies [4] (in the range of 70-700 cm⁻¹), as well as from [5] (4.7-14.7 cm⁻¹), [6] (3.5-5 cm⁻¹), [7] (700-1100 cm⁻¹), and [8] (333-633 cm⁻¹). The MT_CKD-3.5 model reproduces the available experimental data [4-18] much better than its previous versions. At room temperature (296 K), the model on average follows experimental data almost in the whole range of the pure rotational band of the water molecule except for the range of 20-50 cm⁻¹, where the spectral feature related to rotational band of the stable dimer is observed (Figs. 1 and 3). The model smoothes the feature out. Figure 1 also demonstrates that

the variation of the continuum value due to the "pedestal" below the resonance lines (which is originated from the procedure of cutting off the line wings and attributed to the continuum in the MT_CKD, but is preserved to the resonance absorption in our studies) is smaller than the spread of experimental points. The temperature exponent of the MT_CKD-3.5 model was determined similarly to [1,4], particularly, on the basis of Eq. (5) of [4] and continuum cross-sections calculated using version 3.5 (instead of 3.2 used in [1,4]) at 296 K and 326 K. Obtained temperature exponent demonstrates good qualitative agreement with experimental data [4,5,7,11-13,15,16], however, a slight overestimation is still notable (Fig. 2).

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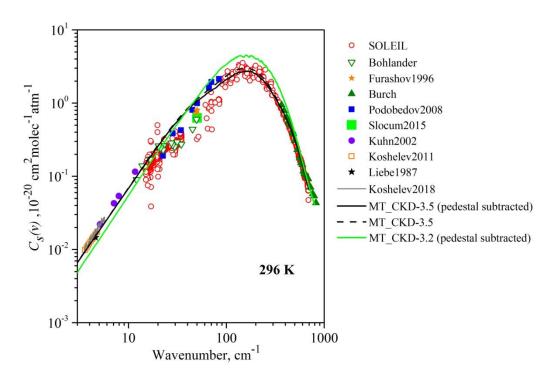


Fig. 1 (analogue of Fig.1 of Paper I). Self-continuum at 296 K: red circles (SOLEIL measurements) [4,9,10], green triangles [7,11], blue squares [12], black star [13], green empty triangles (measurements of R.A. Bohlander) [7], light green square [14], violet circles [15], orange empty squares [16], orange star [17], grey curve [18], green curve (MT_CKD-3.2 model) [2], and dashed and solid black curves are the MT_CKD-3.5 model [2] with and without "the pedestal" (see the text for details), respectively.

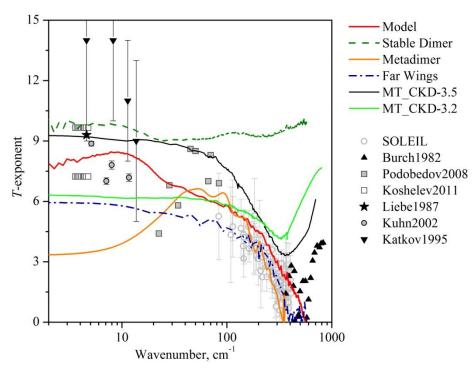


Fig. 2 (analogue of Fig.3 of Paper I). Self-continuum temperature exponent: grey empty circles (SOLEIL measurements) [4], black triangles [7, 11], grey squares [12], black star:[13], grey empty squares [16], black circles [15], black inverted triangles [5], red solid curve (continuum model obtained as a sum of true bound metastable dimers, and far-wings contributions simulated by in [1]), green dash curve (stable dimer) [19], orange solid curve (metastable dimer model), blue dash-dot curve (far wings model), green curve (MT_CKD-3.2 model) [2], and black solid curve (MT_CKD-3.5 model) [2].

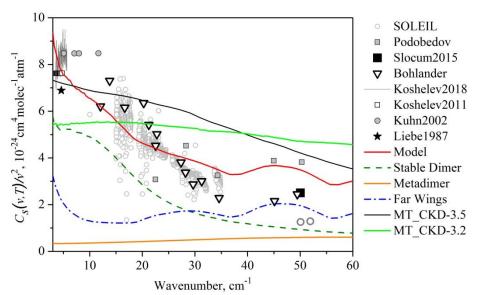


Fig. 3 (analogue of Fig.4 of Paper I). Continuum spectral function: grey empty circles(SOLEIL measurements) [9, 10], black empty triangles [11], grey squares [12], grey curve [18], grey empty squares [16], grey filled circles [15], grey star [17], green dash curve (stable dimer model), orange solid curve (metastable dimer model), blue dash-dot curve (far wings), red solid curve (continuum model obtained as a sum of true bound metastable dimers, and far-wings contributions simulated by in [1]), green curve (MT_CKD-3.2 model) [2], and black thin curve (MT_CKD-3.5 model).

- [1] T.A. Odintsova, A.O. Koroleva, A.A. Simonova, A. Campargue, M.Yu. Tretyakov, The atmospheric continuum in the "terahertz gap" region (15–700 cm⁻¹): Review of experiments at SOLEIL synchrotron and modeling, J. Mol. Spectrosc. 386 (2022) 111603.
- [2] E. J. Mlawer, V. H. Payne, J. L. Moncet, J. S. Delamere, M. J. Alvarado, D. C. Tobin, Development and recent evaluation of the MT CKD model of continuum absorption, Philos. Trans. R. Soc. A Math. Phys. Eng. Sci. 370 (2012) 2520–2556.
- [3] https://github.com/AER-RC/MT_CKD/wiki/What's-New
- [4] T. A. Odintsova, M. Yu. Tretyakov, A. A. Simonova, I. V. Ptashnik, O. Pirali, A. Campargue, Measurement and temperature dependence of the water vapor self-continuum between 70 and 700 cm⁻¹, J. Mol. Structure. 1210 (2020) 128046.
- [5] V. Yu. Katkov, B. A. Sverdlov, N. I. Furashov, Experimental estimates of the value and temperature dependence of the air-humidity quadratic component of the atmospheric water-vapor absorption coefficient in the frequency band of 140-410 GHz, Radiophys. Quantum Electron. 38(12) (1995) 835–844.
- [6] M.Yu. Tretyakov, Spectroscopy underlying microwave remote sensing of atmospheric water vapor, J. Mol. Spectrosc. 328 (2016) 7–26.
- [7] D. E. Burch, R. L. Alt, Continuum absorption by H_2O in the 700-1200 cm⁻¹ and 2400-2800 cm⁻¹ windows, US Air Force Geophysics Laboratory report AFGL-TR-84–0128, Hanscom Air Force Base, MA, USA(1984)
- [8] D.E. Burch, D.A. Gryvnak, Method of calculating H2O transmission between 333 and 633 cm⁻¹, 1979.
- [9] T. A. Odintsova, M. Yu. Tretyakov, O. Pirali, P. Roy, Water vapor continuum in the range of rotational spectrum of H₂O molecule: new experimental data and their comparative analysis, J. Quant. Spectrosc. Rad. Transf. 187 (2017) 116–123.
- [10] T.A. Odintsova, M.Yu. Tretyakov, A.O. Zibarova, O.Pirali, P. Roy, A. Campargue, Farinfrared self-continuum absorption of $\rm H_2^{16}O$ and $\rm H_2^{18}O$ (15–500 cm⁻¹), J. Quant. Spectrosc. Rad. Transf. 227 (2019) 190–200.
- [11] D. Burch, Continuum absorption by atmospheric H₂O, Proc. SPIE.277 (1981) 28–39.
- [12] V. B. Podobedov, D.F. Plusquellic, K. E. Siegrist, G.T. Fraser, Q. Ma, R. H. Tipping, New measurements of the water vapor continuum in the region from 0.3 to 2.7 THz, J. Quant. Spectrosc. Radiat. Transf. 109 (2008) 458–467.
- [13] H.J. Liebe, D.H. Layton, Millimeter-wave properties of the atmosphere: Laboratory studies and propagation modeling, NTIA Rep. (1987) 87–224.

- [14] D. Slocum, R. Giles, T. Goyette, High-resolution water vapor spectrum and line shape analysis in the Terahertz region, J. Quant. Spectrosc. Radiat. Transf. 159 (2015) 69–79.
- [15] T. Kuhn, A. Bauer, M. Godon, S. Buehler, K. Kuenzi, Water vapor continuum: absorption measurements at 350 GHzand model calculations, J. Quant. Spectrosc. Radiat. Transf. 74 (2002) 545–562.
- [16] M.A. Koshelev, E.A. Serov, V.V. Parshin, M.Yu. Tretyakov, Millimeter wave continuum absorption in moist nitrogen at temperatures 261–328 K, J. Quant. Spectr. Radiat. Transf. 112 (2011) 2704–2712.
- [17] N.I. Furashov, B. A. Sverdlov, S.N. Chernyaev, Absorption of electromagnetic radiation by pure water vapor at frequencies near1.5 THz, Radiophysics and Quantum electronics. 39(9) (1996) 754-9.
- [18] M.A. Koshelev, I.I. Leonov, E.A. Serov, A.I. Chernova, A.A. Balashov, G.M. Bubnov, A.F. Andriyanov, A.P. Shkaev, V.V. Parshin, A.F. Krupnov, M.Yu. Tretyakov, New Frontiers of Modern Resonator Spectroscopy, IEEE Trans. on Terahertz Sci. Technol. 8(6) (2018) 773–783.
- [19] Y. Scribano, C. Leforestier, Contribution of water dimer absorption to the millimeter and far infrared atmospheric water continuum, J. Chem. Phys. 126 (2007) 234301.