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WATER DIMER DETECTION AT ATMOSPHERIC CONDITIONS

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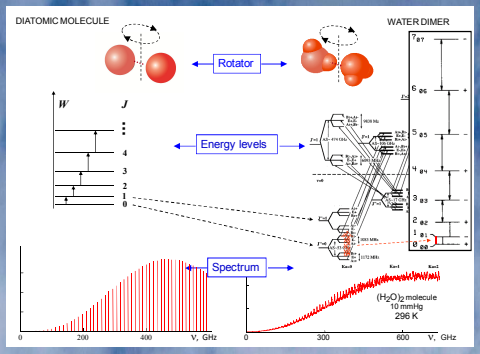
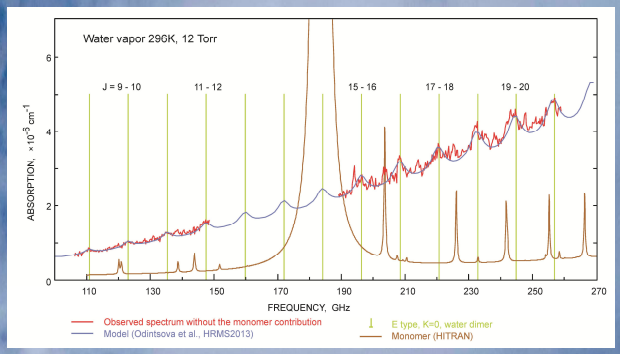
The water dimer, a spectroscopic challenge

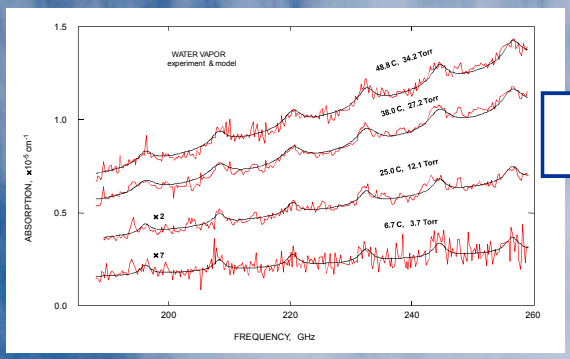
«The nature and importance of water collisional and dimer effects in the atmosphere have been the subject of a great deal of recent interest and controversy ».

A.R.W. McKellar

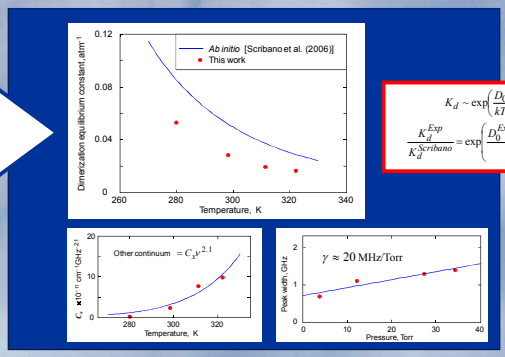




Pure water vapor



Model fitting

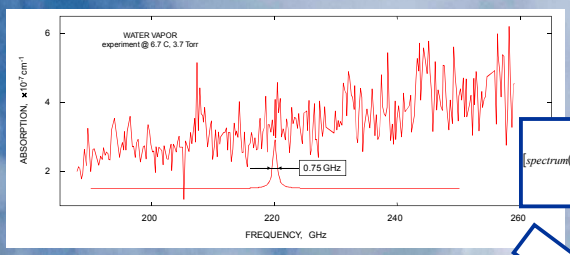


$$K_d \sim \exp\left(\frac{D_0}{kT}\right)$$

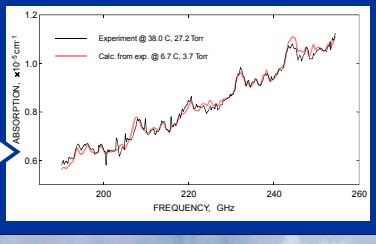
$$\frac{K_d^{Exp}}{K_d^{Scribano}} = \exp\left(\frac{D_0^{Exp} - D_0^{Scribano}}{kT}\right)$$

Dissociation energy D_0, cm^{-1}

This work	1115(25)
Scribano et al. JPC **110** 2006 (*ab initio*)	1230
Shank et al. JCP **130** 2009 (*ab initio*)	1103(4)
Leforestier et al. JCP **137** 2012 (*ab initio*)	1108.2
Rocher-Casterline et al. JCP **134** 2011 (experiment)	1105(10)



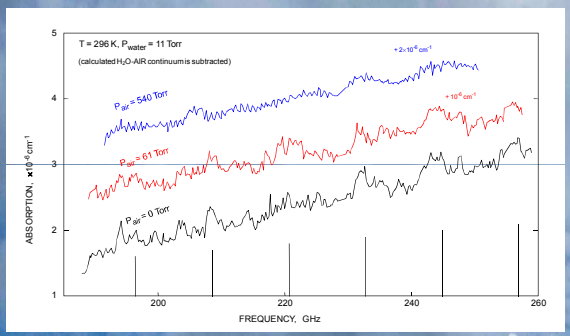
$$[spectrum(P_0,T_0)\otimes Lorentz(C_1)]\times C_2\left(\frac{P_1}{P_0}\right)^2\left(\frac{T_0}{T_1}\right)^{10.15}+C_3\nu^2$$



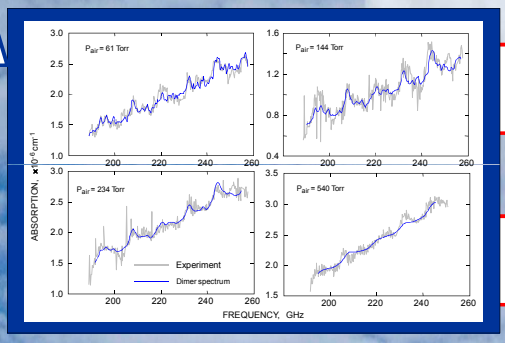
H_2O pressure broadening

$$\gamma_{H_2O} \sim 16 \pm 5 \text{ MHz/Torr}$$

Water vapor with air



Reference spectrum



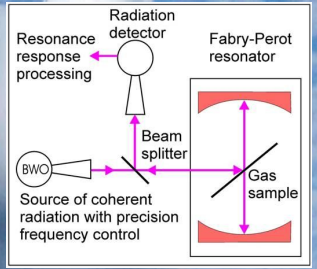
Dimerization constant

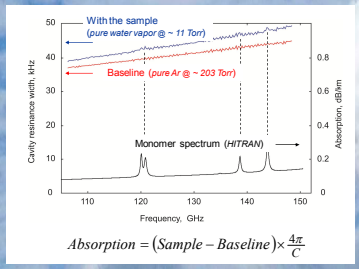
$$\frac{K_d^{air}}{K_d^{H_2O}} \approx 0.8 \pm 0.2$$

Air pressure broadening

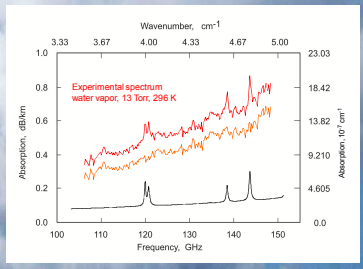
$$\gamma_{air} \sim 4 \pm 0.5 \text{ MHz/Torr}$$

Details of the measurement method





$$Absorption = (Sample - Baseline)\times\frac{4\pi}{C}$$



Related references

1. M.Yu. Tretyakov, E.A. Serov, M.A. Koshelev, V.V. Parshin, A.F. Krupnov, Observation of the rotationally resolved spectrum of the water dimer at room temperature, *Phys. Rev. Letters,* **110**, 093001 (2013).
2. M.Yu. Tretyakov, A.F. Krupnov, M.A. Koshelev, D.S. Makarov, E.A. Serov and V.V. Parshin, Resonator spectrometer for precise broadband investigations of atmospheric absorption in discrete lines and water vapor related continuum in millimeter wave range, *Review of Scientific Instruments*, **80(9)** 093106 (2009).
3. A.F. Krupnov, M.Yu. Tretyakov, C. Leforestier, Possibilities of observation of discrete spectrum of water dimer at equilibrium in millimeter-wave band, *J. Quant. Spectr. Radiat. Transf.*, **110** 427–434 (2009).