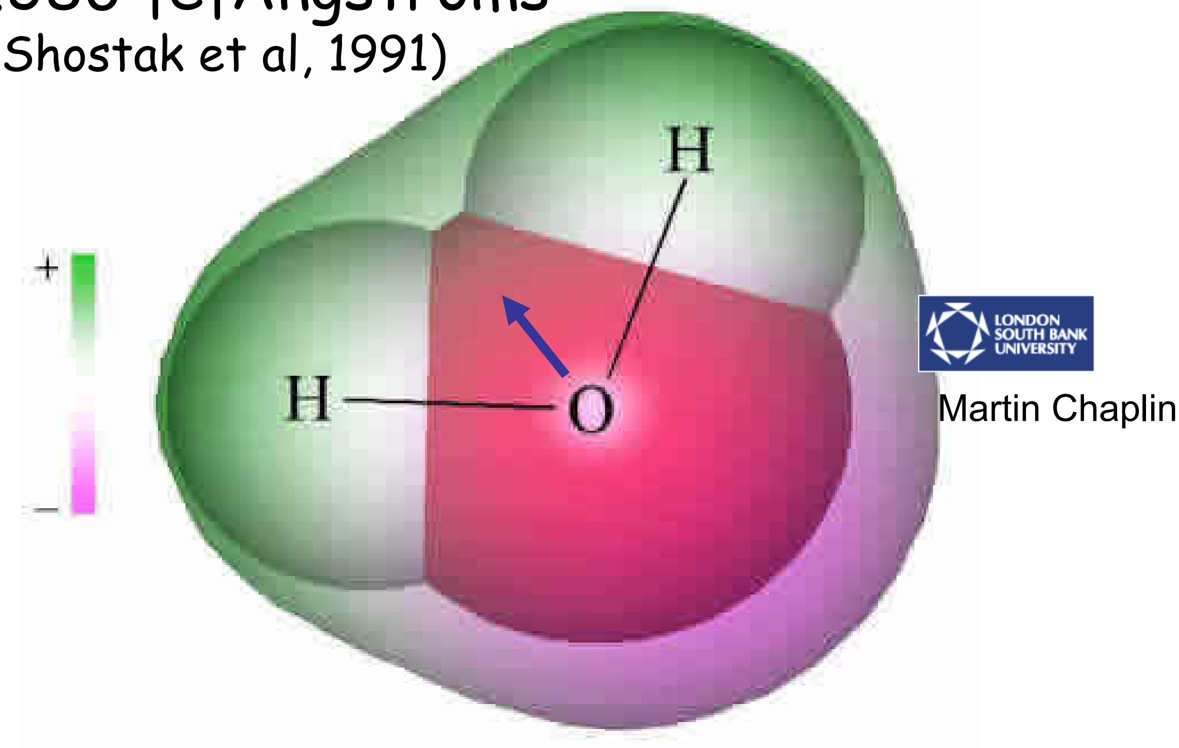
H_2O, Vapor phase dipole moment

μ=1.8550 Debyes

=0.386 |e|Angstroms

(Shostak et al, 1991)



The total molecular dipole moment for liquid water

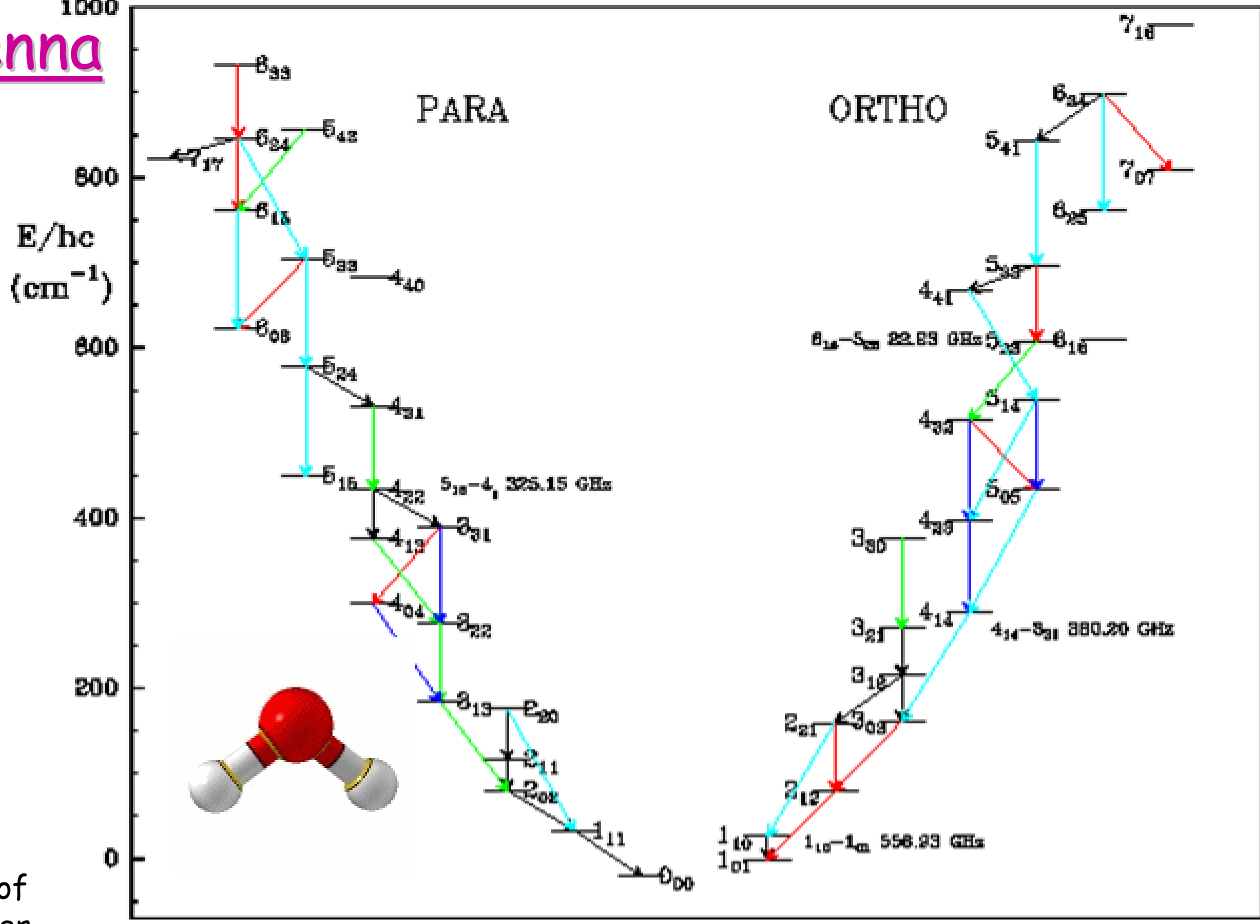
A. V. Gubskaya and P. G. Kusalik J. Chem. Phys. **117**, 5290 (2002).

"An almost 10% variation in the dipole moment with temperature is observed over the range 273 to 373 K. The value obtained for the molecular dipole moment at 300 K, **2.95±0.2 D**, is in excellent agreement with a recently reported result extracted from x-ray scattering data… ."

H_2O – a quantum antenna

Proceedings of the "IRAM Millimeter Interferometry Summer School," S. Guilloteau, Institut de Radio Astronomie Millimétrique, Saint Martin d'Hères, FRANCE

This book is dedicated to the memory of Bernard AUBEUF
Francis GILLET
Henri GONTARD
Roland PRAYER
Patrick VIBERT
and of the other 15 persons who died on 1st of July, 1999, in the tragic accident of the cable car to the IRAM interferometer site on Plateau de Bure.

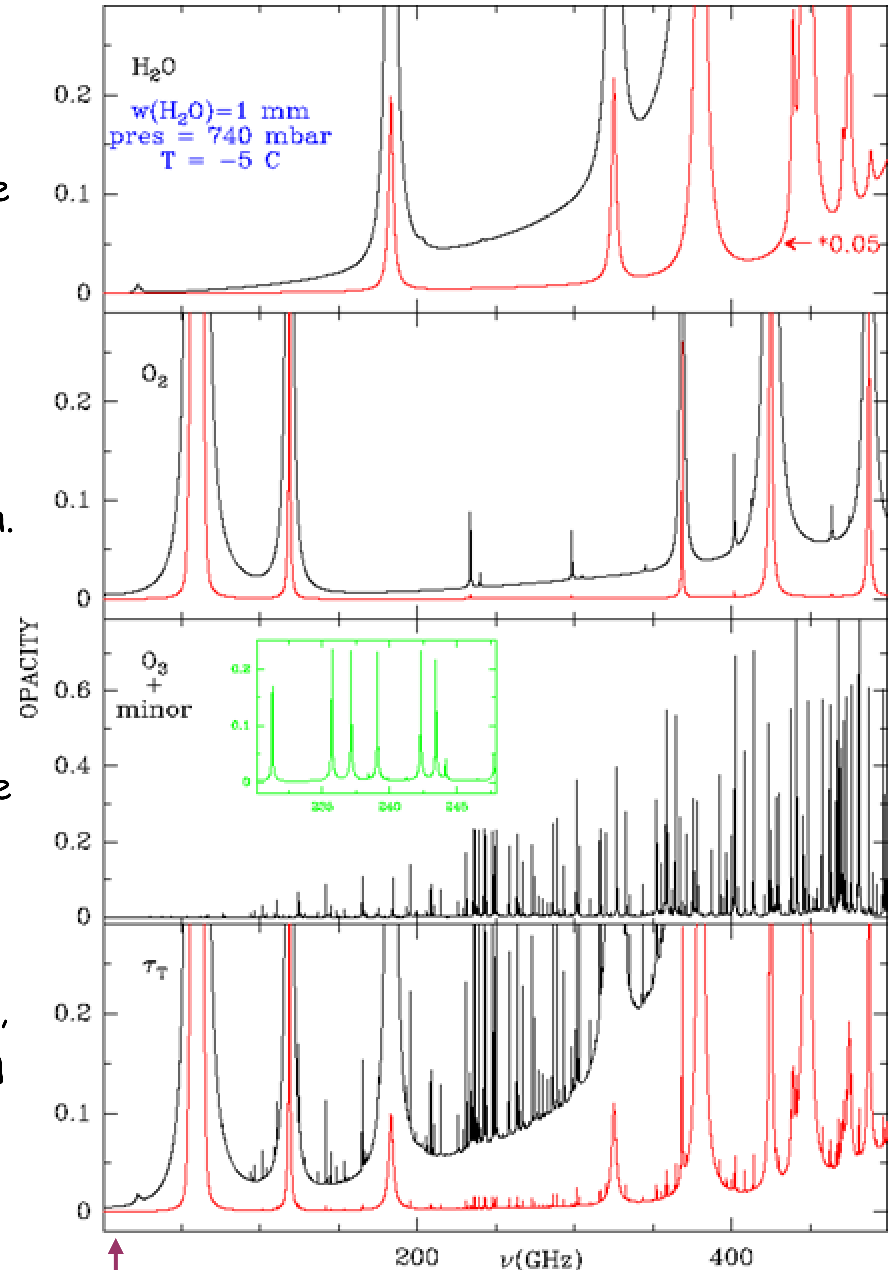


The rotational energy level diagram of water. Each level is denoted by three numbers (J,K-1,K+1). J, which is a ``good'' quantum number, represents the total angular momentum of the molecule; K-1 and K+1 stand for the rotational angular momenta around the axis of least and greatest inertia. The levels with K-1 and K+1 of the same parity are called para levels, those of opposite parity, ortho levels. Transitions between ortho and para levels are forbidden. The **arrows show the transitions which will be observed by the satellite FIRST**.

Zenith opacity of the **standard winter atmosphere** at an altitude of 2.5 km for 1 mm of precipitable water vapor, as a function of frequency (GHz). The contributions of H_2O, O_2 and O_3 are shown in the three upper panels. The red line shows the same zenith opacity at a scale of 1/20. One may note the importance of the water line wings above 150 GHz, compared to those of O_2 (a consequence of the absence of electric dipole moment in the latter molecule) and O_3. Courtesy [Cernicharo & Pardo 1999]

Some of the results for the band 20-500 GHz are shown. One recognizes from left to right, the (blended) forest of fine structure transitions from O_2, near 60 GHz, the 1,1 ← 0,1 fine structure line of O_2 at 118.75 GHz, the third lowest lines of para water (still 200 K above the ground level), at 183.31 GHz, and the fourth ortho water line (420 K above ortho ground level), at 325.15 GHz. The fundamental line of ortho water ($1_{10} \leftarrow 1_{01}$), at 556.94 GHz is visible.

The water and oxygen lines delineate the 4 atmospheric ``windows'' of the millimetre spectrum (called the 3 mm, 2 mm, 1.3 mm and 0.8 mm windows). **Water is seen to dominate completely atmospheric absorption above 150 GHz.**



Microwave oven 2.45 GHz

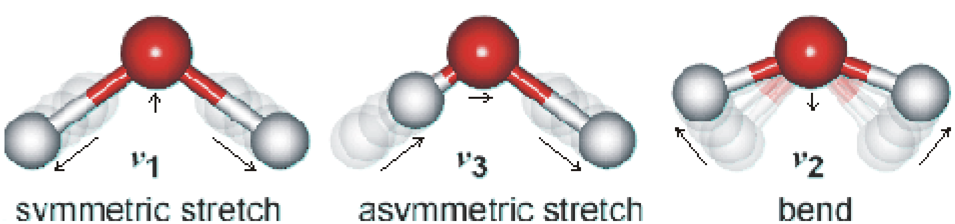
Visible light ν=f > 330,000 GHz

Character table for point group C_{2v}

C_{2v}	E	C_2 (z)	$\sigma_v(xz)$	$\sigma_v(zy)$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	z	x^2, y^2, z^2	z^3, x^2z, y^2z
A_2	+1	+1	-1	-1	R_z	xy	xyz
B_1	+1	-1	+1	-1	x, R_y	xz	xz^2, x^3, xy^2
B_2	+1	-1	-1	+1	y, R_x	yz	yz^2, y^3, x^2y

Vibrational modes of water molecule

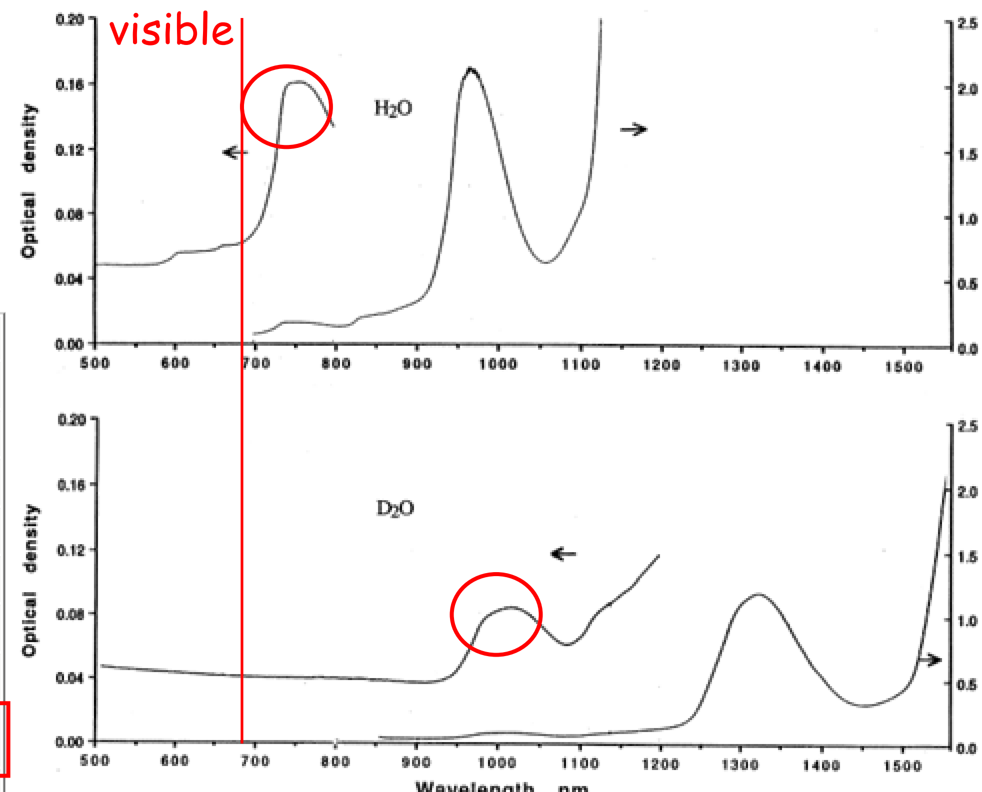
A_1 B_1 A_1



Charles L. Braun and Sergei N. Smirnov,

WHY IS WATER BLUE? J. Chem. Edu., **70**, 612 (1993).

Figure 1. The upper spectrum is that for liquid H_2O in a 10 cm cell at room temperature; the lower spectrum is for D_2O under the same conditions. The absorption below 700 nm in wavelength contributes to the color of water. This absorption consists of the short wavelength tail of a band centered at 760 nm and two weaker bands at 660 and 605 nm



The OH symmetric ($\nu 1$) and antisymmetric ($\nu 3$) vibrational stretching modes are at high enough energy [3650 cm-1 and 3755 cm-1, respectively] so the four quantum overtone ($\nu 1$+ 3$\nu 3$) occurs at 14,318.77 cm-1 (698 nm), just at the red edge of the visible.

gas[a]	assignment[a]	liquid	shift
3.6517	ν_1	3.40[b]	
3.7558	ν_3		
5.332	$\nu_2+\nu_3$	5.15[c]	0.18 7
7.2516	$\nu_1+\nu_3$	6.90[c]	0.35
8.807	$\nu_1+\nu_2+\nu_3$	8.40[c]	0.41
10.613	$2\nu_1+\nu_3$	10.3[c]	0.31
13.831	$3\nu_1+\nu_3$	13.16(760 nm)	0.67
14.319	$\nu_1+3\nu_3$	13.51(740 nm) s	0.81
15.348	$3\nu_1+\nu_2+\nu_3$	15.15(660 nm)	0.20
15.832	$\nu_1+\nu_2+3\nu_3$	15.15(660 nm)	0.681
16.822	$3\nu_3+2\nu_2+\nu_1$		
6.899	$4\nu_4+\nu_1$	16.53(605 nm)	0.37

All liquid phase assignments of gas phase transitions which lie above 10,613 cm-1 are based on Fig. 1 and are speculative.