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WATER STRUCTURE AND SCIENCE
Martin Chaplin

Home

Water Absorption Spectrum

Water absorbs a wide range of electromagnetic radiation with rotational transitions and intermolecular vibrations responsible for absorption in the microwave (~1 mm - 10 cm wavelength) and far-infrared (~10 μm - 1 mm), intramolecular vibrational transitions in the infrared (~1 μ- 10 μ) and electronic transitions occurring in the ultraviolet region (< 200 nm).
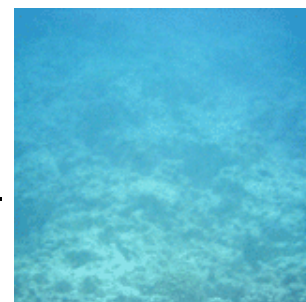
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Water in the atmosphere

Water is the main absorber of the sunlight in the atmosphere; without it, the Earth would be in a permanent ice-age. The 13 million million tons of water in the atmosphere (~0.33% by weight; compare CO_2 ~0.04%) is responsible for about 70% of all atmospheric absorption of radiation, mainly in the infrared region where water shows strong absorption. The average relative humidity [l] of the atmosphere [2474] is about 75% at ground level reducing to about at 45% at 5000 m. See also, water and global warming.
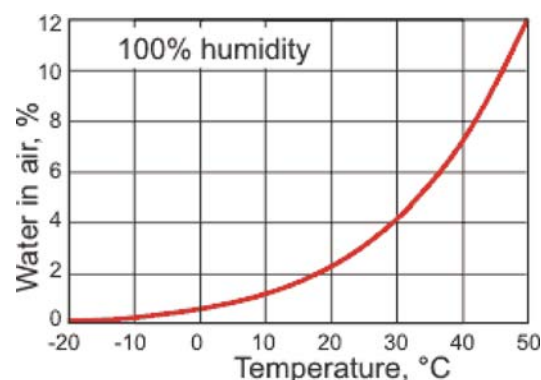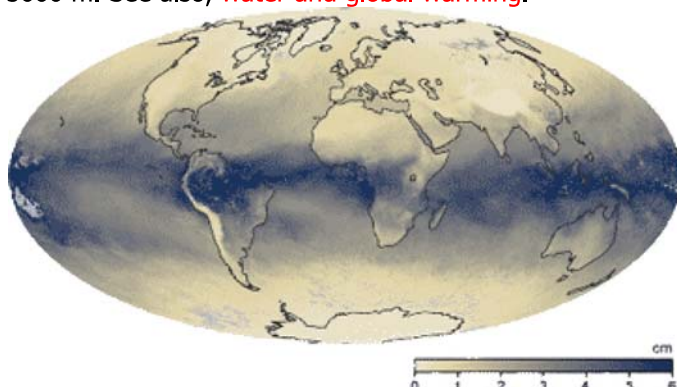
The water absorption spectrum is very complex. Water's vapor spectroscopy has been recently reviewed [348]. The water molecule may vibrate in a number of ways. In the gas state, the vibrations [607] involve combinations of symmetric stretch (v_1), asymmetric stretch (v_3) and bending (v_2) of the covalent bonds with absorption intensity ($H_2^{16}O$) v_1;v_2;v_3 = 0.07;1.47;1.00 [8]. As shown right, there is significant isotope effects with the frequencies in H_2O are higher than those in D_2O and T_2O; the ratios between H_2O, D_2O and T_2O being approximately the square root of the D:H or T:H atomic mass ratios. The stretch vibrations of HDO refer to the single bond vibrations, not the combined movements of both bonds. Gas phase rotations [1701] are complex and are combined with these vibrations. The lowest *ortho-para* transitions are given elsewhere.

Main vibrations of water isotopologues [607, 1728]

| Gas	v_1, cm^{-1}	v_2, cm^{-1}	v_3, cm^{-1}
$H_2^{16}O$	3657.1	1594.7	3755.9
$H_2^{17}O$	3653.1	1591.3	3748.3
$H_2^{18}O$	3649.7	1588.3	3741.6
$HD^{16}O$	2723.7	1403.5	3707.5
$HD^{17}O$	(2716.0)*	1399.7	(3701.5)*
$HD^{18}O$	2709.3	1396.3	3696.3
$D_2^{16}O$	2671.6	1178.4	2787.7
$D_2^{17}O$	(2665.8)*	1174.0	(2772.3)*
$D_2^{18}O$	2660.8	1170.2	2767.5
$HT^{16}O$	2299.8	1332.5	3716.6
$T_2^{16}O$	2237.2	995.4	2366.6

* estimated

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Absorption spectra of liquid and solid water

Shown opposite are the main vibrations occurring in liquid water. Rotations in the liquid phase are totally dominated by hydrogen bonding. The movements are animated using the cursor. The dipole moments change in the direction of the movement of the oxygen atoms as shown by the arrows. As the H-atoms are light, the vibrations have large amplitudes.

v_1 symmetric stretch v_3 asymmetric stretch v_2 bend

x   y   z
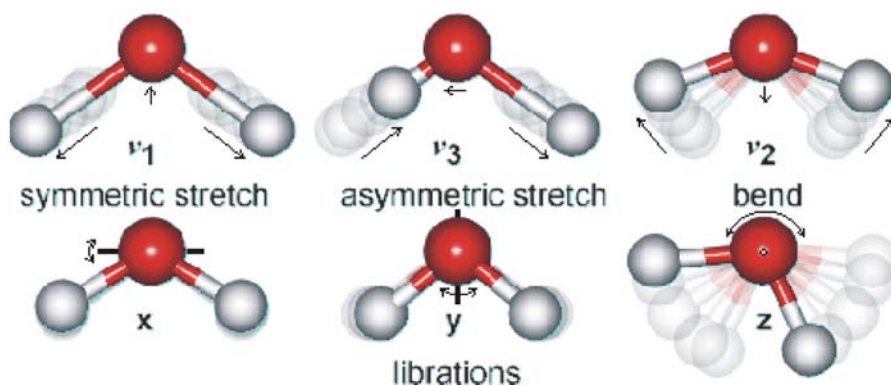
librations

The water molecule has a very small moment of inertia on rotation which gives rise to rich combined vibrational-rotational spectra in the vapor containing tens of thousands to millions of absorption lines. In the liquid, rotations tend to be restricted by hydrogen bonds, giving the librations. Also, spectral lines are broader causing overlap of many of the absorption peaks.
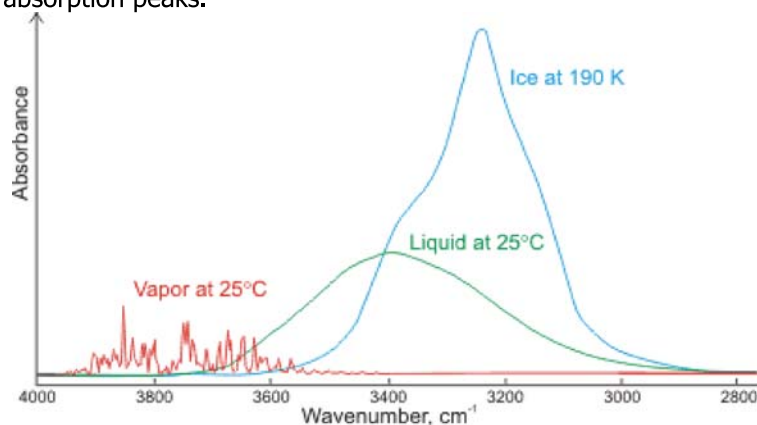
Opposite is shown a comparison of the gas, liquid and solid spectra of the same amount of H_2O [1392]. On mousing over the Figure, the high (HDL) and low (LDL) density liquid water forms are shown [1738]. [j] The main stretching band in liquid water is shifted to a lower frequency (v_3, 3490 cm^{-1} and v_1, 3280 cm^{-1} [8]) and the bending frequency increased (v_2, 1644 cm^{-1} [942]) by hydrogen bonding. As seen, increased strength of hydrogen bonding typically shifts the stretch vibration to lower frequencies (red-shift) with greatly increased intensity in the infrared (but not Raman) due to the increased dipoles. Blue-shifting hydrogen bonds are described elsewhere. [**Back to Top**

▲]

The vibrational spectra of liquid water

Main vibrations of liquid ordinary and heavy water

Vibration(s) [942]	liquid H$_2$O (25 °C)		liquid D$_2$O (25 °C)		liquid T$_2$O [1848]
	v, cm^{-1}	ε_λ, M^{-1} cm^{-1} [d]	v, cm^{-1}	ε_λ, M^{-1} cm^{-1}	v, cm^{-1}
v_2	1643.5	21.65	1209.4	17.10	1024
combination of v_2+ libration	2127.5	3.46	1555.0	1.88	
v_1, v_3 , and overtone of v_2	3404.0 [e]	100.61	2504.0	69.68	2200

HDO (50 mole % H$_2$O plus 50 mole % D$_2$O; ~50% HDO, ~25% H$_2$O, ~25% D$_2$O) has maxima at 3415 cm^{-1}, 2495 cm^{-1} 1850 cm^{-1} and 1450 cm^{-1} assigned to OH stretch, OD stretch, [h] combination of v_2+ libration and HDO bending respectively [786] (see right for comparative spectra). HTO and DTO (50 mole % mixtures as HDO above) have v_2 bend maxima at 1388 cm^{-1} and 1130 cm^{-1} respectively [1848].
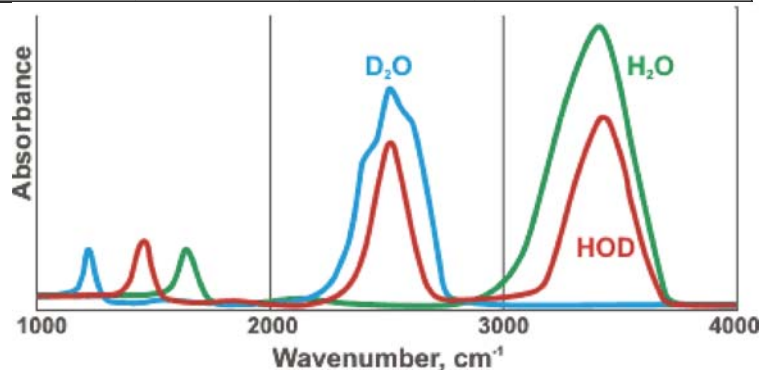

All the vibrational bands in liquid water are made up from contributions from different components from water molecules in different hydrogen bonded environments (see, for example, hydrogen bonds); lower frequency components are attributed to water molecules with stronger hydrogen bonds and higher frequency components have weaker hydrogen bonds [2157].

Variations in the environment around each liquid water molecule gives rise to considerable line broadening with vibration shifts in a hydrogen-bond-donating water molecule being greater than in a hydrogen-bond accepting molecule but both acting in the same direction [679], and accumulating with the number of hydrogen bonds. The strength of the hydrogen

bonding depends on the cooperative/anticooperative nature of the surrounding hydrogen bonds with strongest hydrogen bonds giving the lowest vibrational frequencies [852]. Stretching frequency increases about 360 (at 3.1 Å) -1000 (at 2.6 Å) $cm^{-1}Å^{-1}$ with increasing O····O distance and about 9 cm^{-1} degree^{-1} with increasing O-H····O bend [446]. The absorption intensity of these bands is $v_1; v_2; v_3$ = 0.87;0.33;1.00 [8]. In supercooled water, the spectra is shifted to lower frequency with a 70 cm^{-1} shift of the stretch frequency and 30% increase in its intensity between 298 K and 238 K [1065]. Ultimately a stretch peak at 3120 cm^{-1} dominates, as it also does in amorphous ice (LDA) [1252]. In hexagonal ice, these bands are shifted further (v_1, 3085 cm^{-1}, v_2, 1650 cm^{-1}, v_3, 3220 cm^{-1}).

The O-H stretch band around 3400 cm^{-1} is often broken down into a number of Gaussian peaks supposedly corresponding to different hydrogen bonded water molecules with varying donor (D) and acceptor (A) hydrogen bonds. At 295 K and 0.1 MPa, the Raman spectra of H_2O and D_2O can be deconvoluted into five sub-bands (see the Raman spectra left, from [2830]), located at 3043, 3225, 3432, 3575, 3638 cm^{-1} (H_2O), or 2265, 2382, 2503, 2590, 2666 cm^{-1} (D_2O), which are assigned to OH (OD) vibrations engaged in DAA, DDAA, DA, DDA hydrogen bonding, and free vibrations [1980, 2894]. It can be seen that the two major vibrations are due to the doubly donor-acceptor or singly donor-acceptor water molecules.
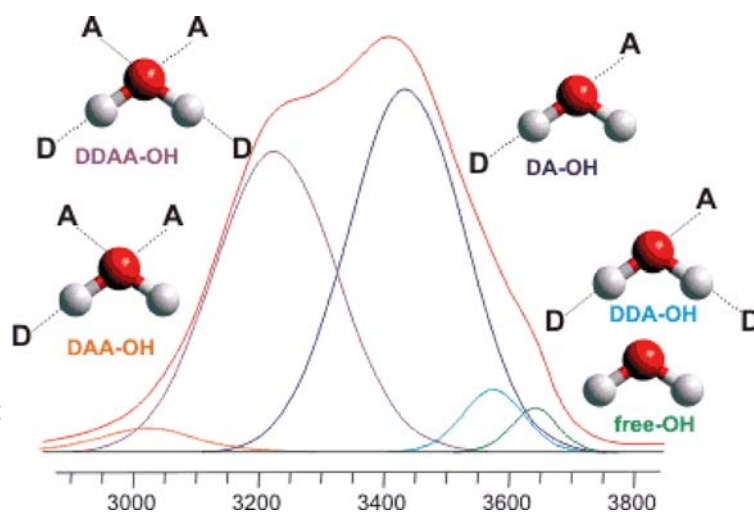
In liquid water the molecular stretch vibrations shift to higher frequency, on raising the temperature (as hydrogen bonding weakens, the covalent O-H bonds strengthen causing them to vibrate at higher frequencies) whereas the intermolecular vibrations shift to lower frequencies and the molecular bend vibration peak shifts to lower frequencies and becomes both narrower [696] and stronger. These differences between stretch and bend vibrations are due to the increased importance of intermolecular hydrogen bonding at lower temperatures that tends to reduce intermolecular bending whilst encouraging stretching. Thus in the extreme non-hydrogen bonded state, the 'dangling' O-H bond stretch frequency at surfaces where the water molecule has three hydrogen bonds (two accepting and one donating) is at 3697 cm^{-1} [1246]. Raising the temperature also lowers the intensity of the stretching bands. This divergent behavior of bending and stretching vibrations allows their contributions to combination bands to be discerned. Thus, combinations of stretching vibrations shift to higher frequency with temperature with this trend reduced when bending vibrations are also combined. As examples, the first overtone combination of symmetric and asymmetric stretching shows a shift from strongly hydrogen-bonded structures (6707 cm^{-1}) to weakly hydrogen bonded structures (7082 cm^{-1}) with increasing temperature [237], and the combination band at about 5200 cm^{-1} shifts to slightly higher wavenumbers with reduced hydrogen bond strength [282]. The second overtone of the stretching band gives rise to a significant peak in the near-infrared spectrum (λ 970 nm).

Recent work, using attenuated total reflectance (ATR) infrared spectroscopy, shows isosbestic points for both ordinary and heavy liquid water, with respect to temperature. For H_2O these are at around 600, 1600, 1680 and 3550 cm^{-1} [1738] (171, 221, 669 and 3535 cm^{-1} [2254]), in agreement with earlier work [530, 699]. [a] Shown opposite are the ATR spectra of liquid water at -4 °C (blue solid line; 61% LD, 39% HD) and 80 °C (red solid line; 31% LD, 69% HD) and those of the low density (LD, blue dashed line) and high density (HD; red dashed line) forms that make up the liquid water [1738] in a linear combination. Similar conclusions have been gained from Raman spectroscopy where the LD peak is analyzed as tetrahedral fully-hydrogen bonded H_2O molecules

and the HD peak analyzed as molecules with single acceptor and donor hydrogen bonds [1980]. Also, similar conclusions (at different wavenumbers) are drawn for D_2O [1738]. Unsurprisingly, such changes in absorption with temperature extend into the near infrared and visible spectrum [1974]. These conclusions are in qualitative agreement with recent wide-angle X-ray diffraction measurements [1755] and supportive of progressively changing two-phase models such as described here.
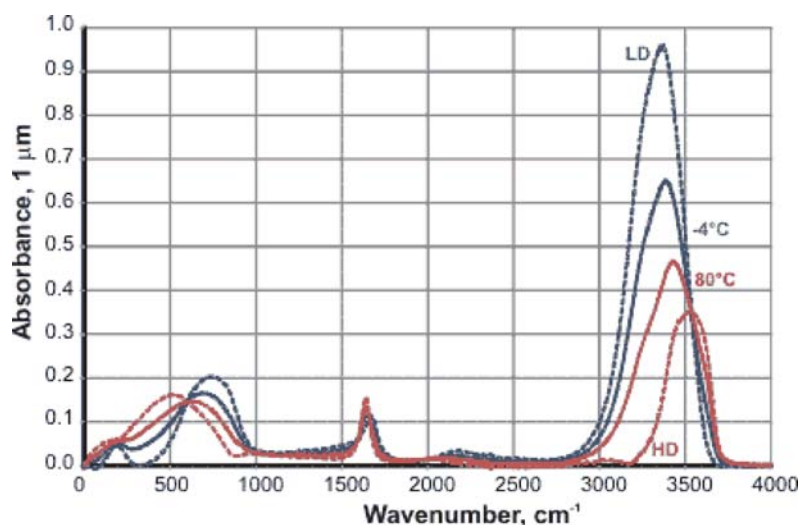
Increasing the pressure on water decreases the O····O distances (graphed elsewhere) so increasing the covalent O-H distances and lowering their stretch frequency [804]. Raised pressure also causes a reduction in long, weak or broken bonds and an increase in bent and short, strong hydrogen bonds [804].

The overtone bands of water (~1100 nm - 2500 nm, in a scientific discipline known as AquaPhotomics) have been shown to be good discriminatory, and non-destructive, indicators of changes in aqueous structuring in disease diagnosis and protein conformation and have aided the understanding of the role of water in biological systems [1615a]. A database of such interactions is being built up [1615b], with comparison being made using polar graphs (Aquagrams) [1615c].

The spectra for isotopic variants of water (for example, HDO, D_2O and $H_2^{18}O$) are all different; in particular the H-O (~3400 cm^{-1}) and D-O (~2500 cm^{-1}) stretching vibrations are not connected in HDO but the related vibrations in H_2O and D_2O involve both hydrogen atoms.

Assignment of the IR vibrational absorption spectrum of liquid water[*]

Wavelength	cm^{-1}	Assignment	Wavelength[**]	cm^{-1}	Assignment
0.2 mm	50	hydrogen bond bend	1200 nm	8330	$a\nu_1 + \nu_2 + b\nu_3$; a+b=2
55 μm	183.4	hydrogen bond stretch	970 nm	10310	$a\nu_1 + b\nu_3$; a+b=3
25 μm	395.5	L_1, librations	836 nm	11960	$a\nu_1 + \nu_2 + b\nu_3$; a+b=3
15 μm	686.3	L_2, librations	739 nm	13530	$a\nu_1 + b\nu_3$; a+b=4
6.08 μm	1645	ν_2, bend	660 nm	15150	$a\nu_1 + \nu_2 + b\nu_3$; a+b=4
4.65 μm	2150	$\nu_2 + L_2$ [b]	606 nm	16500	$a\nu_1 + b\nu_3$; a+b=5 [526]
3.05 μm	3277	ν_1, symmetric stretch	514 nm	19460	$a\nu_1 + b\nu_3$; a+b=6 [526]
2.87 μm	3490	ν_3, asymmetric stretch	449 nm	22270	$a\nu_1 + b\nu_3$; a+b=7 [1937]
1900 nm	5260	$a\nu_1 + \nu_2 + b\nu_3$; a+b=1	401 nm	24940	$a\nu_1 + b\nu_3$; a+b=8 [1937]
1470 nm	6800	$a\nu_1 + b\nu_3$; a+b=2		Note that a and b are integers, ≥ 0.	

* Raman peaks are given in [805].
**Wavelength (nm) = 10^7/wavenumber (cm^{-1}) (nm ~3.3 attosecond); 1 cm^{-1} ~ 0.03 THz

The near-infrared (NIR) bands (at about λ 970-1940 nm) are suited to rapid non-destructive water determination [479], all shifting a few nm to longer wavelength (lower frequency) with strengthening hydrogen bonding due to shifts from high density water (that is, increasing CS) to low density water (that is, increasing ES) [489]. A shoulder at about 3250 cm^{-1} on the side of the only strongly active Raman peak, and recently described in the IR spectrum at 3220 cm^{-1} [699], (symmetric O-H stretch, ν_1) of liquid water has been assigned to the collective in-phase symmetric O-H vibrations of strongly tetrahedrally-bonded water patches. The ratio of this to the remaining peak at about 3400 cm^{-1} has been used to determine the fraction of such water but such comparisons, although commonly used, should be treated with caution, as their absorbencies are unlikely to be identical and other possible vibrations, such as the first bend (ν_2) overtone, will interfere. This remaining peak has been analyzed in many ways (for example, as zero, single, double and triple coordinated hydrogen-bonded water) but most convincingly in terms of three-coordinate (double acceptor single donor, 3400 cm^{-1}; single acceptor double donor, 3535 cm^{-1}) and two-coordinate (single acceptor single donor, 3630 cm^{-1}) hydrogen-bonded water molecules [699]. There is clearly much structural information hidden in the vibrational spectra of water, if only it can be unambiguously interpreted (see methods page). Some success has recently been made using femtosecond mid-infrared nonlinear spectroscopy [189, 190] and the theoretical Raman spectra of water clusters [483].

In liquid water and ice the infrared and Raman spectra are far more complex than the vapor due to vibrational overtones and combinations with librations (restricted rotations; that is, rocking motions). These librations are due to the restrictions imposed by hydrogen bonding (minor L_1 band 395.5 cm^{-1}; major L_2 band 686.3 cm^{-1}; both for liquid water at 0 °C, the absorbance of L_1 increasing with increasing temperature whereas L_2 absorbance decreases but broadens with reduced wavenumber with increasing temperature [177]). Ice has a sharper major band at 819 cm^{-1} (-10 °C) with a very minor band at about 510 cm^{-1} [1219]. The less energetic librations are available to terahertz absorption spectroscopy. The librations depend on the moments of inertia such that the almost doubling of the moments of inertia of D_2O, relative to H_2O, reduces the frequencies by about a factor of √2. Cluster vibrations such as translational vibrations involve combinations of hydrogen bond O-H····O stretching and bending at around 200 cm^{-1} (6 THz) [240] (S or connectivity band, 183.4 cm^{-1} (5.5 THz); at 0 °C, the hydrogen bond stretch absorbance increasing with decreasing temperature [819] [a]; with a major sharp band at 215 cm^{-1} (6.4 THz) and a minor sharp band at 155 cm^{-1} (4.6 THz) in ice Ih at -10 °C [1219]. These involve hydrogen-bonded network movements along linear or near-linear hydrogen bonds [i] and show relatively small differences between H_2O and D_2O, due to their slightly different masses [1004]. These vibrations around 5 THz (165 cm^{-1}) overlap with the longitudinal acoustic (LA) phonon modes (i.e. hydrogen bond

network vibrations in the direction of propagation). The Raman spectrum also involves an overlapping band involving the reorienting of the molecular dipoles around the hydrogen bonds [1384]. Some report bending vibrations of the hydrogen bonds also occur, due to out of alignment translations relative to the hydrogen bonds (B band ~40 - 60 cm^{-1} (1.2-1.8 THz); at 0 °C, the absorbance increasing with temperature [608]) [1004]. It seems likely that this 60 cm^{-1} peak is strongly localized within a local cluster and not connected with the more extensive hydrogen-bonded network [1549]. [f] These vibrations around 1 THz (33 cm^{-1}) overlap with the transverse acoustic (TA) phonon modes (i.e. hydrogen bond network vibrations perpendicular to the direction of propagation). Also in liquid water there is a small but significant combination band (IR and Raman) of the bending (ν_2) and libration modes at 2125 cm^{-1} (2270 cm^{-1} in ice Ih; the 'association band'). [b]

A contribution to the Raman scattering of water at 50 cm^{-1} (1.5 THz) has been attributed to the low-frequency vibrations of oxygen-oxygen bonds at the vertices of pentagonal dodecahedral structures [165] or simply O····O····O bending motions [901]. Such low-frequency features (centered around 60 cm^{-1}, 1.8 THz) are also observed in the spectra of dense non-associated liquids, such as the noble gases, and may be attributed to non-bonded 'cage effects' where translations are frustrated [448]. This same effect, however, may also operate within hydrogen bonded 'cage effects' consistent with the 60 cm^{-1} absorption band [900]. Further confirmation of the hydrogen-bonding source for this absorption comes from the use of an intense source of far infrared radiation showing temperature dependent peaks at a number of wavelengths in the 40-90 cm^{-1} (1.2-2.7 THz) range [656]. The infrared spectrum runs into the β-relaxation band (~0.2 THz; due to rattling of molecules in a cage of surrounding molecules) and absorption due to microwave radiation at longer wavelengths. This interacts with the water dipole, moving the molecules backwards and forwards and so stretching and bending the hydrogen bonds, which generates heat. If the radiation is at too high a frequency (> 1000 GHz, λ < 0.3 mm), the molecules do not have time to react to the electromagnetic field changes and no heat is generated. If the radiation is at lower frequencies (< 1 GHz, λ > 30 cm), the molecules react to the electromagnetic field changes but so slowly that effectively no heat is generated. Pure water is almost totally transparent to such low frequency radiation. The maximum absorption varies to higher frequencies at higher temperatures when the weaker hydrogen bonding allows a quicker response to changes in the field [136]. Microwave ovens typically use radiation at 2.450 GHz (λ 12.24 cm). More details on the response of water to microwave and the far infrared radiation (< 100 THz, < 400 cm^{-1}) are available in the microwave in the complex dielectric sections.

Anions may be classified as kosmotropes or chaotropes according to how the effect the water's stretch vibrations; ionic kosmotropes (for example, F$^-$) causing broadening and movement to lower wavenumbers whereas chaotropes (for example, I$^-$) causing narrowing and movement to higher wavenumbers [758]. Primarily this seems due to water's ability to hydrogen bond to the anions. The vibrational spectra of H$_3$O$_2^-$ and H$_5$O$_2^+$ are described on another page.

The reported structuring absorption of sound by water is not generally accepted. [**Back to Top ▲**]

## The visible and UV spectra of liquid water

Absorption coefficients [d] [k] for water
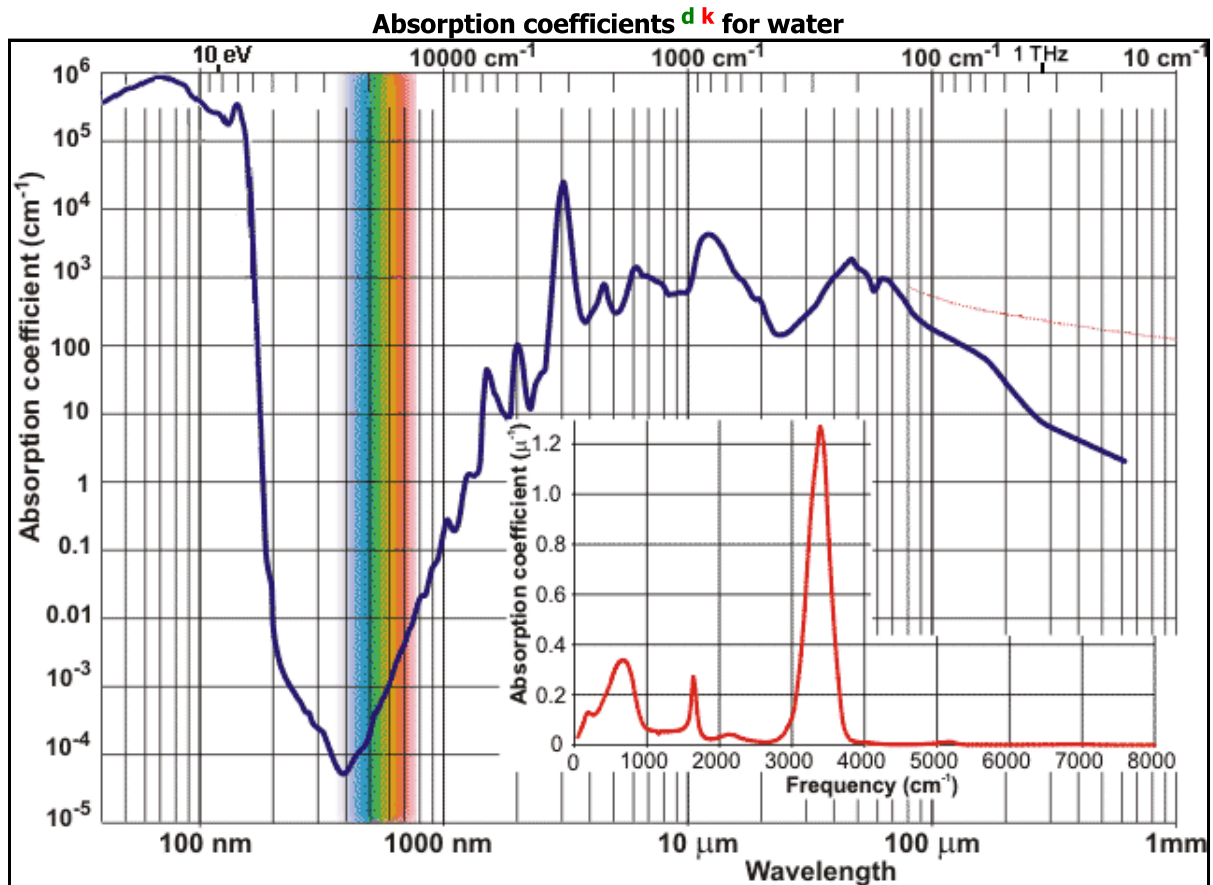
The refractive index of water is given on another page. Water is almost perfectly transparent to 'visible' light, a property which is made good use of by photosynthesis and allowing production of both biomass and oxygen. However, some absorption is achieved by atmospheric water (see right, which shows seven absorption bands). Water is very slightly blue in color [131] [c] as overtone and combination vibrational absorption bands (albeit far less intense, see above [130]) extend through the red part of the visible spectrum with a small peak at 739 nm and shoulder at 836 nm, plus a smaller fourth overtone of the v_1:v_3 stretch at 606 nm, and very small fifth overtone (at 514 nm) and combined overtone (at 660 nm) bands. As an example, the 739 nm peak absorbs only 10% through 1 km of atmosphere at a relative humidity of 57% at 20 °C (the path containing 1 cm of precipitable water).
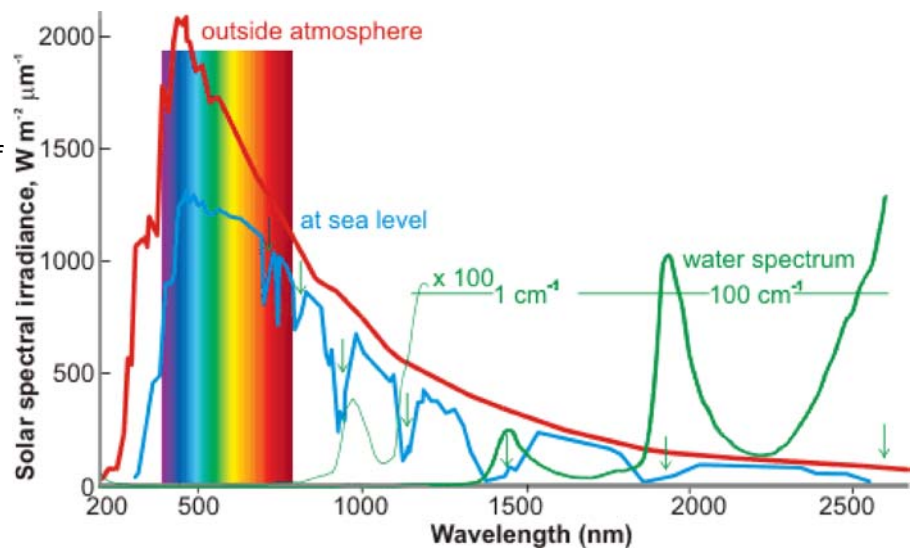
These overtone and combination vibrational bands increase and sharpen somewhat with increasing temperature [268] in line with the expectation from the two state water model. This absorption spectrum of water (red light absorbs 100 times more than blue light), together with the five-times greater scattering of blue light over red light, contributes to the blue color of lake, river and ocean waters. Colloidal silica may contribute to the outstanding blue color of certain, often hydrothermal, pools and lakes [372]. Ice is also blue [159] for similar reasons but liquid D_2O does not absorb in the red region (as the absorption band is shifted into the infrared) and is blue solely because of the light scattering effect [159].

Although the absorptions of water's overtone bands within the visible spectrum are quite small ($\sim$0.3-0.01 m^{-1}), they are sufficient to create spectral niches amongst photosynthetic organisms; thus directing water ecology and evolution [1281].

The first peak in the far UV of gaseous water (166.5 nm [902], shown light blue in the spectrum above) is due to excitation from the occupied p$_z^2$-type molecular $1b_1$ orbital (interactive orbitals are available, COW only [Plug-in, ActiveX]). Absorption of UV close-by ($\sim$125 nm), excites the $3a_1$ orbital leading to dissociation into OH + H

(photodissociation; higher energy absorption produces charged fragments [1299]). Such dissociation can also be achieved by consecutive absorption of two 266 nm photons [589]. Absorption of two higher energy photons, at 200 nm, gives rise to a hydrated electron by $H_2O + h\nu \longrightarrow H_2O^+ + e^-_{aq}$ [1057]. Inelastic x-ray scattering studies find this far UV peak to be absent in liquid water [355], where the major peak is at about 56 nm. [**Back to Top ▲**]

The spectrum of the Zundel cation

The Zundel cation is detected in acid solutions and has been shown to give several characteristic vibrations [2440].

Shuttle ~1200 cm⁻¹   Bend ~1750 cm⁻¹   Stretch ~ 3000 cm⁻¹
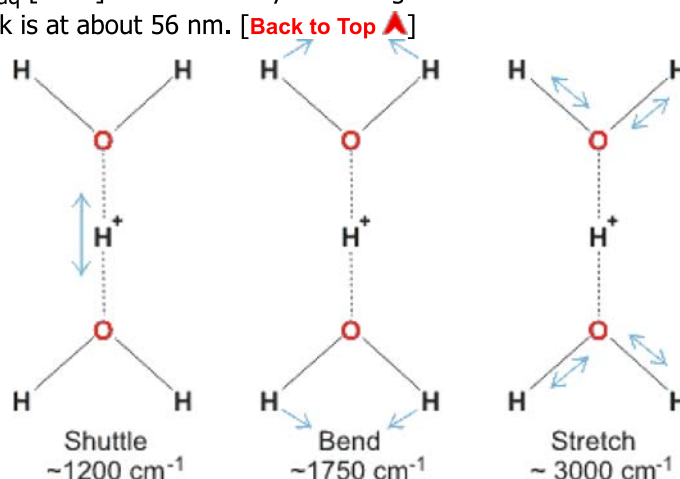
Footnotes

a   Dielectric studies showed an opposite effect with the absorbance at around 200 cm⁻¹ increasing with increasing temperature to about 30 °C before reducing with increasing temperature due to hydrogen bond breakage [608]. The discrepancy may be due to additional relaxation processes detected by these dielectric studies in addition to the hydrogen bond stretching detected by infrared spectroscopy [819]. The Raman absorption at 180 cm⁻¹ has been proposed to be used to monitor tetrahedrally hydrogen bonded water molecules ('bound' water) [1963]. [Back]

b   This liquid water band, also known as the association band, may be due to third overtone of the libration band, with the second overtone introducing asymmetry into the bend (ν_2) vibration [699b]. Other vibrations may contribute, such asa combination of bending and libration, and intermolecular interactions [2871]. There appears to be five sub-bands at increasing wavenumber from ~2020 cm⁻¹ to ~2255 cm⁻¹ corresponding to increasing molecular structure [2871]. The dependence of this band on hydrogen bonding makes it sensitive to changes in liquid and solution structuring, although this importance is seemingly often overlooked. [Back]

c   The sky is blue due to molecular light scattering, with neither tiny air-borne particles nor its small and variable content of gaseous water having significant effect [710]. [Back]

d   **Absorption and penetration.** According to Beer's law (e.g. see K. B. Oldham and J. M. Parnis, Shining light on Beer's law, *ChemTexts* **3** (2017) 5), the intensity of an electromagnetic wave penetrating a material falls off exponentially with distance from the surface. Thus, the rate of decrease in the intensity (I) of light passing through a transparent medium
with distance is proportional to the concentration (c) of the absorbing material and to the local intensity of the light at that point, $I(x)$:

$$\frac{d}{dx}I(x) = -\alpha_\lambda\, cI(x)$$

where α_λ is the absorption coefficient, with units of cm⁻¹, at a particular wavelength (λ). On integration we get:

$$\frac{I}{I_0} = e^{-\alpha_\lambda L}$$

where I is the transmitted intensity of the light, I_0 is the incident intensity of the light and L is the path length (cm). The absorbance (A, in optical density units) is defined by the equation:

$$A = -Log_{10}\left(\frac{I}{I_0}\right)$$

The transmittance (T) of a sample is defined by $T = \left(\frac{I}{I_0}\right)$. The molar extinction coefficient (ε_λ, molar absorptivity, molar extinction coefficient, or molar absorptivity), with units   liters mole⁻¹ cm⁻¹, is defined by the equation $A = \varepsilon_\lambda cL$ where c is the molar concentration (= 55.345 M for liquid water at 25 °C) and l is the path length (cm). Comparison of these definitions shows that $A = \frac{\alpha_\lambda L}{2.303}$ and $\varepsilon_\lambda = \frac{\alpha_\lambda}{2.303c}$ (note that $\log_e(10) \approx 2.303$). The penetration coefficient (δ_P) is the reciprocal of the absorption coefficient ($1/\alpha_\lambda$). δ_P is the thickness of material when the amount of light has reduced to 1/e (i.e. 36.79%) of its original value. The thickness of material when the amount of light has reduced by 50% is Ln(2)/α_λ = 0.693/α_λ. [Back]

[e]   This band in the Raman spectrum has been clearly separated into three peaks at ~3210, 3450 and 3650 cm^{-1} [1310]. The two dominant components at 3210 and 3450 cm^{-1} were assigned to ice-like (for example ES) and disordered (for example CS) [1310]. [Back]

[f]   This assignment, for 40 cm^{-1} in the far infrared, is disputed as being caused by collective vibrations, with no temperature dependence found between 10 °C-70 °C [1676]. [Back]

[g]   The presence of isosbestic points have been disputed [526], but has also been found by Raman spectroscopy of optically levitated supercooled micron-sized water droplets between -34.6 °C and 46.0 °C at about 3340 cm^{-1} [1909] and between -25 °C and 25.0 °C at 3330 cm^{-1} using a confocal micro-Raman system in a backscattering geometry [1980] . The presence of isosbestic points does not necessarily indicate interconverting chemical or structural species [2272], but, in this case the whole actual spectrum can be obtained from two spectra showing isosbestic points, giving proof of a two state equilibrium. [Back]

[h]   The peak at 2495 cm^{-1} can be used to quantify moderate HDO contents. [Back]

[i]   The peak at about 200 cm^{-1} (~6 THz) involves molecular translational vibrations involving the hydrogen bond (but not the O-H covalent bond), such as shown right [1992]. [Back]

[j]   Liquid water can be considered as a mixture of high (HDL) and low (LDL) density liquid water forms. [Back]

[k]   This curve(s) has been generated using data for liquid and frozen water to give a continuous curve showing the main features. For exact data please consult the original references [130]. [Back]

[l]   Humidity is the amount of water vapor in the air, but there are a number of different units describing it [2465]. Absolute humidity is the water content of air at a given temperature (g m^{-3}), changing with both temperature and pressure. Specific humidity (g kg^{-1}) is the mass of moisture per mass of air (including the water vapor). Mixing ratio (g kg^{-1}) is the mass of moisture per mass of dry air. Relative humidity (RH, %) represents the extent to which air is saturated that equals 100 × (actual vapor pressure of water vapor)/(saturation vapor pressure of water vapor at the same temperature). Equilibrium relative humidity (ERH, %) is the value of relative humidity under equilibrium conditions. The saturation vapor pressure of water vapor at different temperatures (T) can be approximately described by the equation:

$$Saturation\ vapor\ pressure = 6.108e^{\left(\frac{17.27T}{T+237.3}\right)}$$

[Back]
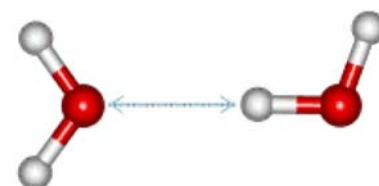
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