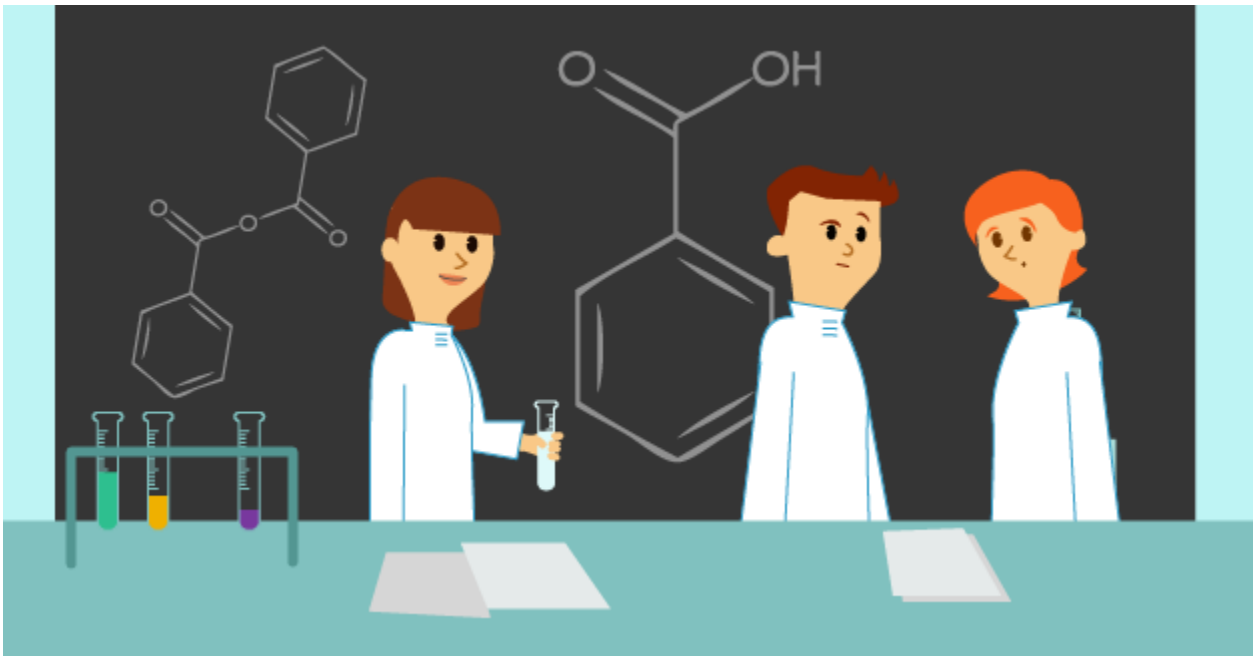
HYDROGEN PEROXIDE STRUCTURE AND SPECTRA



The equilibrium geometry of hydrogen peroxide was established by an electron diffraction study. This was supported by an X-ray study with limited least-squares data reduction, an infrared study, and a microwave study. The infrared study may be regarded as definitive, although the structure of the solid, as determined by X-ray, may be appreciably different from the gas phase. The X-ray study may be questioned, however, because the data analysis used visual intensity estimation and primitive numerical machines. The rotational constants measured in the infrared are A' = 10.356 cm^{-1}, B' = 0.8656 cm^{-1}, C' = 0.8270 cm^{-1}, D_J = 4.5 x 10^{-6} cm^{-1}, D_K = 7.5 x $10^{-4}cm^{-1}$, and D_{JK} = -2 x 10^{-5} cm^{-1}. cm Dipole moments of 3.15 ±0.05 D and 3.24 ±0.05 D were measured for each of the two potential minima. A far infrared study showed the angle τ has two equilibrium values (with the lowest at 111.5 degrees ±0.5) and determined an accurate hindered-rotation potential function.

Hydrogen peroxide forms tetragonal crystals, space group D_4^4 – $P4_12_1$, upon freezing. There are four molecules in the unit cell of dimensions a = 4.061Å and c = 8.001Å. The crystal structure has been completely determined, and the volume of the unit cell is 131.9$Å^3$. This gives a crystal density of 1.70 gm/cc.

Hydrogen peroxide is the simplest molecule having an internal rotation motion, and, therefore, has had fairly extensive study with respect to absorption spectra. Hindered internal rotation effects are observed in all regions of the spectrum. Extensive studies have been conducted on the vapor, the crystalline solid, and dilute solutions. Less work has been spent on the concentrated liquid solutions, because of decomposition effects and the difficulty in finding suitable window materials. Since the spectrum as a whole is very complicated, it is considered beyond the scope of this article; thus, references to H_2O_2 spectrum characterization are provided as a guide for interested individuals.

The infrared absorption by H_2O_2 is not very useful for chemical analysis because the spectrum is quite similar to that of water and since suitable window materials are not widely available. Ultraviolet absorption by H_2O_2 is quite strong, and (although Beer's law does not hold strictly) if the solution is clear and transparent to ultraviolet, direct spectrophotometry measurements are suitable for analysis of dilute solutions.

Source : http://www.diyspaceexploration.com/hydrogen-peroxide-structure-and-spectra/