THE ROTATIONAL SPECTRUM OF THE WATER-HYDROPEROXY RADICAL (H_2O-HO_2) COMPLEX

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Peroxy radicals and their derivatives are elusive but important intermediates in a wide range of oxidation processes. We observed pure rotational transitions of the water-hydroperoxy radical complex, H_2O-HO_2, in a supersonic jet by means of Fourier transform microwave spectroscopy combined with a double-resonance technique. The observed rotational transitions were found to split into two components because of the internal rotation of the water moiety. The molecular constants for the two components were determined precisely, supporting a molecular structure in which HO_2 acts as a proton donor to form a nearly planar five-membered ring with one hydrogen atom of water sticking out from the ring plane. The structure and the spectral splittings due to internal rotation provide information on the nature of the bonding interaction between open- and closed-shell species. They also provide accurate transition frequencies that are applicable to remote sensing of this complex, which may elucidate its potential roles in atmospheric and combustion chemistry.