SPECTROSCOPIC DETECTION OF THE HYDROTRIOXYL RADICAL (HOOO) IN THE GAS PHASE

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Pure rotational spectra of the HOOO and DOOO radicals have been observed in a supersonic jet by using a Fourier transform microwave (FTMW) and FTMW-millimeter wave double resonance spectroscopy with a pulsed discharge nozzle. From a total of 12 observed rotational transitions with fine and hyperfine splittings, precise molecular constants have been determined. The experimentally determined molecular structure is $trans$ planar, which was not expected before the present experimental detection, since the large number of $ab\ initio$ calculations so far reported have predicted its structure to be cis planar. The determined bond length between the HO and O_2 moieties, HO-OO, is fairly long, 1.688 Å, and the molecular structure of HOOO is similar to that of an isoelectronic radical, FOO, which also has a fairly long FO bond.