

FTMW AND FTMW-MMW DOUBLE RESONANCE SPECTROSCOPY OF AN OPEN-SHELL RADICAL COMPLEX, AR-HO₂.

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Although a number of molecular complexes have been studied extensively for a long time, studies on open-shell radical complexes are relatively scarce due to its difficulty of production. Besides, most of them deal with relatively simple rare-gas(Rg)-diatomic systems. We report the first microwave observation of the Rg-open-shell triatomic species, Ar-HO₂. The *a*-type and *b*-type transitions of Ar-HO₂ have been observed using Fourier transform microwave (FTMW) and FTMW-millimeter wave double resonance spectroscopy. The *r*₀ structure of Ar-HO₂ has been determined from the rotational constants by fixing the structure of the HO₂ monomer. The determined molecular structure is *cis* planar, where the argon atom is attached to the hydrogen atom of HO₂; *r*₀(ArH) = 2.622Å, and *θ*₀(ArHO) = 153.9°. *r*₀(ArH) of Ar-HO₂ is shorter than that of Ar-HO, 2.776Å^a, indicating that the Ar-HO₂ bond is relatively rigid. In fact, the binding energy of Ar-HO₂, 292cm⁻¹, calculated by RCCSD(T)/aug-cc-pVTZ + bond function is much larger than that of Ar-HO or other closed-shell Rg-triatomic species. On the other hand, the determined fine and hyperfine structures are almost identical to those of the HO₂ monomer. The large binding energy may be ascribed to the effect of the low-lying first excited state of the HO₂ monomer.

^aY. Ohshima, M. Iida, and Y. Endo, *J. Chem. Phys.* **95**, 7001 (1991)