A THEORETICAL INVESTIGATION OF THE RENNER INTERACTIONS AND MAGNETIC DIPOLE TRANSITIONS IN THE $\widetilde{A} - \widetilde{X}$ ELECTRONIC BAND SYSTEM OF $\mathrm{HO_2}$

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The $\widetilde{A}^2A' \rightarrow \widetilde{X}^2A''$ electronic band system of HO_2 has been simulated in emission using an extended version of the program RENNER [a] [b]. The two electronic states involved in this transition have strongly bent equilibrium geometries but they correlate together to form a $^2\Pi$ state at linearity. As a result the energy level pattern in the states is affected by electronic angular momentum effects (i.e., the Renner effect and spin-orbit coupling). In order to simulate the spectrum, we have calculated *ab initio* the potential energy surfaces, electric dipole moment surfaces, magnetic dipole moment surfaces, spin-orbit coupling parameter, and the electronic angular momentum matrix elements. Some of the forbidden $\Delta K = 0$ transitions occurring in the spectrum are induced by the magnetic dipole transition moment, and the others are electric dipole transitions that gain intensity because of the Renner interaction, spin-orbit coupling, or because of rotation-vibration interaction. All of these effects are allowed for in our calculation. The electric dipole transition moment is very small (0.017 D at the ground state equilibrium geometry) and because of this the magnetic dipole transitions are quite visible; the strongest magnetic dipole transitions are calculated to be about ten times weaker than the strongest electric dipole transitions. In this way previous experimental assignments [c] are confirmed theoretically.

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[b] M. KOLBUSZEWSKI, P. R. BUNKER, W. P. KRAEMER, GERALD OSMANN, AND PER JENSEN, *Mol. Phys.* **88**, 105-124 (1996)
[c] E. H. FINK AND D. A. RAMSAY, *J. Mol. Spectrosc.* **185**, 304-324 (1997)