THE EFFECTS OF PARTIALLY QUENCHED ORBITAL ANGULAR MOMENTUM ON THE INFRARED BAND STRUCTURE, MICROWAVE SPECTRUM, AND MAGNETIC HYPERFINE SPLITTING IN THE OH–WATER COMPLEX

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As a result of the significant splitting of the OH monomer orbital degeneracy into $^2A'$ and $^2A''$ electronic states upon formation of the OH–water complex, the OH monomer electronic orbital angular momentum is partially quenched. This quenching and the associated decoupling of the electron spin from the a inertial axis have dramatic effects on the microwave spectrum and rotational band structure of the infrared spectrum of the OH–water complex. Similarly, magnetic hyperfine splittings in the microwave spectrum, due to couplings between the hydrogen nuclear spins and the unpaired electron, are considerably affected by the partial quenching and the $^2A' -^2 A''$ energy separation. The infrared and microwave spectra, as well as the hyperfine splittings, have a noticeably different appearance than the well-established limiting cases of fully quenched or completely unquenched orbital angular momentum. Analysis of gas-phase OH-water spectra, such as those obtained using Fourier transform microwave spectroscopy by Brauer, *et al.*[a] and Ohshima, *et al.*[b], requires explicit consideration of this quenching phenomenon.

[a] C. S. Brauer, G. Sedo, E. M. Grumstrup, K. R. Leopold, M. D. Marshall, and H. O. Leung, Chem. Phys. Lett. 401, 420 (2005).
[b] Y. Ohshima, K. Sato, Y. Sumiyoshi, and Y. Endo, J. Am. Chem. Soc. 127, 1108 (2005).