FINE AND HYPERFINE INTERACTIONS, AND PSEUDOROTATIONAL TUNNELING IN Na_3

L. H. COUDERT, *Laboratoire de Photophysique Moléculaire, C.N.R.S., Bât. 210, Université Paris-Sud, 91405 Orsay Cedex, France*.

The Na_3 cluster has proven to be interesting from the experimental and theoretical point of view, and two of its electronic states, the A and B states, have been subject to several spectroscopic investigations. The A state, and the ground state, are dominated by Jahn-Teller induced rovibronic effects, while in the B state an almost free pseudorotational motion takes place. Although the two former states can be treated as ordinary asymmetric rotors[a] and the latter one using a newly developed model,[b] it is not yet possible to fully understand observed electronic spectra mainly because of the large fine and hyperfine splittings.[a]

In this paper a formalism will be presented which make possible the calculation of fine and hyperfine patterns of Na_3 in the ground and A electronic states. The approach involves treating simultaneously the pseudorational tunneling motion and the fine and hyperfine interactions since they are of the same order of magnitude.[a] The tunneling motion leads to splitting of the rotational levels into two sublevels. Depending on their symmetry, fine and hyperfine interaction operators can have nonzero matrix elements between or within the two tunneling sublevels. In the paper this will be discussed and we hope to be able to show calculated hyperfine patterns.

[a] D. T. Vituccio, O. Golonzka, and W. E. Ernst, *to be published.*

[b] N. Ohashi, M. Tsuura, and J. T. Hougen, *J. Molec. Spectrosc.* **173,** 79–99.