THE BARRIER TO FREE PSEUDOROTATION IN THE SODIUM TRIMER

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In the $\tilde{B}$ state of Na_3, the three sodium nuclei can perform an almost free pseudorotational motion in the molecular plane. The purely vibrational movement is slightly hindered in the lowest vibronic level due to the small potential barriers which separate the three equivalent nuclear configurations of this X_3-type molecule. Optical-optical double resonance spectroscopy in conjunction with resonant two-photon ionization was used to record the lowest vibronic bands (u=0, j=0, 1, 2, and 3) in the $\tilde{B}$-$\tilde{X}$ system with rotational resolution. The recently developed effective rotation-pseudorotation Hamiltonian of Ohashi *et al.*[a,b] was applied in the rotational analysis of the spectra. The Hamiltonian is described in Refs. 1 and 2 in detail and contains two terms $F j_P^2 + \frac{1}{2}V_3(1 - \cos 3\chi_P)$ which represent the three-identical-well particle-on-a-ring pseudorotational problem. While previously measured higher vibronic levels[c] do not indicate the presence of any barrier, a fit of the lowest bands yields a value V_3=10.15 cm^{-1} for the pseudorotational barrier. In their theoretical treatment of the pseudo Jahn-Teller coupling of a $^2A_1'$ and a $^2E'$ state which are believed to form the three-surface potential called the $\tilde{B}$ state of Na_3, Meiswinkel and Köppel[d] derived pseudo Jahn-Teller coupling parameters which correspond to a barrier height of 15.2 cm^{-1}. The results will be compared and supplemented by a discussion about a recently published rovibronic coupling model.[e]

[a] N. Ohashi, M. Tsuura, and J. T. Hougen, *J. Mol. Spectrosc.* 173, 79-99 (1995).
[b] N. Ohashi, M. Tsuura, J. T. Hougen, W. E. Ernst, and S. Rakowsky, to appear in *J. Mol. Spectrosc.*
[c] D. T. Vituccio, O. Golonzka, and W. E. Ernst, to appear in *J. Mol. Spectrosc.*
[d] R. Meiswinkel and H. Köppel, *Chem. Phys.* 144, 117-128 (1990).
[e] M. Mayer, L. S. Cederbaum, and H. Köppel, *J. Chem. Phys.* 104, 8932-8942 (1996).