JAHN-TELLER AND PSEUDO JAHN-TELLER INTERACTIONS IN THE B STATE MANIFOLD OF THE SODIUM TRIMER

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The B state of Na_3 is the result of the vibronic coupling of a $^2E'$ and a $^2A_1'$ state. The three states mix by pseudo Jahn-Teller (PJT) and Jahn-Teller (JT) interactions giving rise to three potential surfaces the lowest of which allows for free pseudorotational motion of the Na nuclei. Energy levels in the corresponding lowest vibronic states are well described by a new model Hamiltonian[a] which includes rotation and pseudorotation.

In this talk, we link experimentally determined molecular parameters from the Ohashi-Hougen Hamiltonian to the potential surface picture used by molecular dynamics theorists[b,c]. Of particular interest is the potential barrier to the pseudorotation which lies well below the lowest vibronic state. This small barrier can be caused by PJT or JT interaction or by a combination of both. The Hamiltonian parameter corresponding to the effective barrier height has been well determined from our analysis of high resolution spectra. Measured barrier parameters for different vibronic states allow to distinguish the influences of JT and PJT coupling on the shape of the barrier. Our study suggests that the lowest potential surface is dominated by linear PJT interaction with some smaller amount of quadratic PJT and linear JT coupling.

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[b] F. Cocchini, T.H. Upton and W. Andreoni, J. Chem. Phys., Vol. 88, No. 10, 6068-6077 (1988).
[c] R. Meiswinkel and H. Köppel, Chem. Phys. 144, 117-128 (1990).