APPLICATION OF THE DIABATIC CORRELATION METHOD TO LABELING SPECTRA OF MOLECULES CONTAINING AN INTERNAL ROTOR

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Labeling problems for rotational energy levels of asymmetric-top molecules containing a noncoaxial internal rotor are investigated by using Rose and Kellman's diabatic correlation methods. We find that $v_t = 2$ and $v_t = 3$ rotation-torsion eigenstates for acetaldehyde, which lie just below and just above the barrier to internal rotation, can be unambiguously and meaningfully labeled by nominal quantum numbers K_a corresponding to eigenstates of a suitably chosen zeroth-order symmetric-top Hamiltonian. Such a K_a labeling is shown to be superior to that based on eigenvector composition for this near-prolate asymmetric rotor. The K_a assignments from the diabatic correlation method agree with assignments made using the criterion, based on spectroscopic intuition, of smooth variation of the B value along a series of levels of given K_a and increasing J. As a second example, the $v_t = 0$ state of acetamide lies near the top of the very low barrier in this near oblate top molecule. For these torsion-rotation states also, meaningful K_a labels can be determined from the diabatic correlation method. A discussion of the method and of the results obtained for these two example molecules will be presented.