TUNNELING SPLITTING AND HYPERFINE STRUCTURE IN THE Na_3 CLUSTER

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The hyperfine structure of non-rigid molecules is of great interest especially for molecules in which the identical nuclei exchanged by the large amplitude motions(s) are also those giving rise to the hyperfine coupling.

The Na_3 cluster in its ground electronic $^2B_2$ state illustrates this case quite nicely. In this cluster the large amplitude pseudorotational motion corresponds to an interchange of the three sodium atoms and allows them to sample different electronic environments of the isosceles triangle shaped equilibrium configuration. This alters the effects of the magnetic spin-spin hyperfine interaction. For non-degenerate *A*-type tunneling levels, a completely symmetrical effective hyperfine Hamiltonian invariant under any operation of the S_3 permutation group arises. For doubly degenerate *E*-type levels, a less symmetrical effective hyperfine Hamiltonian arises.

The goal of the present talk is to understand the hyperfine pattern spectra which have been recorded for the Na_3 cluster. Although no assignments of the microwave lines are possible yet, a preliminary analysis seems to indicate that the tunneling splitting is on the order of magnitude of the hyperfine coupling. In this paper the implications of this result will be discussed considering two limiting cases: the tunneling splitting will be assumed to be either large or small compared to the hyperfine coupling. In the former case, the effective hyperfine Hamiltonians mentioned in the previous paragraph are sufficient to predict hyperfine patterns. In the latter case, *A* and *E*-type levels must be treated simultaneously. Also, as the present microwave spectra were obtained using optical-optical double resonance techniques, the way the choice of the pump transition modifies the hyperfine patterns will be tentatively described in each limiting case.