HYPERFINE EFFECTS IN NON-RIGID MOLECULES WITH FIVE EQUIVALENT NUCLEI

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The hyperfine structure of non-rigid molecules with five equivalent nuclei exchanged by one or several large amplitude motions has not yet been thoroughly investigated. This hyperfine structure should be of great interest for two reasons: *(i)* the form of the effective hyperfine coupling Hamiltonian to be used for the hyperfine energy level calculation depend on the nature of the tunneling sublevel being considered and *(ii)* hyperfine patterns depend on the symmetry species of the tunneling sublevels as a consequence of the Pauli principle. Such effects have already been studied in the case of non-rigid molecules with 3[a] and 4[b] equivalent nuclei, but not in the case of 5 equivalent nuclei. In all three cases, the hyperfine energy level calculation requires the so-called genealogical coefficients[c] which allow us to build symmetry-adapted nuclear spin wavefunctions characterized by a given value of the total nuclear spin angular momentum I and by a given symmetry species of the S_N group, which is the permutation group of N identical particles. These coefficients are known for $N = 3$[a] and 4[b], but not for $N = 5$.

In this paper, the calculation of the genealogical coefficients for 5 identical nuclei will be carried out. They will be applied to the calculation of the hyperfine structure of non-rigid species with 5 identical nuclei such as PF_5, $H_5{}^+$, and $D_5{}^+$. For these species, the effective hyperfine coupling Hamiltonian will be derived and the genealogical coefficients will be used to diagonalize this Hamiltonian, to select the hyperfine energy levels obeying the Pauli principle, and to obtain hyperfine patterns.

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