SPIN EIGENFUNCTIONS AND OPERATORS FOR THE D_n GROUPS

HERBERT M. PICKETT, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109*.

An automated procedure for determining symmetry-adapted spin eigenfunctions is developed for the D_n symmetry groups with n equivalent spins for arbitrary size of I and for $n = 3, \ldots, 6$. These eigenfunctions are also eigenfunctions of the vector sum of the n-equivalent nuclear spins. Generalized hyperfine spin operators are developed that have real matrix elements and that exploit the full symmetry. These spin operators can be combined with operators for other spins and molecular rotation using only real arithmetic.