# AN EFFECTIVE-HAMILTONIAN APPROACH TO $CH_5^+$, USING IDEAS FROM ATOMIC SPECTROSCOPY

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In this talk we present the first steps in the design of an effective Hamiltonian for the vibration-rotation energy levels of $CH_5^+$. Such a Hamiltonian would allow calculation of energy level patterns anywhere along the path travelled by a hypothetical $CH_5^+$ (or $CD_5^+$) molecule as it passes through various coupling cases, and might thus provide some hints for assigning the observed high-resolution spectra. The steps discussed here, which have not yet addressed computational problems, focus on mapping the vibration-rotation problem in $CH_5^+$ onto the five-electron problem in the boron atom, using ideas and mathematical machinery from Condon and Shortley's book on atomic spectroscopy. The mapping ideas are divided into: (i) a mapping of particles, (ii) a mapping of coordinates (i.e., mathematical degrees of freedom), and (iii) a mapping of quantum mechanical interaction terms. The various coupling cases along the path correspond conceptually to: (i) the analog of a free-rotor limit, where the H atoms see the central C atom but do not see each other, (ii) the low-barrier and high-barrier tunneling regimes, and (iii) the rigid-molecule limit, where the H atoms remain locked in some fixed molecular geometry. Since the mappings considered here often involve significant changes in mathematics, a number of interesting qualitative changes occur in the basic ideas when passing from B to $CH_5^+$, particularly in discussions of: (i) antisymmetrization and symmetrization ideas, (ii) $n, l, m_l, m_s$ or $n, l, j, m_j$ quantum numbers, and (iii) Russell-Saunders computations and energy level patterns. Some of the mappings from B to $CH_5^+$ to be discussed are as follows. Particles: the atomic nucleus is replaced by the C atom, the electrons are replaced by protons, and the empty space between particles is replaced by an "electron soup." Coordinates: the radial coordinates of the electrons map onto the five local C-H stretching modes, the angular coordinates of the electrons map onto three rotational degrees of freedom and seven bending vibrational degrees of freedom. The half-integral electron spins map onto half-integral proton spins or onto integral deuterium spins (for $CD_5^+$). Interactions: the Coulomb attraction between nucleus and electrons maps onto a Morse-oscillator C-H stretching potential, spin-orbit interaction maps onto proton-spin-overall-rotation interaction, and Coulomb repulsion between electrons maps onto some kind of proton repulsion that leads to the equilibrium geometry.