

RENNER-TELLER COUPLING IN OPEN-SHELL COMPLEXES: THE ROVIBRONIC STRUCTURE OF CH(A²Δ)-Ne

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Open-shell complexes that involve radicals in orbitally degenerate states exhibit weak-field Renner-Teller coupling effects. The CH(A²Δ)-Ne complex is an interesting example as both the anisotropy of the intermolecular potential energy surface and the spin-orbit coupling constant are small. The level splittings produced by the interaction with Ne produce a dense manifold of states. Consequently, the congested fluorescence excitation spectra observed for the A-X bands of CH-Ne could not be analyzed. The spectra have been simplified using fluorescence depletion techniques. Hole-burning of the B-X fluorescence via the A-X bands provides well-resolved spectra for the latter. Even so, unambiguous assignment of the lines still could not be achieved using a conventional combination difference analysis. To resolve the ambiguities we are predicting the ro-vibronic structure of CH(A)-Ne using high-level *ab initio* methods. Potential energy surfaces have been calculated using the CASSCF-MRCI(SD) level of theory^a. The bound states supported by these surfaces are calculated using product basis sets for the angular coordinates, combined with an optimized DVR treatment of the radial coordinate. The results of these calculations and assignments for the A-X bands of CH-Ne will be presented.

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^aU. Schnupf, Ph. D. Thesis, Dept. of Chemistry, Emory University 1995.