NON ADIABATIC EFFECTS IN THE PHOTELECTRON SPECTRA OF Al_6N^-

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The experimental photodetachment spectra of Al_6N at 193 nm [1], for the first seven low-lying electronic states, are interpreted theoretically using the vibronic coupling theory. Here, the potential energy curves (PECs) obtained through ab initio electronic structure calculations provide the Hamiltonian parameters corresponding to the model vibronic Hamiltonian[2] . These PECs also ascertained the presence of non-adiabaticity among closely spaced electronic states. Furthermore, the theoretical spectra were obtained utilising the time dependent and time-indipendent quantum chemistry approaches by following uncoupled and coupled dynamics. In the uncoupled dynamics, the vibrational structures of all spectral bands are examined and discussed through Poisson intensity distribution and wave packet density plots. At the same time, in the coupled dynamics, we studied the nonadiabatic effects through reduced dimensional calculations and diabatic electronic population transfer.

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