

Abstract Submitted
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Multi channel quantum defect theory calculations of the Rydberg spectra of HCO¹ NICOLAS DOUGUET, ANN OREL, University of California at Davis — We present a first-principles theoretical study of the photoionization spectra of vibrationally autoionizing Rydberg states converging to excited states of HCO⁺. The clamped-nuclei scattering matrix, quantum defects parameters and transition dipole moments are explicitly calculated using the complex variational Kohn technique. The multi-channel quantum defect theory and vibrational frame transformation are then used to calculate the absorption spectrum. The results are compared with experimental data on double-resonance spectroscopy of the high Rydberg states of formyl radical.

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