A THEORETICAL STUDY OF CN SPECTROSCOPY FROM THE IR TO THE VUV

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We have carried out first principles calculations of the spectrum of CN. We have included Rydberg states, spin-orbit and non-adiabatic coupling between different electronic states, and an accurate treatment of the ro-vib-spin-electronic wavefunctions. Doublet, quartet and sextet spin states are included in our calculations. These wavefunctions are used with electric dipole and quadrapole and magnetic dipole transition moments to predict spectra. We consider both bound-bound, bound-free and free-bound transitions. When possible, comparisons are made with experimental results, both for energy levels and radiative lifetimes. Many previously uncharacterized bands are predicted.