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Vibratonal Spectra and DFT calculations of dipicolinic acid and its calcium salt[1] KATHLEEN MCCANN, JAAN LAANE, Texas A&M University, College Station, Texas — The infrared and Raman spectra of dipicolinic acid (DPA) and calcium dipicolinate have been recorded in the solid phase and their vibrations have been assigned. DFT calculations using B3LYP/6-311++G** have been used to calculate the spectra of the free dipicolinic acid molecule and its ion in an environment free of intermolecular interactions. Calculations have also been carried out to better understand the effects of intermolecular hydrogen bonding and the interactions between water and DPA. The calculated frequencies agree well with the experimental values after scaling.

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