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Effect of nuclear motion on the absorption spectrum of dipicolinic acid[1] PETRA SAUER, YURI ROSTOVTSEV, ROLAND ALLEN, Texas A&M University — A current scientific challenge is the rapid detection of chemical and biological substances, including bacterial spores. A significant component of spores is the molecule dipicolinic acid (DPA or 2,6-pyridinedicarboxylic acid) and its salts. A variety of spectroscopic detection schemes are being explored, including fluorescence spectroscopy, ultraviolet and visible resonant Raman spectroscopy, and FAST CARS. Using semiclassical electron-radiation-ion dynamics (SERID), we have examined the effect of nuclear motion, resulting from both finite temperature and the response to a radiation field, on the line broadening of the excitation profile of DPA. With nuclei fixed, we find a relatively small broadening associated with the finite time duration of an applied laser pulse. When the nuclei are allowed to move, the excitation spectrum exhibits a much larger broadening, and is also reduced in height and shifted toward lower frequencies. In both cases, the excitation is due to well-defined π to $\pi*$ transitions. The further inclusion of thermal motion at room temperature broadens the linewidth considerably because of variations in the molecular geometry: Transitions that had zero or negligible transition probabilities in the ground state geometry are weakly excited at room temperature.

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