Spectroscopic Studies of Cyclic Enones in Triplet Excited States

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The main goal of this grant is to characterize the structure and dynamics of low-lying triplet excited states of monocyclic enones. We use the highly sensitive cavity ringdown (CRD) spectroscopic technique to contend with the spin-forbiddenness of the singlet-triplet transitions originating in the electronic ground state. During year 2 of the grant we focused on the molecules 2-cyclohexen-1-one (2CH) and 4-cyclopenten-1,3-dione (4CPD).



In 2CH, as well as the 2-cyclopenten-1-one (CP) molecule studied previously, we found significant differences when comparing ring vibrational frequencies in the singlet vs. triplet (n,π^*) excited states. To investigate whether this is a general property of the conjugated cyclic enones, we recorded the first $T_1(n,\pi^*) \leftarrow S_0$ CRD absorption spectrum of the 4CPD molecule. The spectrum is shown at left along with vibronic assignments. Analysis of combination differences shows that the v_{19} (ring pucker) fundamental frequency in the $T_1(n,\pi^*)$ and $S_1(n,\pi^*)$ states is nearly the same, whereas the v_{14} (ring twist) frequency is 20% lower in T_1 than in S_1 .