第197回 化学コロキウム 日時:3月22日13時から 会場:8-301教室 News from ELISA

. 13:00-14:00 *Lisbeth Munksgaard Nielsen* (Aarhus Univ.) Circular Dichroism Fingerprint of the Thymine Photodimer

Thymine photodimers can be formed in DNA where two neighboring thymine bases are present. In this study short DNA single strands of thymine in solution were exposed to UV light at 254 nm to form photodimers. Absorption data reveals that a constant fraction of 45% of the maximum possible photodimers is formed in the thymine single strands. Furthermore, we determine the circular dichroism fingerprint of a thymine photodimer within the thymine single strands. This fingerprint is found to be independent of the strand length.

14:00-15:00 *Kristian Stochkel* (Aarhus Univ.) Absorption spectrum of the firefly luciferin anion isolated in vacuo

The excited-state physics of the firefly luciferin anion depends on its chemical environment, and it is therefore important to establish the intrinsic behavior of the bare ion. Here we show the electronic absorption spectra of the anion isolated *in vacuo* obtained at an electrostatic ion storage ring and an accelerator mass spectrometer (SEP1) where ionic dissociation is monitored on a long time scale (from 33 μ s and up to 3 ms) and on a short time scale (0 to 3 μ s), respectively. In the ring experiment the yield of all neutrals (mainly CO₂) as a function of wavelength was measured whereas in the single pass experiment, the abundance of daughter ions formed after loss of CO₂ was recorded to provide action spectra. We find maxima at 535 nm and 265 nm, and that the band shape is largely determined by the sampling time interval, which is due to the kinetics of the dissociation process. Calculations at the TD-B3LYP/TZVPP++ level predict maximum absorption at 533 nm and 275 nm for the carboxylate isomer in excellent agreement with the experimental findings. Our data serve to benchmark future theoretical models for bioluminescence from fireflies.