Action (dissociation) spectroscopy of pyrene dimer cations in the gas phase

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Beams of dimer cations of pyrene $(C_{16}H_{10})_2^+$ can be produced with a broad internal energy distribution using an electron cyclotron resonance (ECR) ion source. These dimer cations have been stored up to 2 ms in a compact, home designed in ILM (Lyon, France), electrostatic ion storage ring, so-called the Mini-Ring. The photo-dissociation spectrum shown in Figure 1 has been recorded by scanning the wavelength of an OPO laser and counting the neutral fragments exiting the Mini-Ring. Two bands have been observed corresponding to the charge resonance (CR, shown in Figure 1) and the local excitation (LE, not shown in figure 1). Theoretical spectra have been computed in Toulouse using using a Density Functional based Tight Binding approach modified to treat charge/excitation resonance at different temperatures from 10 K to 500 K (also displayed in figure 1). The calculations show that the CR band is not only broadened when increasing temperature but also shifted towards lower energy. Twisting motion of the monomers induced by temperature effects leads to configurations in which the CR can be strongly weakened, which leads to a shift of the excitation towards lower energy. The experimental spectrum would better correspond to an intermediate temperature between 300 K and 500 K.

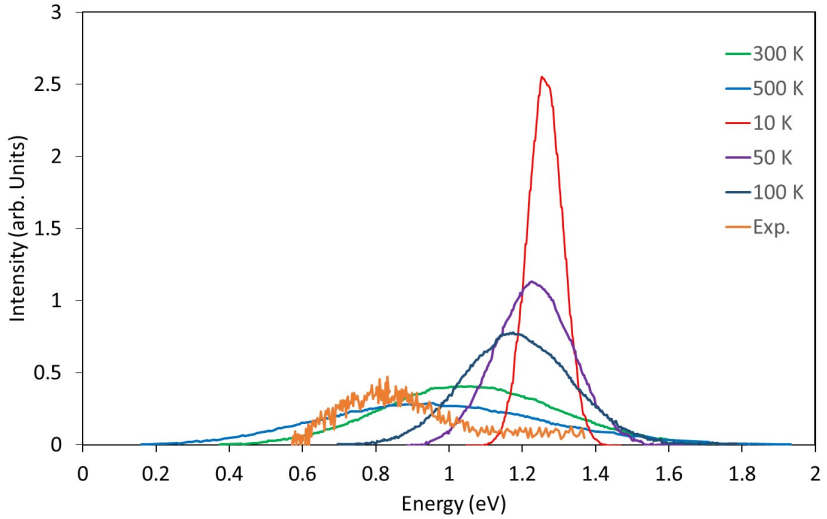

Figure 1: Experimental photo-dissociation spectrum (orange line) of pyrene dimer cations and theoretical absorption spectra calculated at different temperatures from 10 K to 500 K.

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