Phosphorescence of hydrogen-capped polyenes in solid neon at 20 K

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Linear carbon chain molecules are highly reactive and thought to be reaction intermediates converted to carbon nanostructures such as fullerenes, nanotubes, and graphene. Terminated by hydrogen or chemically inert moieties such as a cyano-group, the carbon chain molecules acquire intrinsic stability to be isolated in solutions at ambient temperature. We have developed a method to produce, isolate, and concentrate in solutions a series of hydrogen-end-capped molecules, namely polyynes $H(C{\equiv}C)_nH$ (n = 4-8), to characterize them by UV absorption, IR absorption [1], and resonance Raman spectroscopy [2]. Formation mechanism of cyanopolyynes, $H(C{\equiv}C)_nC{\equiv}N$ (n = 3-6), was also investigated by NMR spectroscopy using ^{13}C isotope-enriched samples [3]. Recently, phosphorescence spectra were reported for cyanopolyynes through HC_5N to HC_9N in solid rare-gas matrices [4-6]. In the present work, size-separated polyynes were co-condensed with the solvent molecules of hexane at 20 K in vacuum and subjected to phosphorescence spectroscopy.

Figure 1: Phosphorescence spectrum of C_8H_2 in solid hexane at 20 K. Peaks in vibrational progression of the symmetric stretching ν_2 mode of the *sp*-carbon chain (~2190 cm^{-1}) are conspicuous at 532, 603, 694, 815, and 988 nm for 0-ν bands (ν = 0-4). Inset shows phosphorescence lifetime of ~31.0 ms for the $a^3\Sigma_u^+ \rightarrow X^1\Sigma_g^+$ transition of C_8H_2 at 20 K.

References

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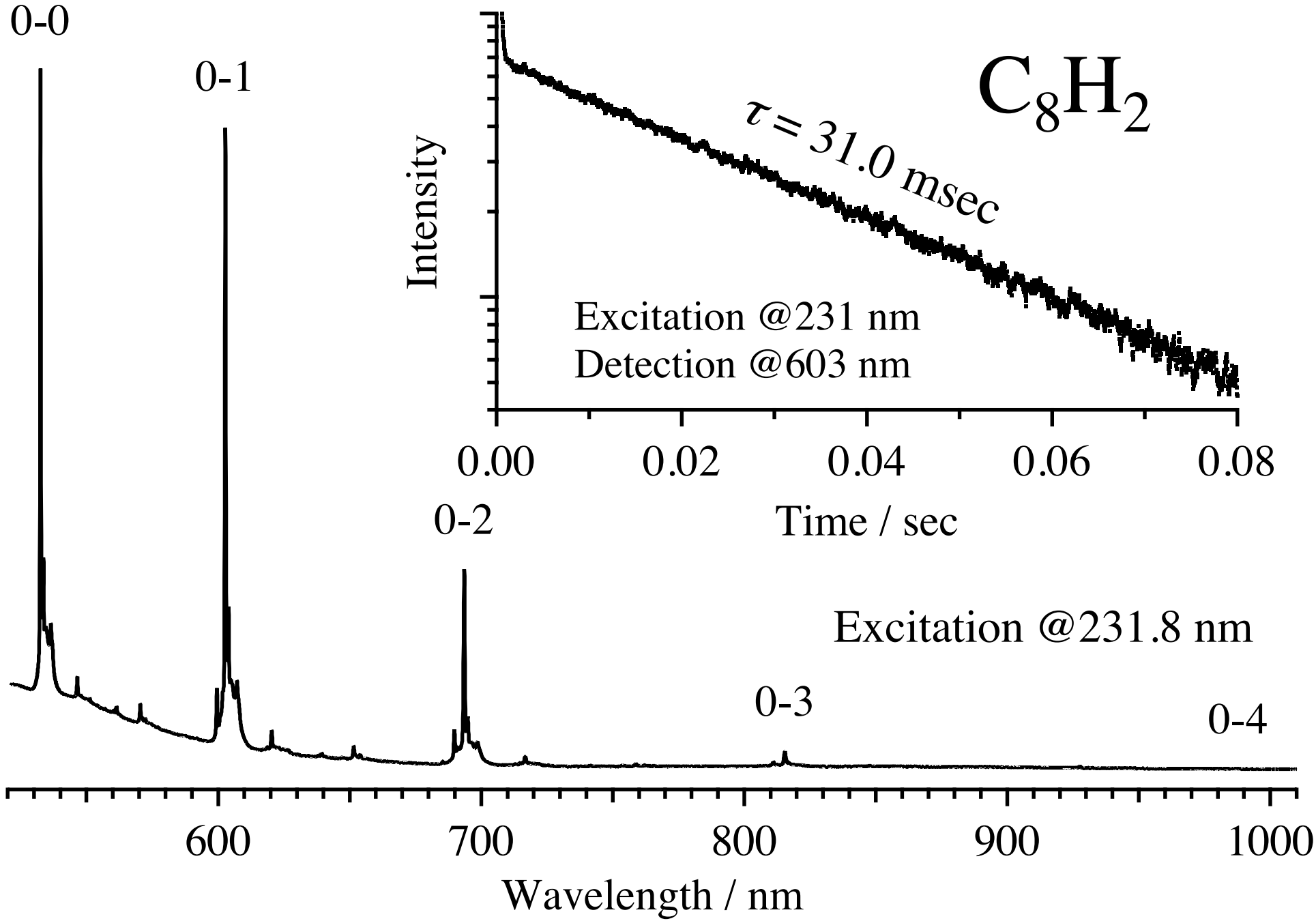
0-0
0-1
0-2
0-3
0-4
C_8H_2
$\tau = 31.0$ msec
Intensity
Excitation @231 nm
Detection @603 nm
0.00
0.02
0.04
0.06
0.08
Time / sec
Excitation @231.8 nm
600
700
800
900
1000
Wavelength / nm