

Electron energy loss spectra of thiophene

Reference: Knut R. Asmis and Michael Allan, Université de Fribourg (unpublished).

Knut R. Asmis, Ph.D. thesis, Fribourg 1996

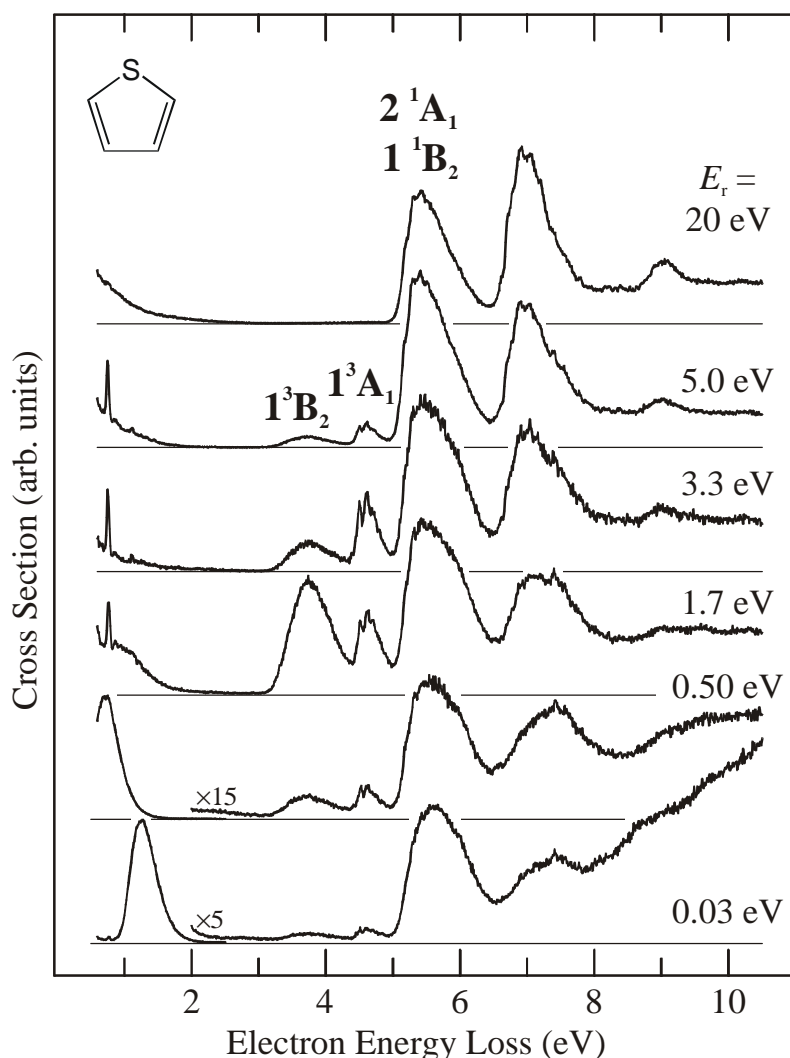


Fig. 1 Survey EEL spectra of thiophene measured at constant residual energies between 0.03 and 20 eV. The two lowest valence triplet states are found at 3.74 and 4.62 eV. The band observed in the region from 4.9 to 6.5 in the $E_r = 20$ eV has a maximum at 5.43 eV, with weak vibrational structure visible on the band envelope. At $E_r = 0.03$ eV the onset of the now structureless band is moved to 5.0 eV and the maximum to 5.61 eV. A magnetic circular dichroism study (Håkansson *et al.* 1977) has reported at least two transitions in this region of the spectrum, at 5.26 and 5.64 eV. The CASPT2 study by Serrano-Andrés *et al.* (1993c) predicts two valence singlet-singlet transitions with similar oscillator strength at 5.33 (2^1A_1 , $f = 0.09$) and 5.72 eV (1^1B_2 , $f = 0.07$). Our spectra confirm this assignment, placing the 2^1A_1 state at 5.43 and the 1^1B_2 state at 5.61 eV. (see K. R. Asmis, Ph.D. thesis, for details.)

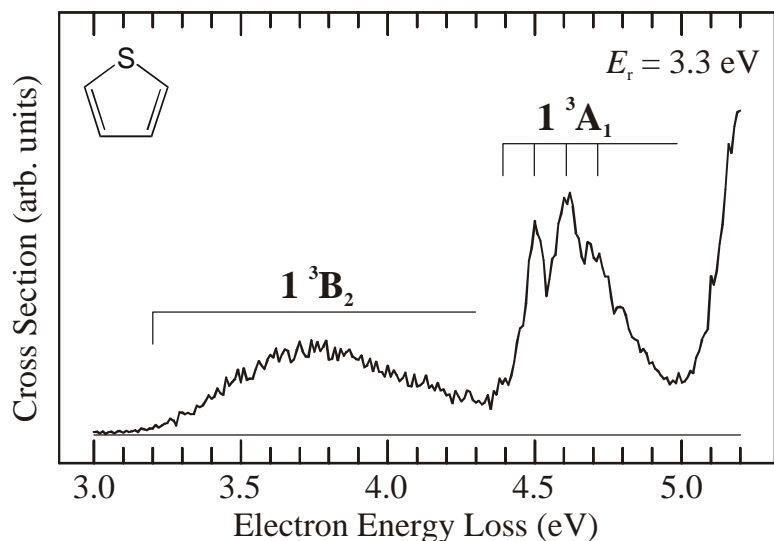


Fig. 2 Detail of the triplet states measured at $E_r = 3.3 \text{ eV}$. The 1^3B_2 band peaks at 3.74 eV. In contrast to previous electron impact studies the second triplet band shows vibrational structure starting with a weak shoulder at 4.38 eV, followed by peaks at 4.50 and 4.62 eV. The shoulder is assigned to the 0-0 transition and the observed peaks could be members of a single vibrational progression with a spacing of 0.12 eV (970 cm^{-1}).

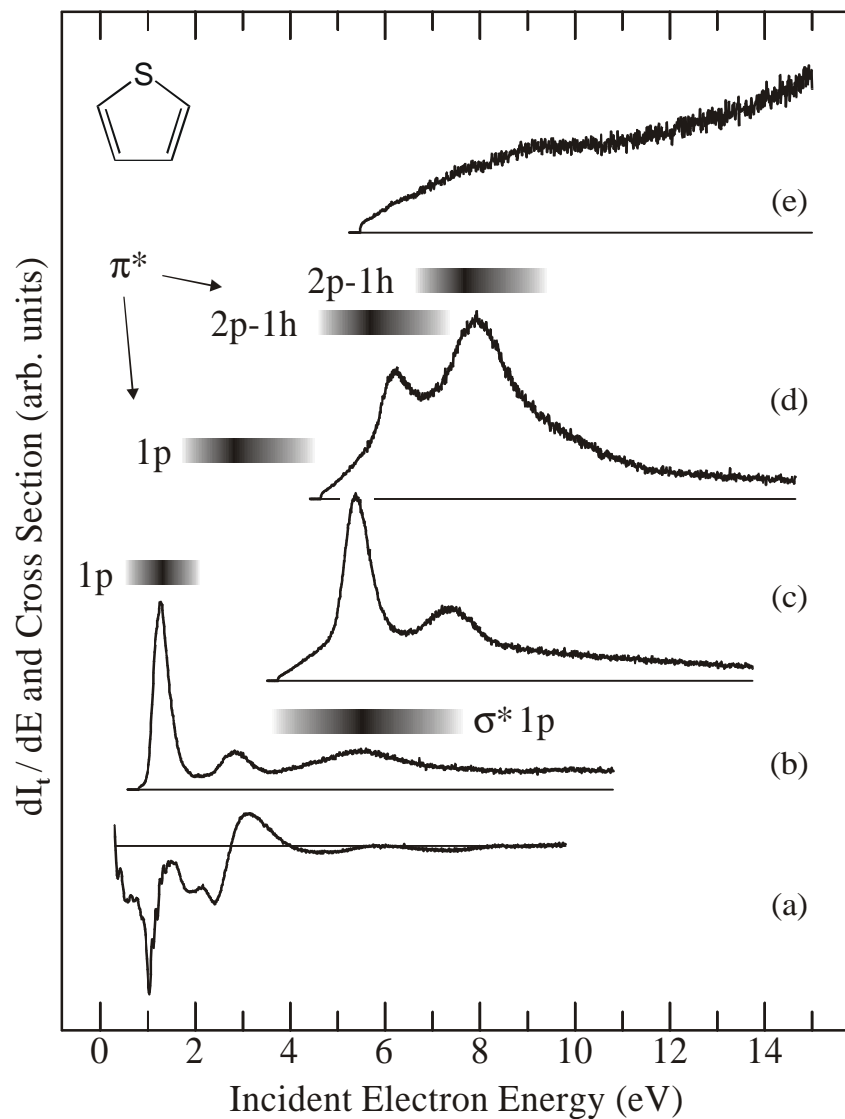


Fig. 3 Electron transmission spectrum spectrum (a) of thiophene compared to vibrational (b: $\Delta E = 0.78$ eV) and electronic excitations functions, measured at the vertical excitation energies of the 1^3B_2 (c: $\Delta E = 3.72$ eV), 1^3A_1 (d: $\Delta E = 4.62$ eV) and 2^1A_1 (e: $\Delta E = 5.45$ eV) state. (see K. R. Asmis, Ph. D. thesis, for details)