Electron energy loss spectra of pyrrole

Reference: Knut R. Asmis and Michael Allan, Université de Fribourg (unpublished).

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

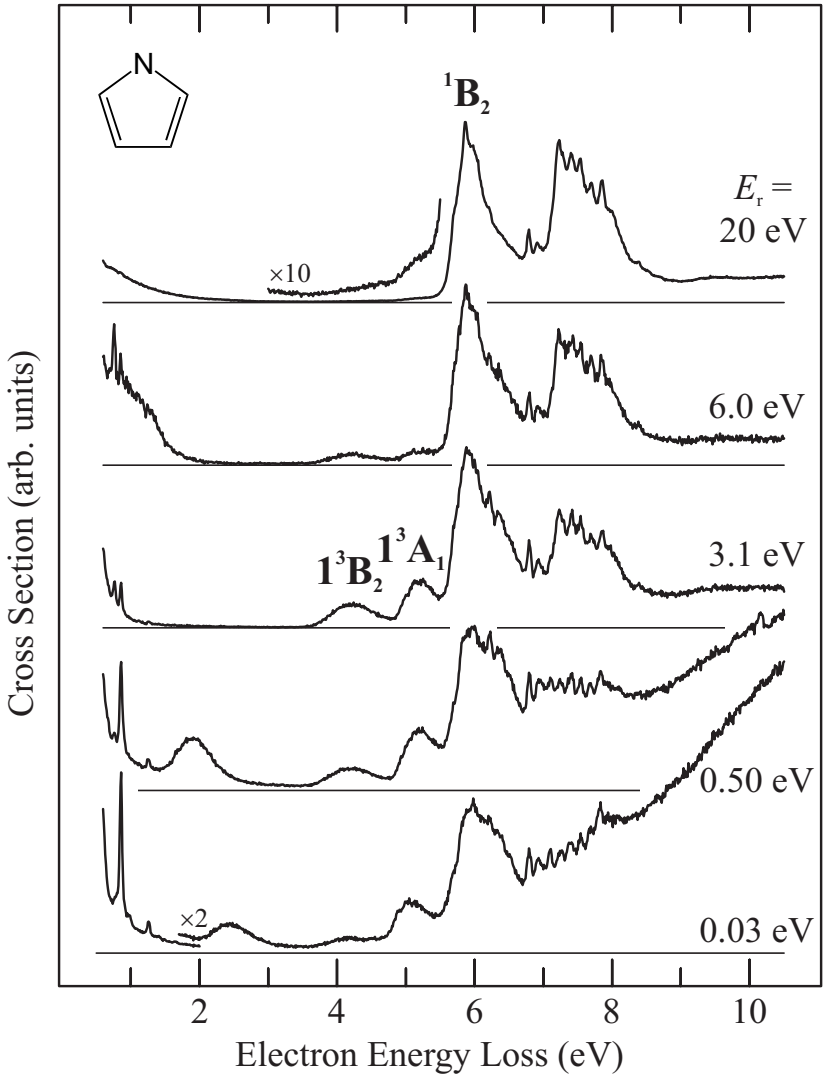

Fig. 1 Survey EEL-spectra of pyrrole. At medium and low residual energy ($E_r \leq 6.0$ eV) two triplet bands at 4.21 and 5.17 eV are observed, previously assigned to the transitions into 1^3B_2 and 1^3A_1 valence excited triplet states (Van Veen 1976). The shoulder seen between 4.9 and 5.4 eV in the E_r = 20 eV spectrum is not attributed to the 1^3A_1 state, but believed to result from a dipole-forbidden spin-allowed transition (Flicker *et al.* 1976). A similar, weak feature is observed in the vapor absorption spectrum and is absent in the crystal spectrum (Bavia *et al.* 1976). It has been assigned to the $^1(\pi,3s)$ Rydberg state. The intense band extending from 5.4 to 6.7 eV is the result of various optically allowed Rydberg and valence transitions. The largest contribution is expected from the valence $^1B_2$ excitation (5.98 eV peak, E_r = 0.03 eV). Signal due to $^1(\pi,3p)$ Rydberg transitions move the maximum of this band to 5.86 eV at E_r = 20 eV. (see K. R. Asmis, Ph.D. thesis, for details.)

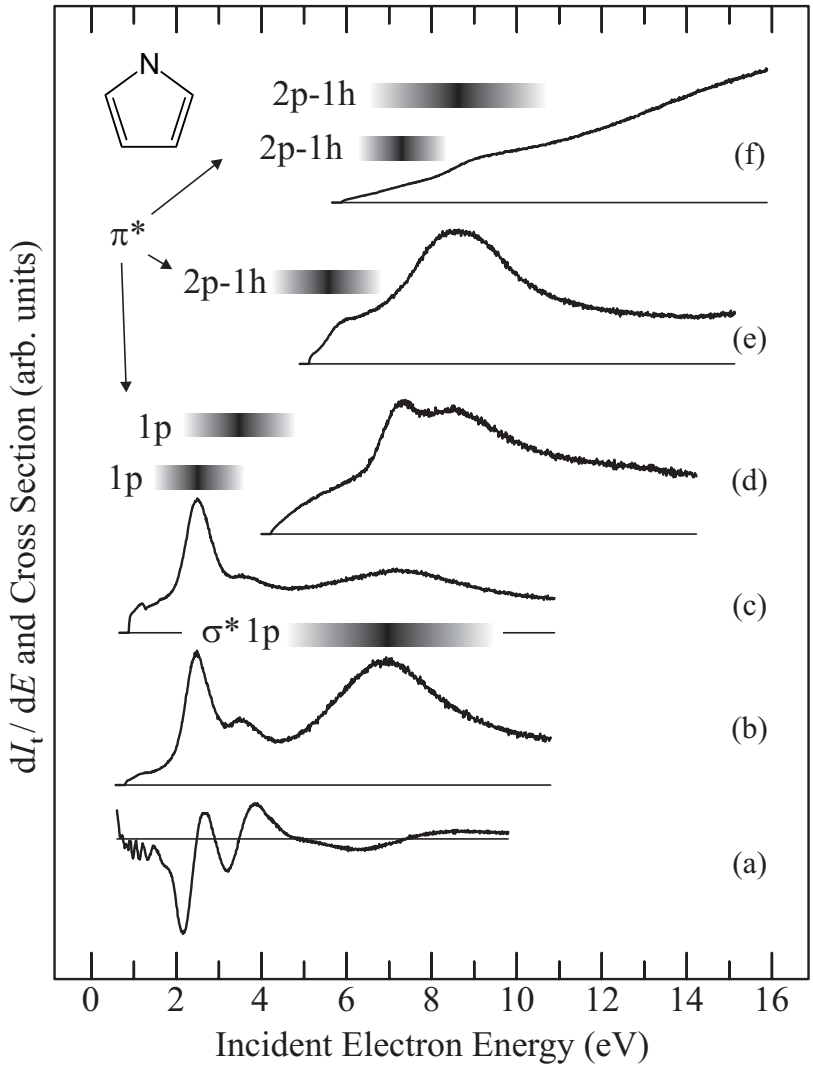

Fig. 2 Electron transmission spectrum (a) of pyrrole compared to excitations functions of pure vibrational excitation (b and c: $\Delta E = 0.77$ and 0.86 eV), the lowest triplet state (d: $\Delta E = 4.20$ eV), the second lowest triplet state (e: $\Delta E = 5.10$ eV) and the first optically allowed valence transition (f: $\Delta E = 5.86$ eV). The shaded rectangles indicate assignment of the bands to "one-particle" (1p) and "two particles – one hole" (2p-1h) resonances. (see K. R. Asmis, Ph. D. thesis, for details)