Electron energy loss spectra of furan

Reference: Knut R. Asmis and Michael Allan, Université de Fribourg (unpublished).

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

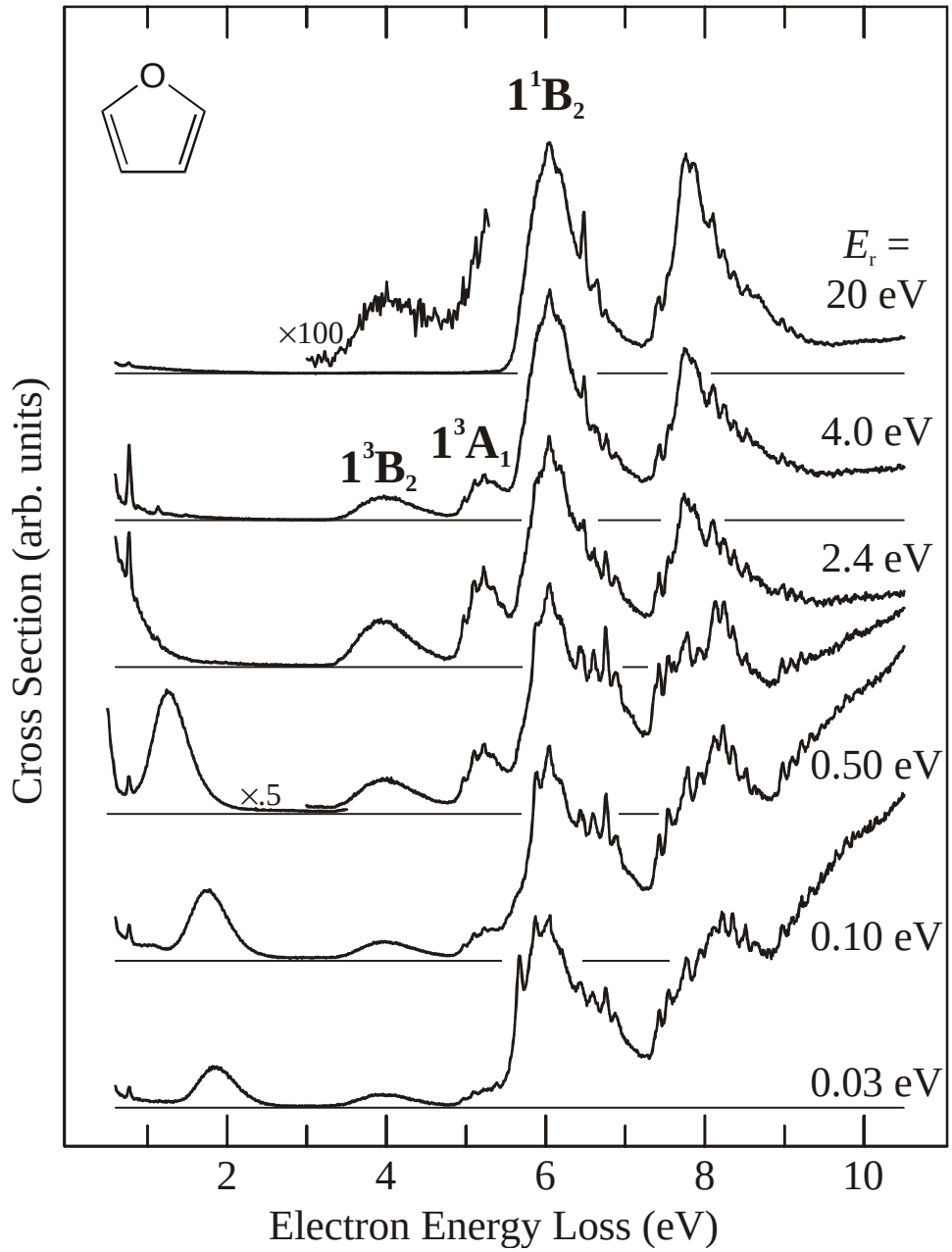

Fig. 1 Survey EEL spectra of furan. The two bands, best seen in the E_r = 2.4 eV spectrum, extending from 3.3 to 4.8 and 4.8 to 5.6, centered at 3.95 and 5.22 eV respectively, have been assigned to the two lowest valence triplet states (Van Veen 1976). The band observed between 5.5 and 7.3 eV is the result of various valence and Rydberg excitations. Its form and position change noticeably with changing E_r. For E_r = 20 eV the maximum lies at 6.04 eV and has been assigned to the vertical excitation energy of lowest valence excited singlet state 1^1B_2, which is believed to contribute predominantly at this residual energy. The weak

features observed in the VUV absorption spectrum on the low energy side of the strong 1^1B_2 band have been attributed to the 2^1A_1 valence state, which has been determined to lie at 5.80 eV (Roebber *et al.* 1980). It is of interest to note, that the two sharp peaks at 5.67 and 5.87 eV observed in the E_r = 0.03 eV spectrum have not been reported before. We assign them to the $^2(\pi,3s^2)$ Feshbach resonance. Its parent state $^1(\pi,3s)$ is known to lie at 5.91 eV (Roebber *et al.* 1980), resulting in a Feshbach decrement of 0.24 eV. (see K. R. Asmis, Ph.D. thesis, for details.)

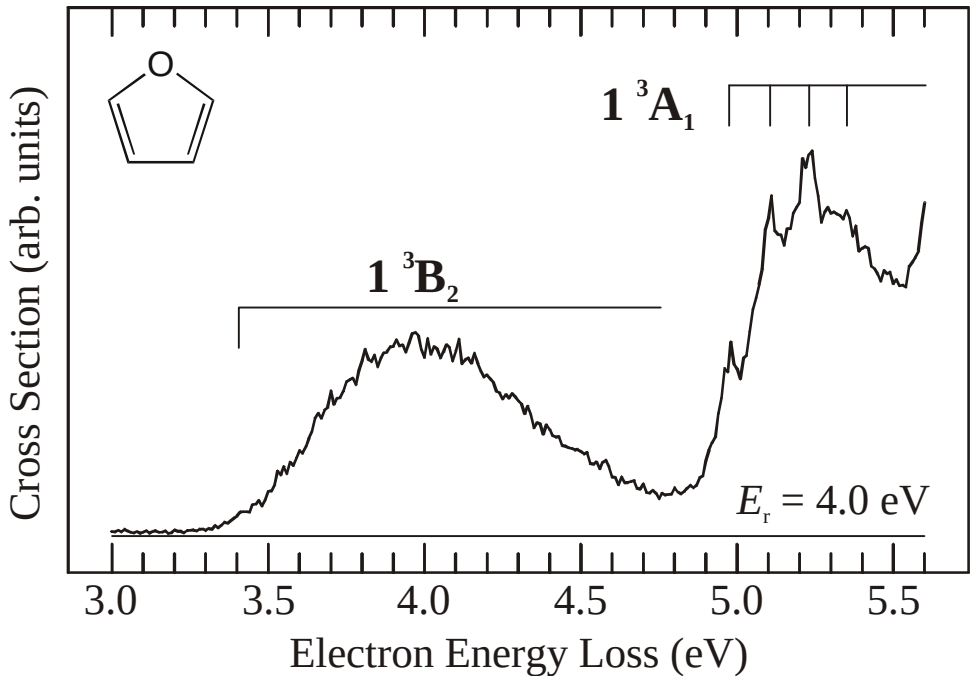

Fig. 2 Detail of the triplet states.

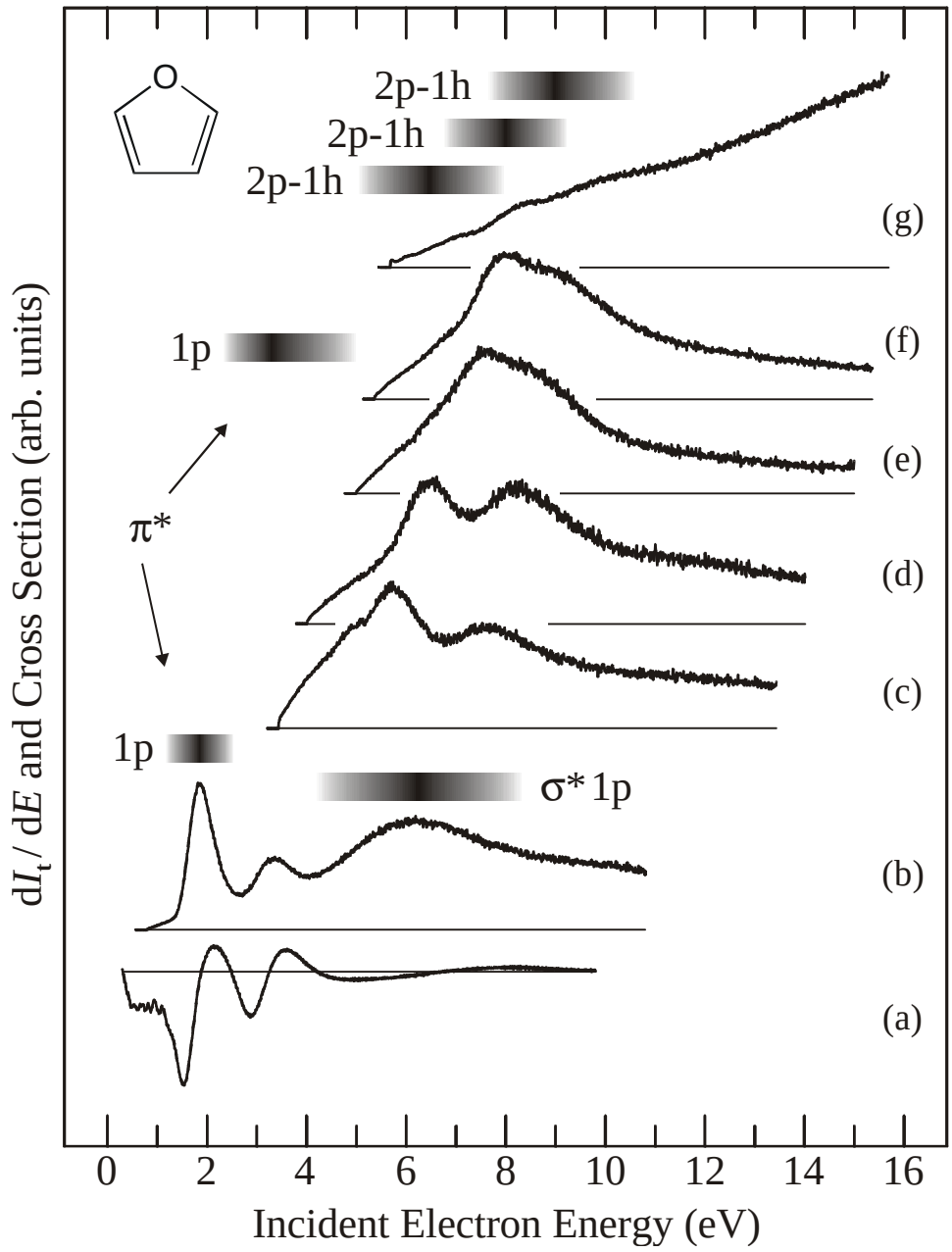

Fig. 3 Electron transmission spectrum (a) of furan compared to excitations functions of pure vibrational excitation (b: $\Delta E = 0.77$ eV), the lowest triplet state (c and d: $\Delta E = 3.41$ and 3.99 eV), the second lowest triplet state (e and f: $\Delta E = 4.97$ and 5.34 eV) and the first dipole-allowed transition (g: $\Delta E = 5.66$ 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)