

## Electron energy loss spectra of *trans*-butadiene

Reference: Knut R. Asmis, Dunja M. Frey and Michael Allan, Université de Fribourg (unpublished).

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

Dunja M. Frey, diploma thesis, Fribourg 1994

M. Allan, *Chimia* 48 (1994) 372.

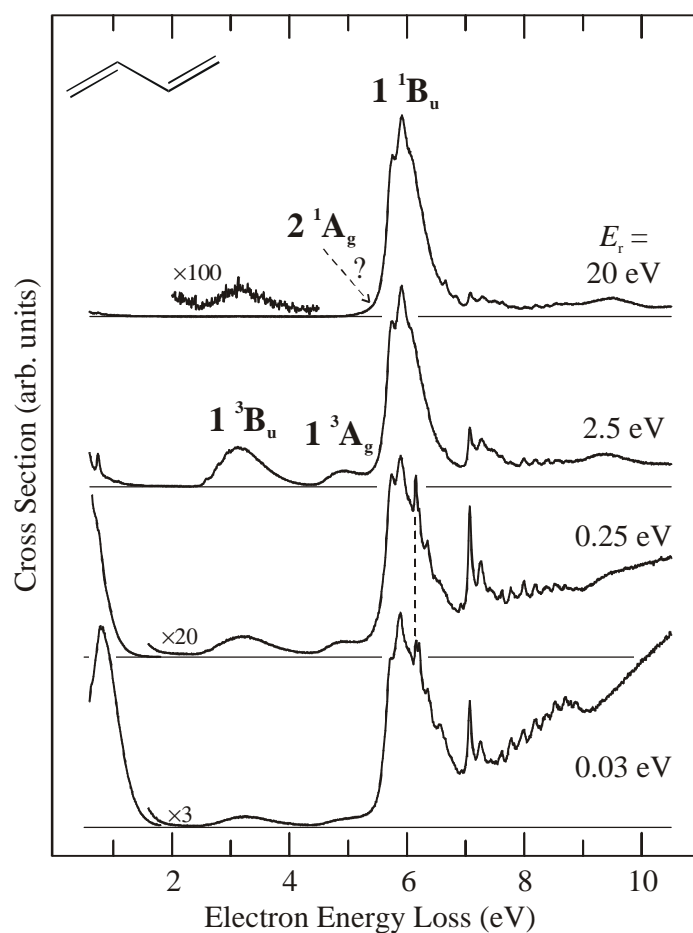


Fig. 1 Survey EEL-spectra of butadiene at residual energies of 0.03, 0.25, 2.5 and 20 eV. The transitions into the lowest two triplet states are enhanced at medium residual energies. The bands below 2 eV are due to resonant vibrational excitation. The spectra were recorded with the magnetically collimated spectrometer — they show the sum of  $0^\circ$  and  $180^\circ$  DCSs. (from K. R. Asmis, Ph.D. thesis)

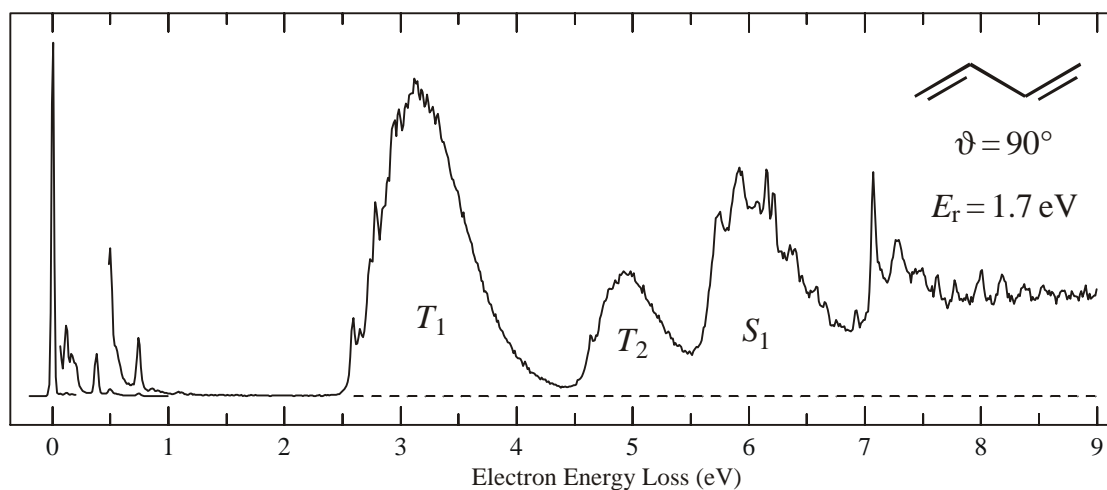


Fig. 2 EEL spectrum recorded with the spectrometer with hemispherical analysers. The conditions emphasize spin-forbidden transitions. (see also M. Allan, *Chimia* 48 (1994) 372)

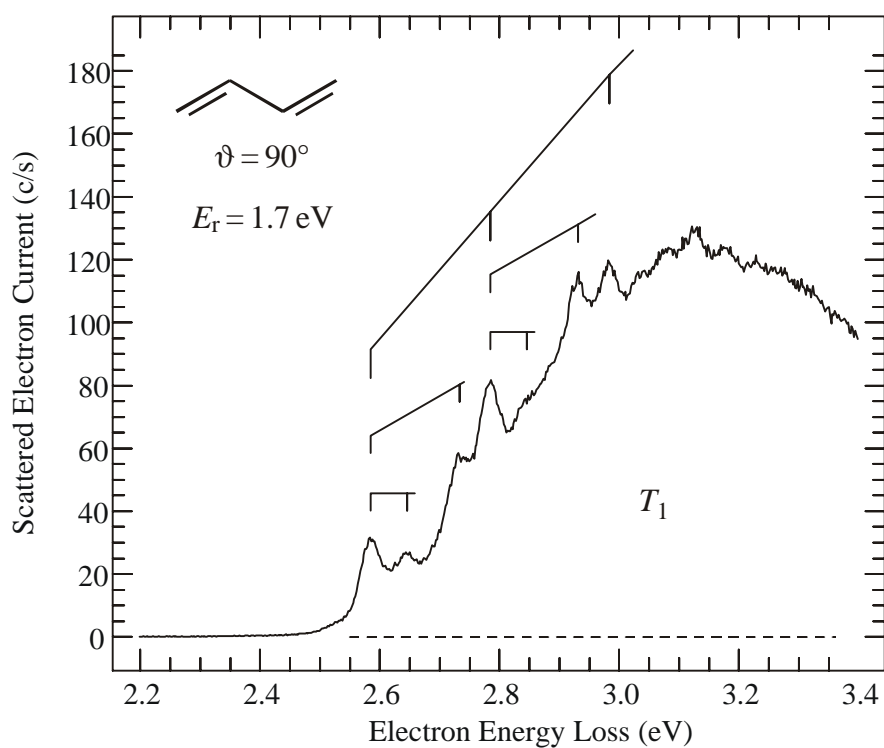


Fig. 3 Detailed recording of the first triplet band. Three vibrational spacings can be identified as indicated.

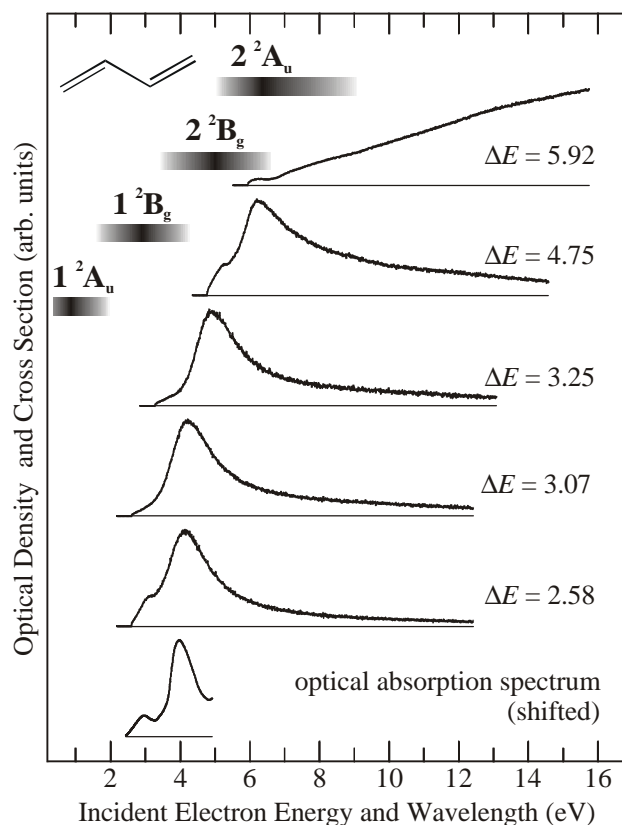


Fig. 4 Excitation functions of the  $1^3B_u$  ( $\Delta E = 2.58, 3.07$  and  $3.25$  eV),  $1^3A_g$  ( $\Delta E = 4.75$  eV) and  $1^1B_u$  ( $\Delta E = 5.92$  eV) states of butadiene. The optical absorption spectrum (T. Shida and W. H. Hamill, *J. Am. Chem. Soc.* 88 (1966) 5371) of the radical anion has been shifted by 0.80 eV. The centers and widths of the lowest four resonances are indicated by the shaded rectangles. The spectra were recorded with the magnetically collimated spectrometer — they show the sum of  $0^\circ$  and  $180^\circ$  DCSs. (see K. R. Asmis, Ph. D. thesis, for details)

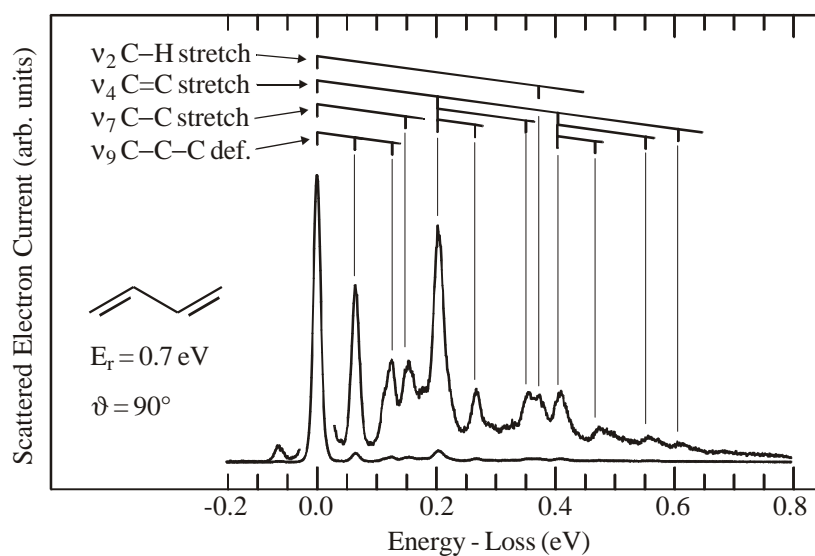


Fig. 5 Typical vibrational EEL spectrum. (from M. Allan, *Chimia* 48 (1994) 372)

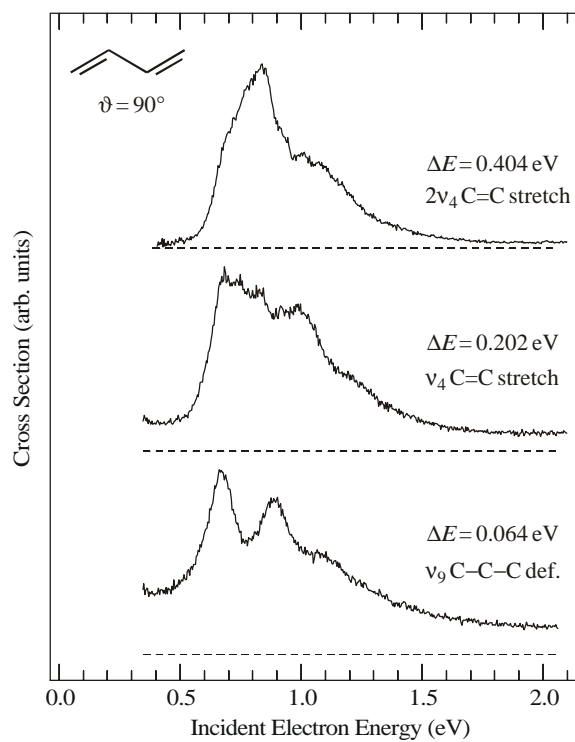


Fig. 5 Typical vibrational excitation functions. As in benzene, the shape of the boomerang structures depends strongly on the choice of the final channel.