High Resolution Photoabsorption Studies at the Carbon and Oxygen K Edges of Small Organic Molecules

K.C. Prince¹, M. de Simone², R. Richter¹, and M. Coreno³

¹Sincrotrone Trieste, ss 14, km 163.5, Area Science Park, I-34012

Basovizza (Trieste), ITALY

²Università di Roma III ed Unità INFM, Via della Vasca Navale 84, I-00146 Rome, ITALY

³INFM- TASC, Laboratorio ELETTRA, I-34012 Trieste, ITALY

We report the carbon and oxygen K edge x-ray absorption spectra of a series of oxygen containing organic molecules (formaldehyde, formic acid, acetaldehyde, acetone, methanol and dimethyl ether), with measured the cross-section determined in absolute units.

At the carbon K edge, most species show vibrational structure; the spectrum of formaldehyde is in good agreement with that of [1], whereas few high resolution spectra of the other gases have been reported. Tentative assignments are given and the vibrational structure discussed in terms of the equivalent core molecule.

At the oxygen K edge, only formaldehyde shows vibrational structure, indicating that the O 1s excited state of the carbonyl chromophore is bound. This is important as it suggests that for the very similar molecules acetaldehyde and acetone, the structure is not absent due to lifetime broadening, but is obscured by many overlapping vibrational bands due to the larger number of degrees of freedom. This implies that the excited states of aldehdydes and ketones are most likely bound. For oxygen K edge spectra of the saturated molecules methanol, formic acid (OH) and dimethyl ether no vibrational structure is observed, but more states are observed than in previous EELS studies [2-4].

The changes in the distribution of oscillator strength near threshold as a function of the molecular structure is discussed.

References.

- 1. G. Remmers et al, Phys. Rev. A 46 (1992) 3935.
- 2. I. Ishii and A.P. Hitchcock, J. Electron Spec. and Rel. Phenomena **46** (1988) 55.
- 3. A.P. Hitchcock and C. E. Brion, J. Electron Spec. and Rel. Phenomena 19 (1980) 231.
- 4. B.X. Yang, J. Kirz and T.K. Sham, Phys. Rev. A 36 (1987) 4298.