

THE PHOTOIONIZATION MASS SPECTROMETRIC STUDY OF THE THREE-MEMBERED RING SYSTEMS C_3H_6 , C_2H_4O and C_2H_4S AND THEIR OPEN CHAIN ISOMERS.

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A previous contribution to this volume [1] reported about a the investigation of three-membered ring systems, i.e. Cyclopropane, Oxirane and Thiirane. We briefly described their V-UV photoabsorption spectra. These are essential tools for the understanding of the photoionization of these molecules which will briefly be reported here. The same work has been performed for the open chain isomers, i.e. propene and acetaldehyde. The thio-derivative corresponding to the latter compound is very unstable and therefore could not be investigated here.

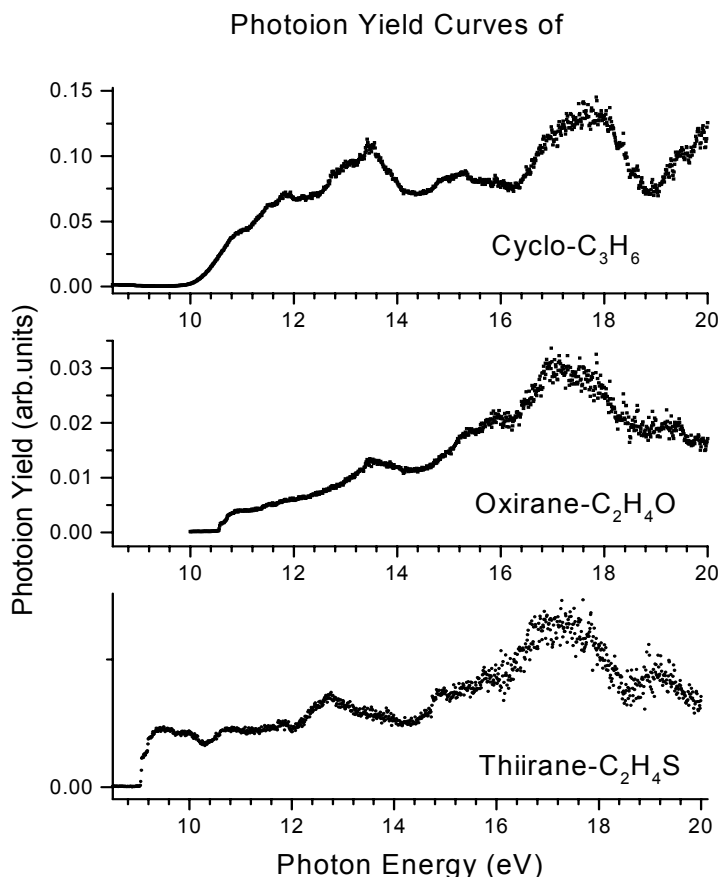


Fig.1: Photoionization efficiency curves of the Cyclopropane, Oxirane and Thiirane molecular ions.

The most extensive photoionization study dedicated to two of these molecules, i.e. C_3H_6 and C_2H_4O (ring and open chain isomers), has been published by Kraessig et al. [2] using synchrotron radiation. Most of the fragmentation pathways were considered. More recently, a low resolution dissociative photoionization study of Oxirane by synchrotron radiation has been reported [3], completed by quantum mechanical calculations. The threshold energy for almost all dissociation channels was measured.

For Thiirane the literature data are very scarce. Only one dissociative photoionization work, restricted to the molecular ion and two fragments, i.e. $m/z=59$ and $m/z=45$, has to be mentioned [4].

The present dissociative photoionization study has been performed on the 3m-NIM monochromator, equipped with a 600 ℓ/mm Al-grating and slit

widths adjusted at 20 μ m (resolution about 5 000).

Fig.1 shows the ionization efficiency curve for the three parent ions, i.e. of Cyclopropane, oxirane and thiirane respectively. Up to about 15 eV the signal/noise ratio is satisfactory. Above this energy this ratio decreases dramatically owing to the 90% reflectivity loss of the grating installed on the monochromator. However, the main and usually structureless features remain measurable. Fig. 2 displays the threshold region of the ion yield curve of $C_2H_4O^+$ and $C_2H_4S^+$ near threshold. The crude numerical first differential is inserted

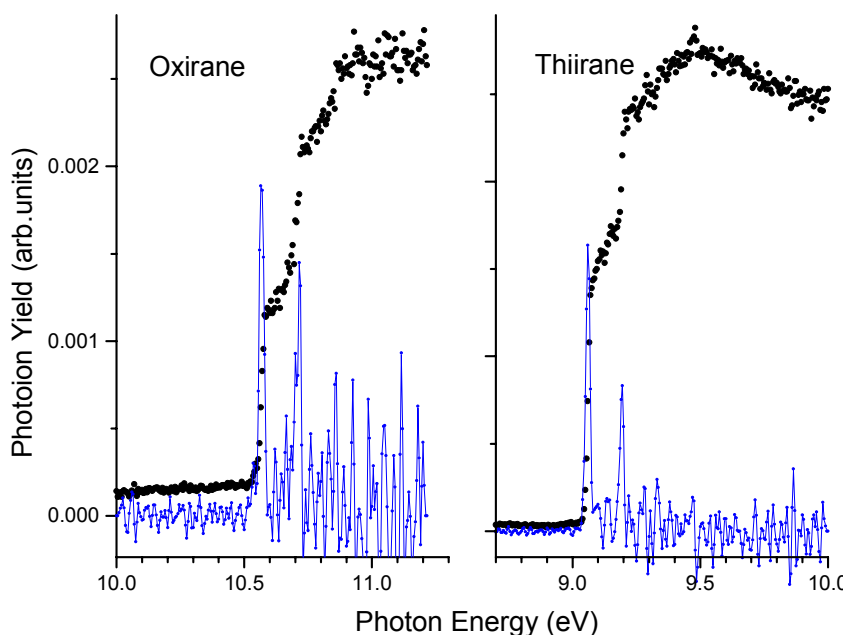


Fig.2: Direct (black) and numerically first differentiated (blue) photoion yield curves of $C_2H_4O^+$ and $C_2H_4S^+$ near threshold.

in this figure to compare the vibrational intensity distribution with that observed in the He(I) photoelectron spectrum measured in the laboratory. The modifications have to be ascribed to the contribution of vibrational autoionization to the population of the individual vibrational levels.

The ionization efficiency of all the fragment ions have been recorded as far as their intensity is larger than 1% of the total ionization. This work has been completed by the measurement of the

kinetic energy distribution of these fragment ions at photon energies of 21.22 eV (HeI), 16.85 eV (NeI) and 13.47 eV (ArII).

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References.

- [1]. R. Locht, B. Leyh, H.W. Jochims, H. Baumgärtel, BESSY Jahresbericht (2004).
- [2]. R. Kraessig, D. Reinke, H. Baumgärtel, Ber.Bunsenges.Phys.Chem. 78 (1974) 116.
- [3]. F. Liu, F. Qi, H. Gao, L. Sheng, Y. Zhang, S. Yu, K.C. Lau, W.K. Li, J.Phys.Chem. A (1999) 4155.
- [4]. J.J. Butler, T. Baer, Org.Mass Spectrom. 18 (1983) 248.

