THRESHOLD PHOTOELECTRON SPECTRA OF ISOXAZOLE OVER THE PHOTON ENERGY RANGE 9-30 eV

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Isoxazole C_3H_3NO is a five-member heterocycle molecule containing carbon ring in which two neighbouring carbon atoms are replaced by oxygen and nitrogen. It is used for synthesis of antibiotic, antitumour and anti-HIV agents *e.g.* [1] and is also considered as an analogue for biological molecules which are fragments of sugar-phosphate backbone of DNA.

We report results of threshold photoionization studies which used penetrating field technique (Fig. 1) [2]. The threshold photoelectron spectrometer [3] was used to collect spectra over the photon energy range from 9.9 eV to 30 eV beyond the previous He I measurements [4, 5]. The overall energy resolution was estimated to be better then 15 meV. This work was carried out at Synchrotron Radiation Source in Daresbury, UK using the five meter McPherson high resolution monochromator providing radiation in the 5–35 eV range with the highest resolution of 2 meV.

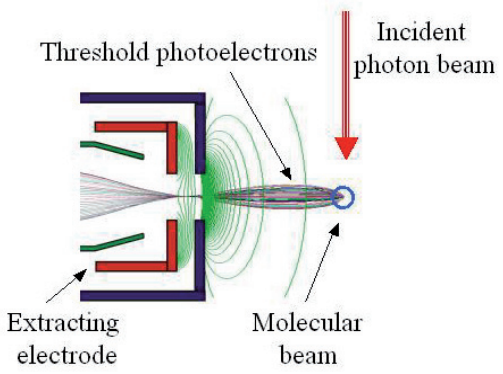

Figure 1. Penetrating field technique.

The complete threshold photoelectron spectrum of isoxazole is presented in Fig. 2. It consists of several bands with the first ionization threshold at 9.977 eV. The first band with resolved fine vibrational structures originates from ionization from the highest occupied molecular orbital *3a''*(π_3). The next band in the 11-13 eV range, can be associated with the *2a''*(π_2) and the *15a'*(LP_n) (nitrogen lone pair) orbitals. At higher energy, apart from clearly visible bands, fitting procedure revealed few further underlying bands.

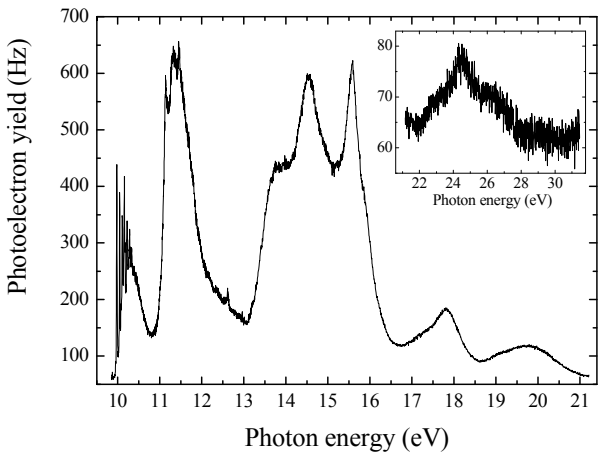

Figure 2. Threshold photoelectron spectrum of isoxazole measured in the energy range 9.9-30 eV.

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