

# Electron Momentum Spectroscopy Investigation of Valence Electronic Structures of CH<sub>3</sub>I

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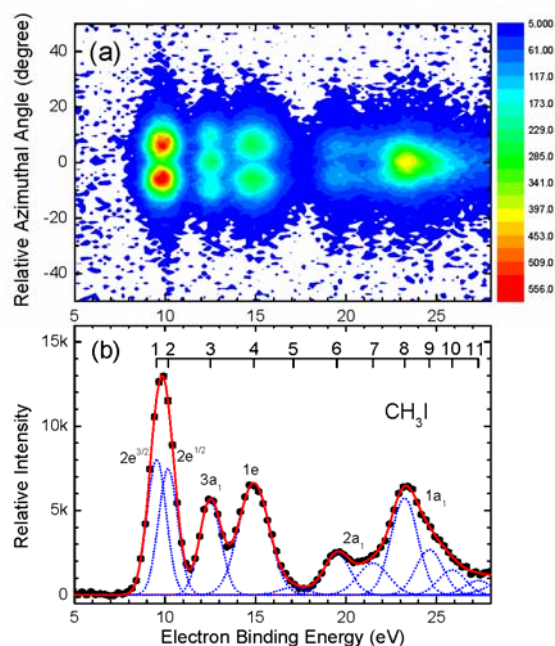
**Synopsis** The binding energy spectrum and electron momentum distributions of valence orbitals of methyl iodide are measured using the high-sensitivity electron momentum spectroscopy apparatus. Detailed theoretical analysis including relativistic, electron correlation and vibrational effects is performed to illuminate the valence electronic structures.

Electron momentum spectroscopy (EMS) [1] has been demonstrated to be a robust technique for exploring the electronic structure of atoms and molecules for its unique ability of detecting electron momentum distributions for individual orbitals. It is a coincidence experiment based on the kinematically complete (e, 2e) reaction near the Bethe ridge condition, in which a fast incident electron is scattered by a target atom or molecule and an electron is knocked out from the target. Within a series of approximations including Born-Oppenheimer and plane wave impulse approximations, the triple differential cross section of the (e, 2e) reaction is proportional to the modulus square of the wavefunction of the ionized orbital in momentum space, i.e., electron momentum profile.

In this work, the valence electronic structure of methyl iodide (CH<sub>3</sub>I) is investigated in detail by EMS by measuring the binding energy spectrum and electron momentum distributions of the valence orbitals. The experiment—in which the symmetric non-coplanar kinematics is employed [2], was carried out at impact energy of 1200 eV plus binding energy. The instrumental energy and momentum resolution were determined to be ~1.2 eV (full width at half maximum (FWHM)) and ~0.2 a.u. ( $\Delta\theta = 0.8^\circ$ ,  $\Delta\phi = 2.2^\circ$ ), respectively, by measuring Ar 3p orbital before the CH<sub>3</sub>I experiment.

The experimental two-dimensional energy and relative azimuthal angle spectrum and binding energy spectrum of present work is displayed in Figure 1. Electron momentum profiles of eleven ionization bands are inferred through a fitting of angular resolved binding energy spectra using Gaussian curves.

Due to the complexity of polyatomic molecules, electron correlation, relativistic effects, Jahn-Teller effects, vibrational effects are taking into account to interpret the electron momentum distributions of the resolved ionization bands. More details will be showed on the poster.



**Figure 1.** (a) Two-dimensional energy and relative azimuthal angle spectrum of CH<sub>3</sub>I. (b) Binding energy spectrum of CH<sub>3</sub>I. The dotted lines represent the 11 Gaussian peaks corresponding to individual molecular orbitals and the solid line is the sum.

## References

- [1] Weigold E. and McCarthy I. E., 1999 *Electron Momentum Spectroscopy* (New York: Kluwer).
- [2] Tian Q. G. *et al.* 2011 *Rev. Sci. Instrum.* 82 033110.

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