Valence electronic structures of isopropyl iodide investigated by using electron momentum spectroscopy

Minfu Zhao*,†, Xu Shan*,[1], Shanshan Niu*, Yaguo Tang*, Zhaohui Liu*, Xiangjun Chen*

[*] Hefei National Laboratory for Physical Sciences at the Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, 230026, China
[†] The Center of Basic Laboratory, West Anhui University, Lu'an 237012, China

Synopsis: We report the two-dimensional electron density map of binding energies and relative azimuthal angles (*i.e.*, electron momenta) for the valence molecular orbitals of isopropyl iodide. The binding energy spectra and electron momentum distributions of the valence orbitals can be obtained. Combined with the theoretical calculations, the influences of the spin-orbit coupling and intramolecular orbital interactions are analyzed.

Electron momentum spectroscopy (EMS), also known as binary (e, 2e) spectroscopy, is a powerful technique for exploring the electronic structures of atoms and molecules [1]. The principal value of the EMS for understanding the electron behavior lies in its unique ability to measure the electron density distribution in momentum space for the ionized orbital. During the past decades, the EMS measurements, combined with the theoretical calculations, have been applied to investigate the intramolecular interactions such as the electron correlation effect, the conformational effect, the spin-orbit coupling effect, the hyperconjugative or orbital interaction, etc.[1-7] Such interactions can coexist and compete in one single molecule like halogenated alkanes.

Isopropyl iodide ($CH_3CH_2ICH_2$) molecule is one of the smallest molecules undergoing spin-orbit coupling effects and hyperconjugative interactions simultaneously. In this abstract, we report the first EMS experiment on the ionizations of the valence molecular orbitals of isopropyl iodide, measured by our highly sensitive electron momentum spectrometer with noncoplanar symmetric geometry at the impact energy of 1.2 keV 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. ($\Delta\theta$ = 0.8º, $\Delta\phi$ = 2.2 º), respectively, by measuring Ar 3p orbital before the experiment of isopropyl iodide.

Figure1 shows the measured two-dimensional electron density map (2D map) including the information on the orbital electron binding energy and momentum, as well as the orbital symmetry. From this 2D map, the binding energy spectra and electron momentum distributions for the valence orbitals of isopropyl iodide can be deduced and compared with the theoretical calculations using various methods. The influence of the spin-orbit coupling and intramolecular orbital interactions are analyzed. More information will be presented in the poster.

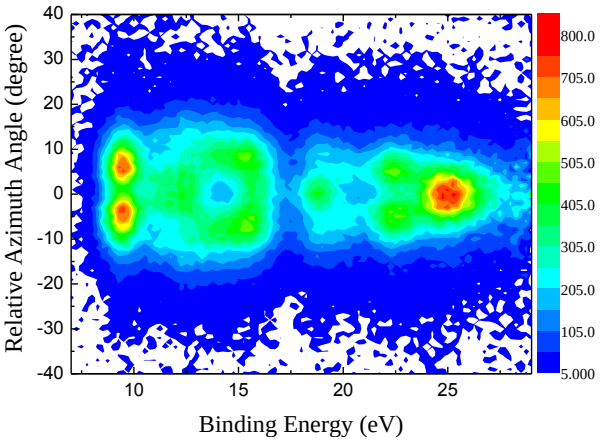

Figure 1 Two-dimensional electron density map of binding energies and relative azimuthal angles of isopropyl iodide.

References

[1] I. E. McCarthy and E. Weigold, 1991 *Rep. Prog. Phys.* **54** 789
[2] M. Takahashi et al. 1999 *Chem. Phys. Lett.* **308**, 195
[3] X. J. Chen *et al.* 2009 *Chem. Phys. Lett.* **472**, 19
[4] Y. Zheng *et al.* 1995 Science **270**,786
[5] M. S. Deleuze *et al.* 2001 *J. Am. Chem. Soc.* **123**, 4049
[6] Z. J. Li *et al.* 2008 *Chem. Phys. Lett.* **457**, 45
[7] K. Liu et al. 2009 *Phys. Rev. A* **80** 022716
[8] Q. G. Tian *et al.* 2011 *Rev. Sci. Instrum.* **82** 033110

[1] E-mail: xshan@ustc.edu.cn