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Absolute Photoionization cross section of C_{70} at 25-120 eV.

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Fullerenes show characteristic properties such as collective plasmon oscillation of valence electrons. Thus excitation dynamics of a single molecule of this family[1,2] has attracted widespread interest. Single-photon ionization of C_{60} and C_{70} has studied by Hertel et al. from ionization potential (~7.6 eV for C_{60} and 7.3 eV for C_{70}) to 35 eV and showed that photoionization yield was dominated by a strong resonance at about 20 eV. Later, our group has recognized the fine peaks at $h\nu$ = 26 and 34 eV and a flat area ranging from 40 – 50 eV in the yield curve of C_{60}^+ and C_{70}^+ produced from C_{60} and $C_{70,}$ respectively, and ascribed these peaks to shape resonance [2,3]. In 2004 Kou et al. reported relative partial cross sections for production of singly- and doubly-charged ions from C_{60} and C_{70}[3] at $h\nu$ = 24.5 to 150 eV. From the sum of the two partial cross sections they obtained a relative total photoionization cross section σ_T of C_{60} and C_{70}. Nevertheless, the resultant σ_T of C_{60} was inconsistent with the theoretical total photoabsorption cross section by Colavita et al. [4] since Kou et al. neglected both the contribution of triply charged ions and the *m/z*-dependence of the detection efficiency. Hence the cross section derived by Kou et al. at a higher $h\nu$ region was deviated from the true total photoionization cross section. Very recently Mitsuke et al.[5] reinvestigated the ion yield curves of singly- and multiply-charged ions C_{60}^{z+} (z = 1 - 3), C_{70}^{z+} (z = 1 - 2), and C_{84}^{z+} (z = 1 - 3) by taking account of the dependence of the relative detection efficiency η of the ion detector on the mass-to-charge ratio *m/z.* Specifically, the absolute partial cross section $\sigma_{abs}(m,z+)$ can be expressed as

$$\sigma_{\mathrm{abs}}(m,z+) \propto \frac{R(m,z+)}{\Phi\, D} \cdot \frac{1}{\eta\ (\mathrm{C}_m^{z+})} \equiv \sigma(m,z+) \qquad (1)$$

Here, R(m,z+) is the signal count rate of the ions in a charge state z from C_m sample (m = 60,70,84), Φ is the photon flux of synchrotron radiation, D is the mass deposition rate of the thickness monitor, η (C_m^{z+}) is the relative overall detection efficiency of the apparatus for C_m^{z+}. Evaluation has been made of η (C_m^{z+}) as follows: first we have experimentally estimated absolute overall detection efficiencies η (Rg^{z+}) of our mass spectrometer for singly- and doubly-charged photoions produced from three rare gases (Rg = Ar, Kr, Xe).Second, we have determined a functional form of η by fulfilling the least-squares fitting of the data points of η (Rg^{z+}) to an empirical formula proposed by Twerenbold et al. [5,8].From the m/z versus η curve it was found that η values of C_m^{2+} and C_m^{3+} are larger than that of C_m^+ by factors of ~ 3 and ~ 6, respectively. Thus introducing a plausible functional form of η has brought about appreciable modification of the relative partial cross sections for the multiply charged ions. Eventually the total photoionization cross section curves of C_{60} and C_{70} have been substantially modified.

Moreover, applying essentially the same method for estimating a partial cross section $\sigma_{abs}(60,z+)$ for the formation of the ions in a charge state z from C_{60} as that employed in our previous papers [5,6], we have reevaluated [7] the absolute total photoionization cross section $\sigma_{abs,T}$ of C_{60} at $h\nu$ = 25 to 120 eV (specifically in that work, instead of relative detection efficiency, we have determined the absolute value of the η in order to determine absolute cross sections). $\sigma_{abs,T}$ of C_{60} was then obtained by summing up $\sigma_{abs}(60,+)$, $\sigma_{abs}(60,2+)$, and $\sigma_{abs}(60,3+)$ and compared with previous experimental works, demonstrating a fairly good agreement in the wide above mentioned energy range as shown in the Fig.1. Moreover, the oscillator strength was derived with the aid of previously published results from 3.5 to 120 eV and observed results were compared with value reported by Berkowitz [8].

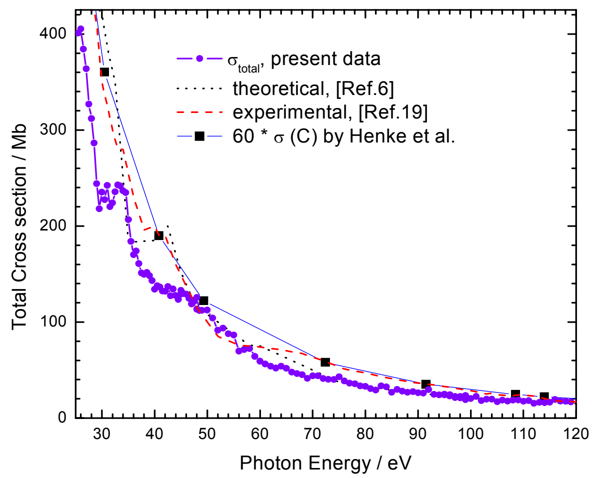

Fig. 3. Total photoionization cross section σ_T (C_{60}) of C_{60}. Closed circles, the present results; dotted curve, theoretical total photoabsorption cross section [4]; dashed curve, experimental data [10]; closed squares, 60 times the total photoabsorption cross section of a C atom [11].

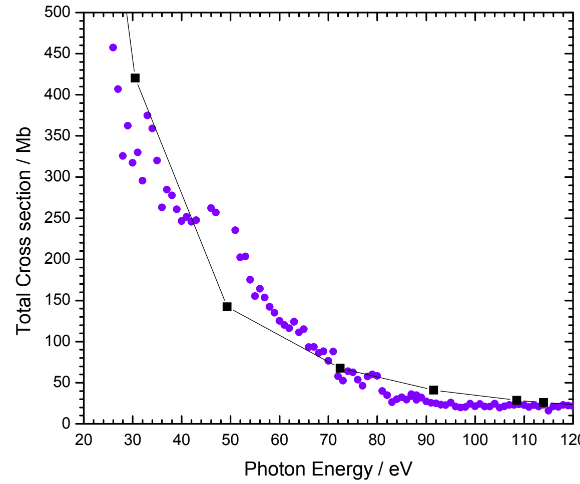

Fig.2. Closed circles represent the total photoionization cross section σ_T (C_{70}) of C_{70} obtained from the sum of the σ(C70,+) and σ (C70·2+).Closed squares, 60 times the total photoabsorption cross section of a C atom [11]. σ_T (C_{70}) curve is normalized to the curve with solid squares at *hν* = 70 eV.

We have re-examined the partial cross sections σ(70,+) and σ(70,2+) for the formation of C_{70}^{+} and C_{70}^{2+}, respectively, measured by Kou et al. [3] by considering dependence of the relative detection efficiency of MCP on the m/z ratio of the detected ion. The σ (70,+) and σ (70,2+) were estimated by Eq. (1) [5] and summed up these partial cross sections in order to obtain relative total cross section σ_T. In Fig. 2 closed squares depict 70 times the total photoabsorption cross section of a C atom [11]. σ_T curve (closed circles) is normalized to the curve with solid squares at *hν* = 70 eV. After normalization to the curve by Henke et al. the cross section value becomes 457 Mb at 26 eV. In order to test the reliability of the σ_T curve, we are trying to reevaluate relative cross sections by recalibrating our TOF spectrometer with rare gases for C_{70} experiment[5]. Moreover, to achieve the reproducibility of ion yields, and the ratios of multiply charges to singly charge produced from C_{70} is most essential (indeed, we observed a very good reproducibility among different experiments in the case of C_{60}, which we could not be observed in higher fullerenes C_{70} and C_{84}). Our current effort is to carefully check the factors, which may affect the above mentioned parameters, such as discrimination level to be set into the discriminator for discarding the voltages generated in the MCP by background ions or other sources.

After constructing the reliable relative photoionization cross section over the visible to EUV region, we are trying to determine the absolute photoabsorption cross section and inspect the consistency of the calculated oscillator strength with the TKR sum rule will be made, as have been performed for C_{60} by Berkowitz.

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