

Supplementary Materials

Anisotropy parameters from two-body dissociations

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Simulations - additional figures

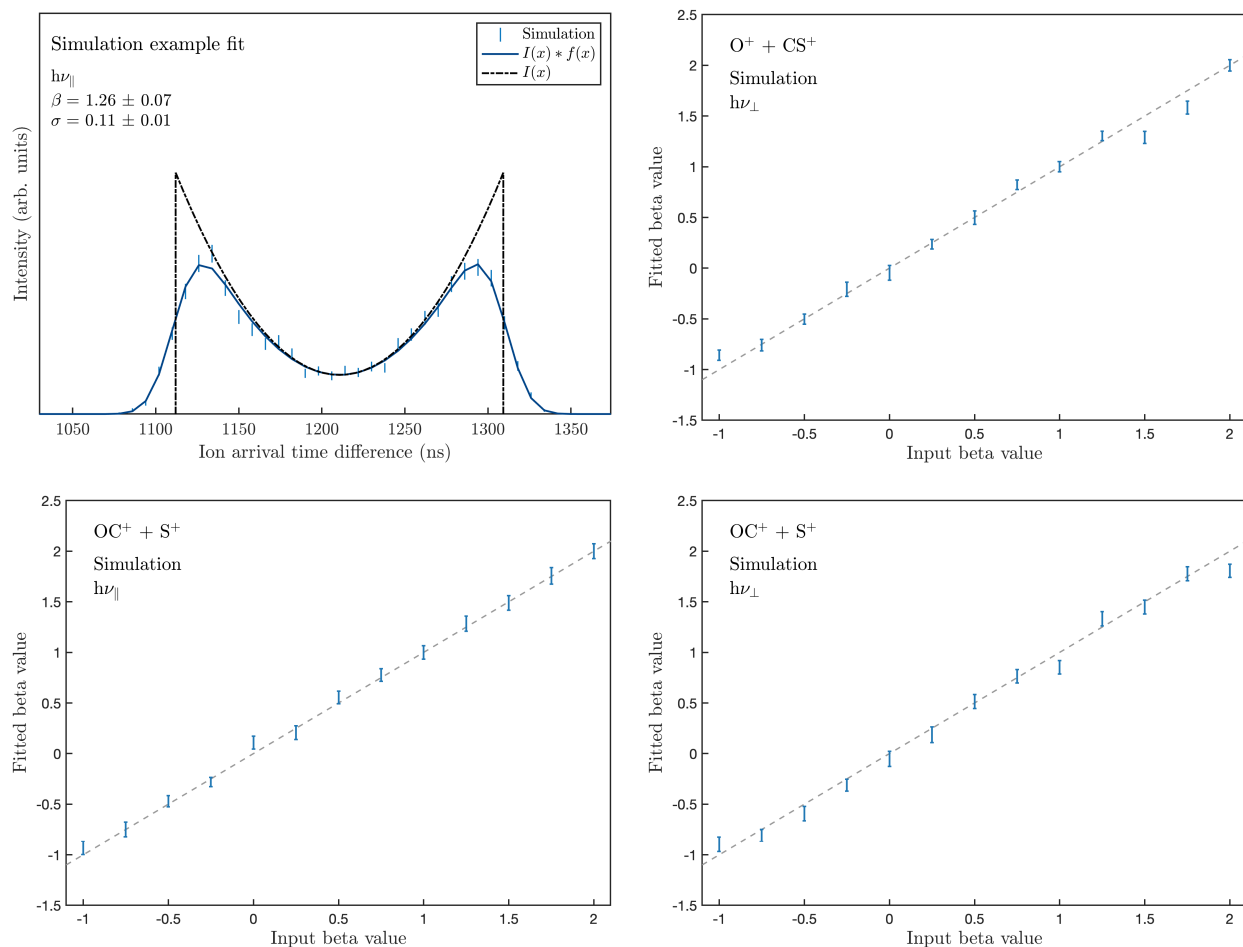


Figure S1. Example peak shape from the simulations (top left), for which the input β was 1.25. Comparison of the simulation input β and fitted β values for the $O^+ + CS^+$ dissociation for $h\nu_{\perp}$ (top right), and for the $OC^+ + S^+$ dissociation in the bottom panels, for $h\nu_{\parallel}$ (left) and $h\nu_{\perp}$ (right). The data point lengths represent 95 % confidence interval for β . For the bottom two panels the fit interval for $I(x)$ was limited to obtain good fits.

Experimental - additional figures

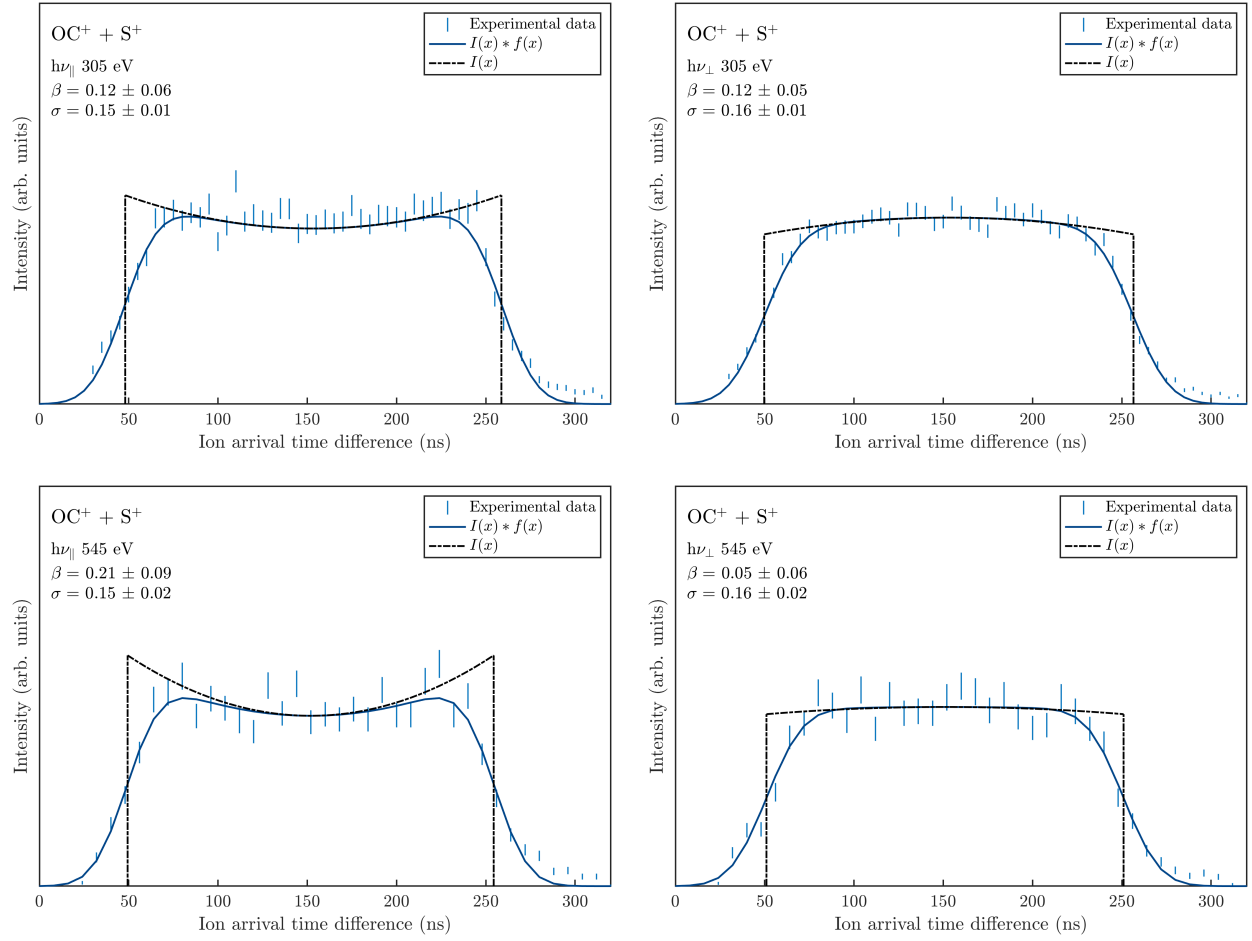


Figure S2. PIPICO peak shapes for the $\text{OC}^+ + \text{S}^+$ dissociation at 305.0 eV (top panels), and 545.0 eV (bottom panels), for $h\nu_{\parallel}$ (left) and $h\nu_{\perp}$ (right). For the bottom right panel, $h\nu_{\perp}$ at 545.0 eV, the fit interval has been set to be equivalent to the interval found for $h\nu_{\parallel}$ (bottom left). The blue solid line shows the fitted function, and the black dashed line is $I(x)$ plotted with the obtained β parameter. One dissociation channel at a specific photon energy should have the same β parameter regardless of polarization.

Algebraic expression for the convolution $I(x) * f(x)$

The two functions convoluted are

$$I(x) = \frac{1}{4\pi} \left(1 + \frac{\beta}{2} (3x^2 - 1) \right)$$

and

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\left(-\frac{x^2}{2\sigma^2}\right)},$$

where $I(x)$ is 0 outside $[-1,1]$ for x . Using Mathematica¹ and assuming only real values for x , the convolution $I(x) * f(x)$ is simplified, giving the following expression:

$$I(x) * f(x) = a \left(-3\sqrt{2}\sigma\beta e^{-\frac{(1+x)^2}{2\sigma^2}} \left(1 - x + e^{\frac{2x}{\sigma^2}} (1+x) \right) + \sqrt{\pi} \left(2 + \beta(-1 + 3\sigma^2 + 3x^2) \right) \left(\operatorname{erf}\left(\frac{1+x}{\sqrt{2}\sigma}\right) - \operatorname{erf}\left(\frac{-1+x}{\sqrt{2}\sigma}\right) \right) \right)$$

which is further simplified by approximating the error functions with

$$\operatorname{erf}(x) \approx \tanh\left(\frac{2}{\sqrt{\pi}}\left(x + \frac{11}{123}x^3\right)\right),$$

again under the assumption of only real-valued x .

References

1. Inc., W. R. Mathematica, Version 14.0. Champaign, IL, 2024.