VUV Photoionization Dynamics of the C₆₀ Buckminsterfullerene: 2D-Matrix Photoelectron Spectroscopy in an Astrophysical Context - Supplementary Information

Helgi Rafn Hrodmarsson,^{1,2}* Gustavo A. Garcia,¹ Harold Linnartz,² Laurent Nahon¹ ¹Synchrotron SOLEIL, L'Orme des Merisiers, St Aubin, BP 48, Gif sur Yvette, France ²Laboratory for Astrophysics, Leiden Observatory, Leiden University, PO Box 9513, NL-2300 RA Leiden, the Netherlands

Supplementary Information

Several fixed photon energy data acquisitions were performed to measure the anisotropies of the observed bands. To correct for the detector gain inhomogeneities and to obtain a flat response on the delay line anode PSDs, a Xenon mask was recorded at 27 eV at the same accelerator voltage. The mask was fitted with a 20-dimensional polynomial contour surface function which were subsequently used to correct the recorded fixed photon energy electron images of C_{60} (see Figure S1).



Figure S1. An electron image of Xe photoionized at 27 eV, accumulated for one hour. Plotted over the surface are the fitted contours of the multidimensional polynomial 2D-surface function which is used to calibrate the detector spatial response.

An example of one of the inverted images of the mass-filtered signal at 10.5 eV is presented in Figure S2.



Figure S2. Abel-inverted image of the photoelectron signal accumulated at 10.5 eV. The polarization axis is set horizontal in the image.

Fixed photon energy i²PEPICO acquisitions were performed at 8.5 eV, 10.5 eV, 11.5 eV, 12.5 eV and 13.5 eV. The anisotropy parameters are presented in Figure S3, overlaid on the measured TPES of the first three bands. Averaging the anisotropy parameter over the first band allows comparison with calculated anisotropies.^{1,2} For the second and third bands Venuti *et al.* calculated the anisotropies of the photoelectrons ejected from the individual orbitals, i.e. $6g_g$, $10h_g$, etc. Thus, a direct comparison is moot.



Figure S3. (Upper left corner) Anisotropy parameters over the first photoelectron band. (Upper right corner) Anisotropy parameters (black squares) that have been averaged over the first photoelectron band, and theoretical values obtained by Venuti *et al.* and Ponzi *et al.* (Lower left corner) Anisotropy parameters over the second band. (Lower right corner) Anisotropy parameters over the third band.

References

- 1 M. Venuti, M. Stener, G. De Alti and P. Decleva, Photoionization of C-60 by large scale onecenter density functional explicit continuum wave-function, *J. Chem. Phys.*, 1999, **111**, 4589– 4597.
- 2 A. Ponzi, S. T. Manson and P. Decleva, Photoionization of C-60: Effects of Correlation on Cross Sections and Angular Distributions of Valence Subshells, *J. Phys. Chem. A*, 2020, **124**, 108–125.