Supplementary Information: Threshold Energies for Single Carbon Knockout from Polycyclic Aromatic Hydrocarbons

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October 28, 2015

In Figure 1, we show the results of Gaussian fits to the experimental mass spectra from Figure 1 in the main text. These or fits over the region from the tail of the parent ion ($C_{14}H_{10}^{+}$) peak, the CH_x-loss and C_2H_y-loss peaks. At the low energies, the contribution of CH_x-loss becomes negligible.

In Figure 2, we show the absolute cross sections for carbon knockout for the three PAHs studied in our MD simulations. Single- and double-carbon knockout cross sections are given separately, along with their sums. The solid lines are fits from which the A values in Table 1 in the main article are obtained.

In Figure 3, we show the energy lost from the He projectile in collisions with a particular C atom in anthracene, ΔE_{He}, as a function of center-of-mass energy in the He-PAH system. Each curve shows results of our MD simulations conducted for face-on trajectories with different impact parameters b. For trajectories with $b = 0$ Å, the transferred energy follows a linear dependence of the collision energy. This trend deviates increasingly from the linear one as the impact parameter increases. The mean energy transfer averaged over all impact parameters and molecular orientations follows a power law, as shown in Figure 4 in the main text.

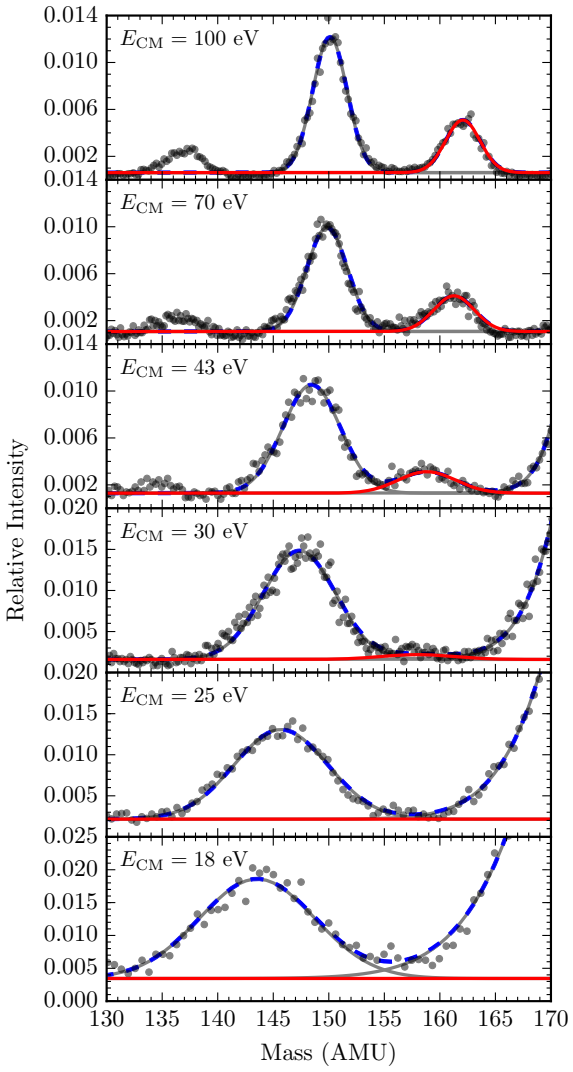

Figure 1: Gaussian fits to parts of the experimental spectra from Figure 1 in the main text. At the lowest energies, the contribution from CH_x-knockout (red line) is negligible.

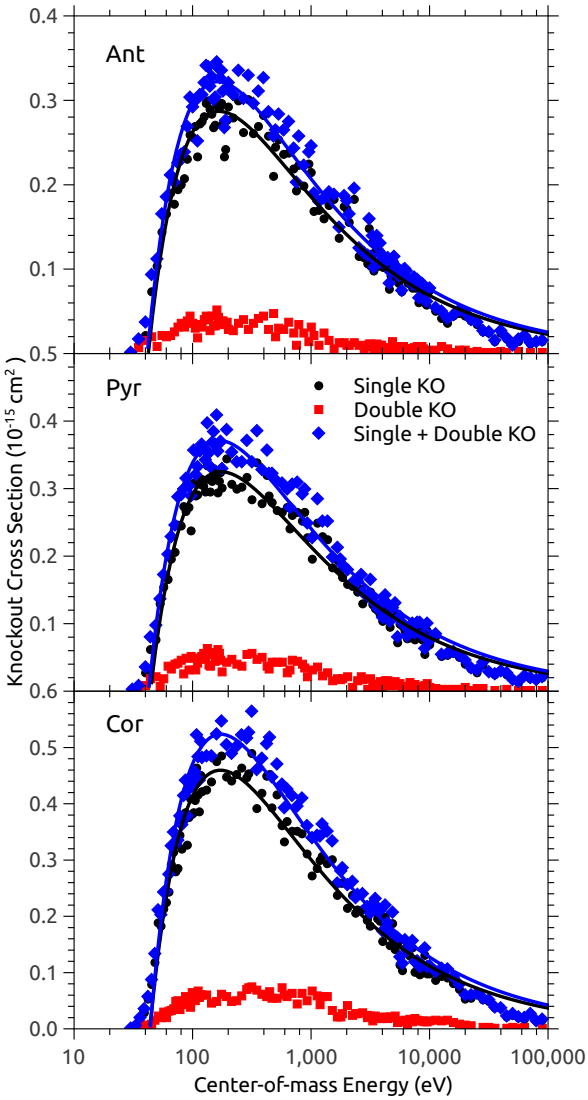

Figure 2: Simulated absolute carbon knockout cross sections for anthracene (Ant), pyrene (Pyr) and coronene (Cor) colliding with He atoms. Single- (black circles) and double- (red squares) carbon knockout cross sections are given, along with their sums (blue diamonds). The solid lines are fits from which the A values in Table 1 in the main article are obtained.

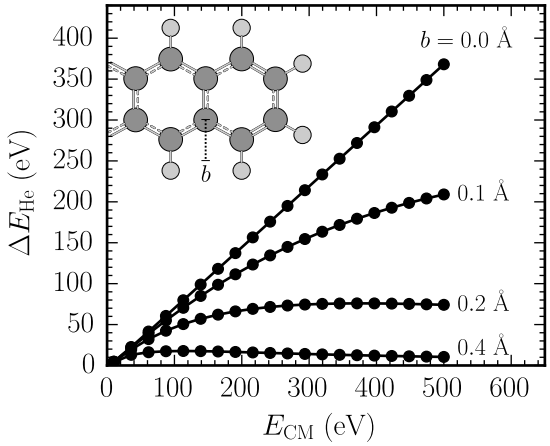

Figure 3: Transferred energies, ΔE_{He}, calculated from MD simulations of a He projectile colliding with a C atom in anthracene along trajectories perpendicular to the molecular plane as a function of of He-PAH center-of-mass collision energy, E_{CM}, and impact parameter, b. For trajectories with $b = 0$ Å, the transferred energy follows a linear dependence of the collision energy. This trend deviates increasingly from the linear one as the impact parameter increases.