Shape and Core-excited Resonances in Thiophene

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Figure S1: Energy loss spectra recorded in the forward (lower panel) and backward (upper panel) directions. The forward direction spectrum shows nearly exclusively dipole allowed transitions. The backward direction spectrum, recorded with a low residual energy, is dominated by triplet states, but weak excitation of the singlet states also contributes. The first (T1) and second (T2) triplet states as well as the first excited singlet state (S1) are clearly identifiable in the energy loss spectra below and are consistent with earlier calculations and experiments. Three other bands, above ~5.4 eV, are also clearly identifiable in the experiments, but their assignation to specific states is less clear: the band labelled Tn may correspond to the $1^{3}B_{1}$ and $1^{3}A_{2}$ states with contributions from the $2^{3}A_{1}$ $2^{3}B_{2}$ states. The Tm experimental feature could be due to (overlapping) $3^{3}A_{1}$ and $2^{3}A_{2}$ states. We are not able to identify which singlet state or states contribute to the Sn band.



Figure S2: Elastic differential cross sections in thiophene. The yellow circles indicate the absolute values obtained by the relative flow method at discrete incident energies. The red continuous line is the excitation function, obtained by sweeping the incident and scattered electron energies, and normalized to the discrete values.

