Time Delay in Molecular Photoionization - Supplementary Materials

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This document presents the full sets of dipole matrix elements resulting from the calculations discussed in the manuscript, and used in the angle and energy-dependent Wigner delay maps therein.

Here, the matrix elements are presented for all (l,m) partial-waves, for each accessible ionization continuum (i.e. each allowed final state symmetry).

In the plots, the magnitudes and phases of each (l,m) channel are shown, along with the coherent sum over the channels. The partial-wave resolved Wigner delays τ are also shown, along with the full Wigner delay (resulting from the coherent sum over all channels).

For reference, the direct sum of the channel-resolved Wigner delays is also shown, and denoted "sum τ" in the figure legends. This corresponds to an incoherent sum over the partial-wave channels.

Additional line-plots of the cross-sections and Wigner delays are also included. These show cuts through the full surfaces (figs 1 & 2 in the manuscript) at various angles, equally spaced over $0 \leq \theta \leq 90^\circ$ for N_2 and $0 \leq \theta \leq 180^\circ$ for CO. Note that singularities appear in some regions, but these correspond to minima in the cross-sections (and concommittant sign-changes in the phases), hence are not physically meaningful.

N$_2$ ePS, raw matrix elements by l-wave (σ_u continuum, m=0 only)
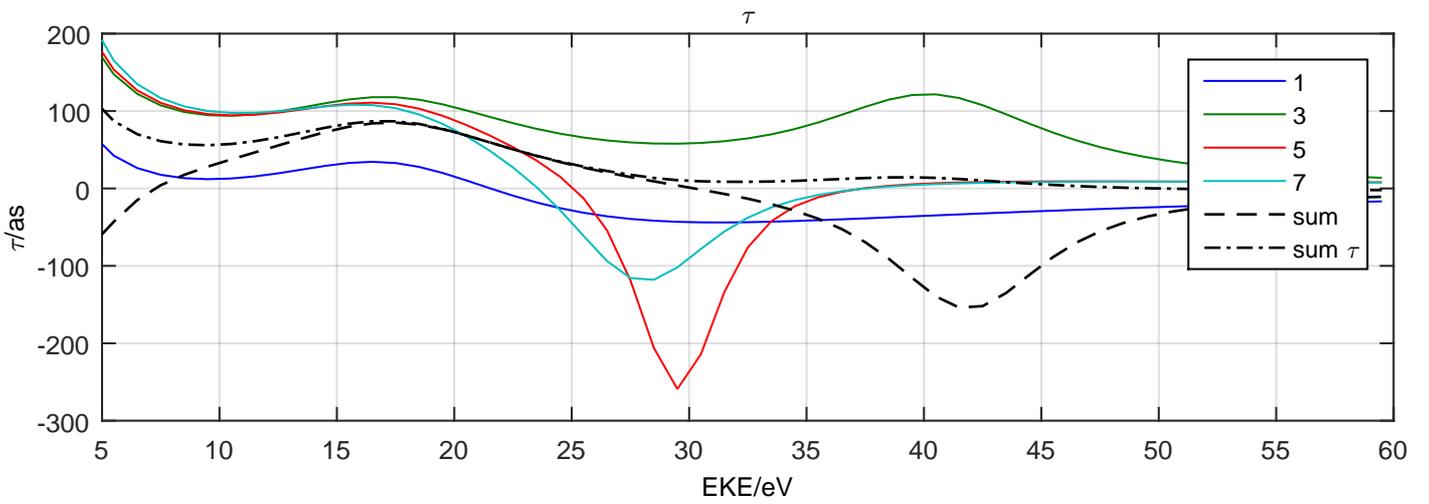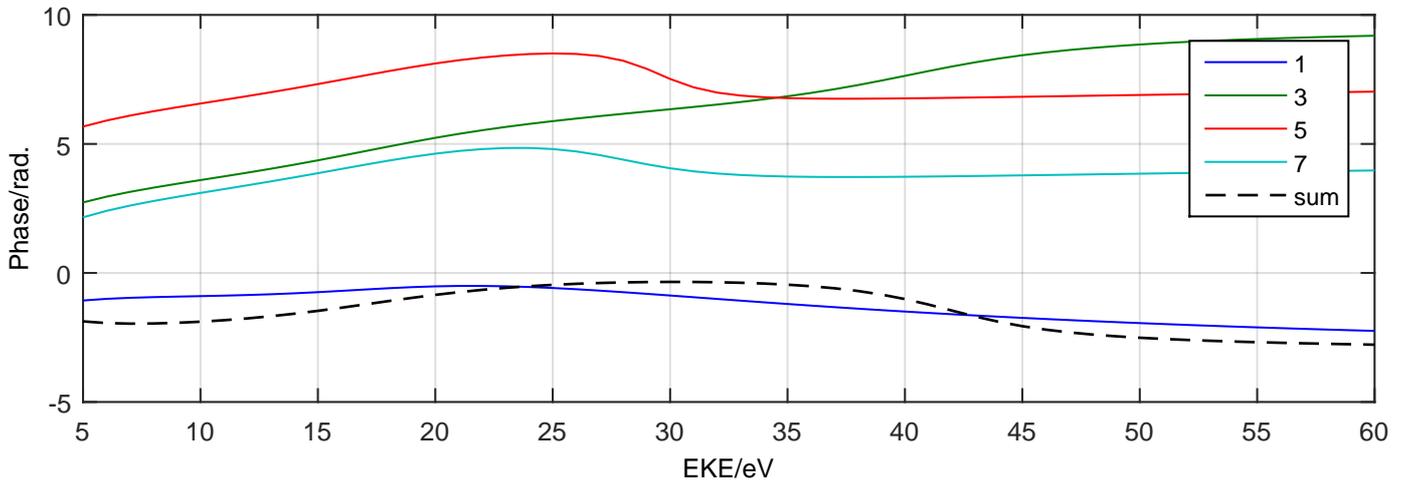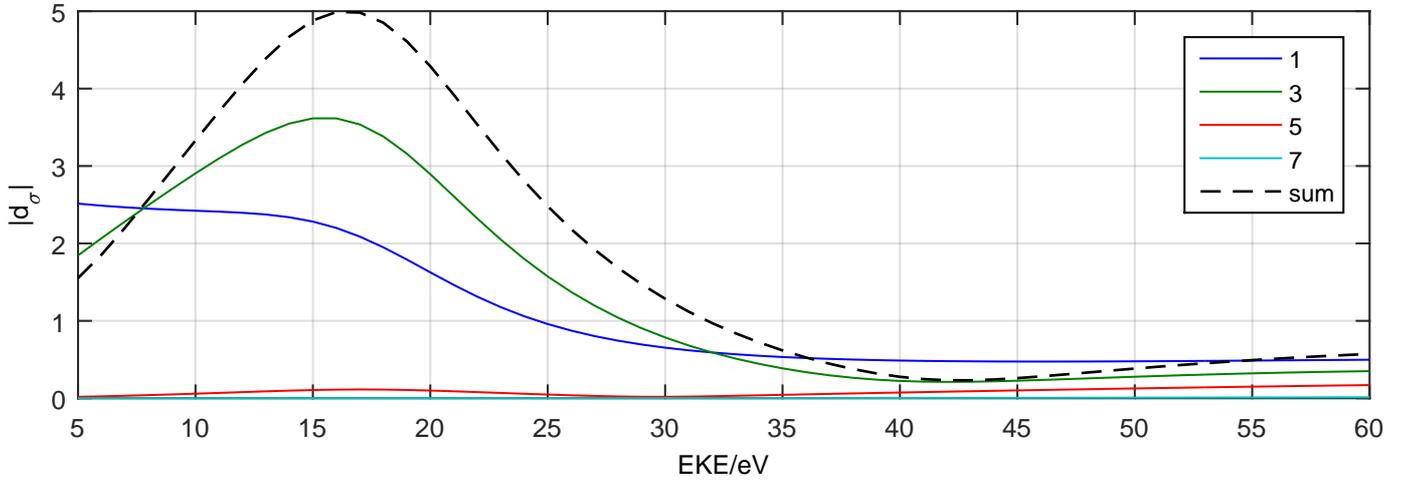
N$_2$ ePS, raw matrix elements by l-wave (π_g continuum, |m|=1 only)
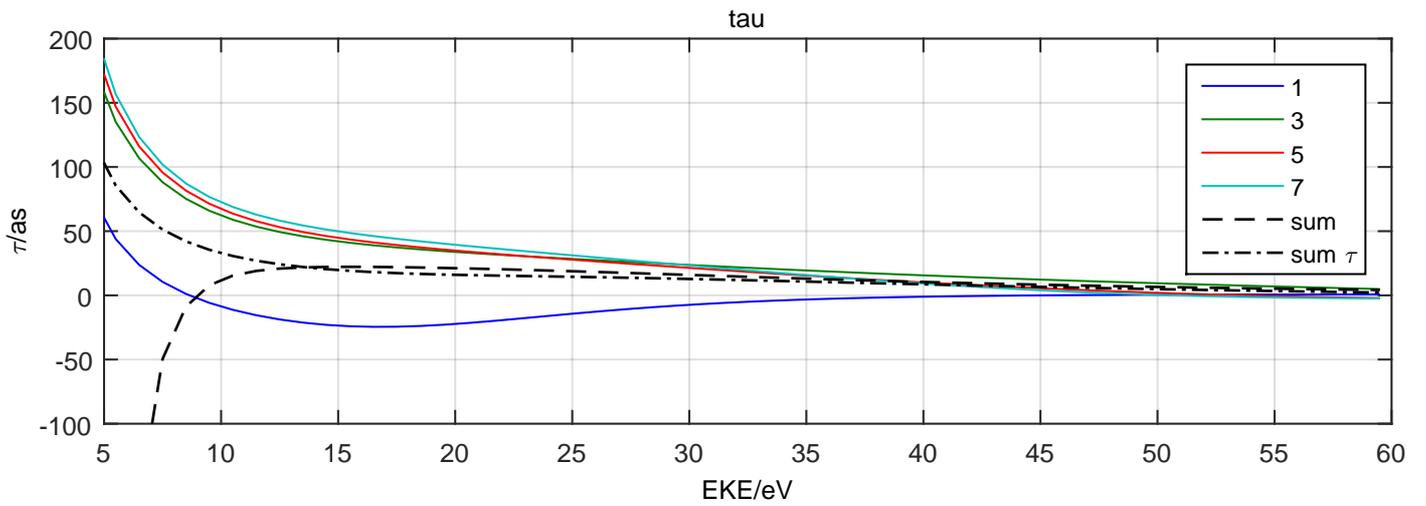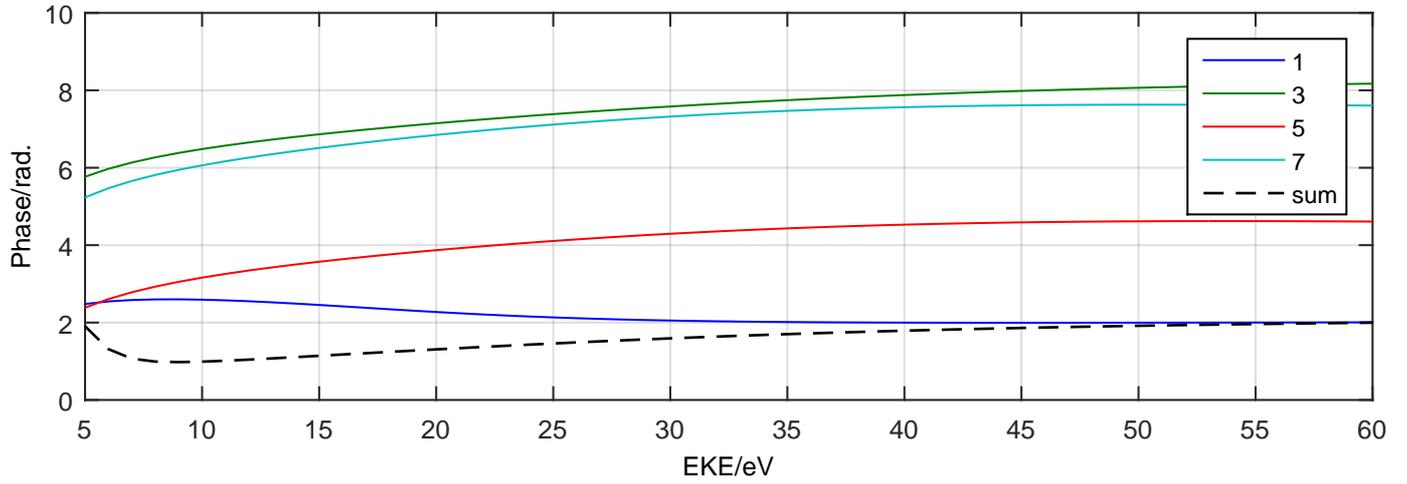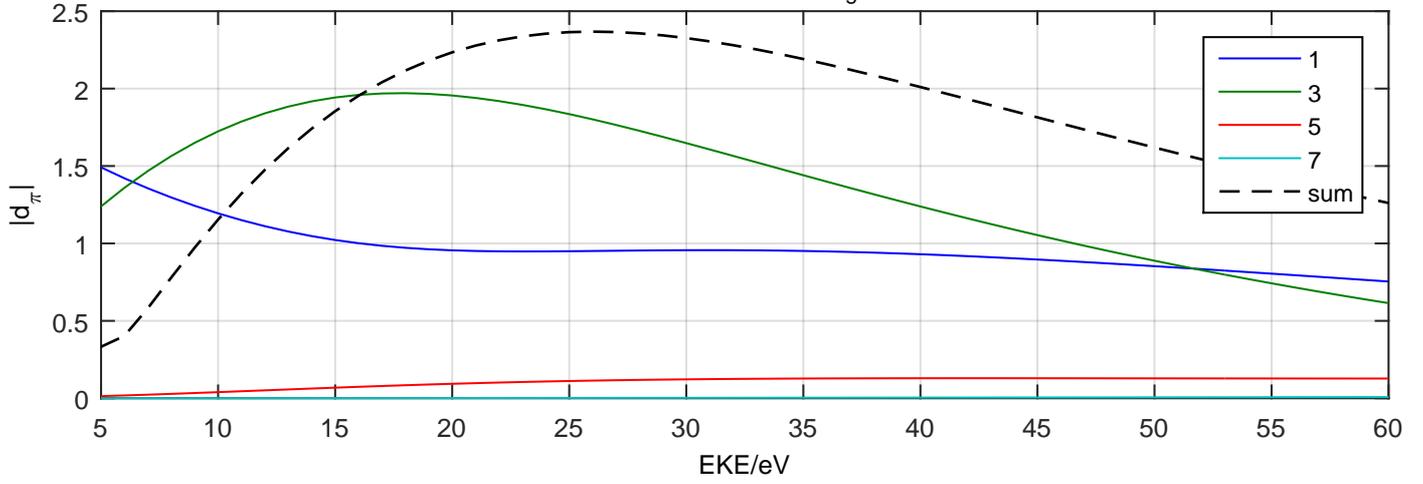
CO ePS, raw matrix elements by l-wave (σ continuum, m=0 only)
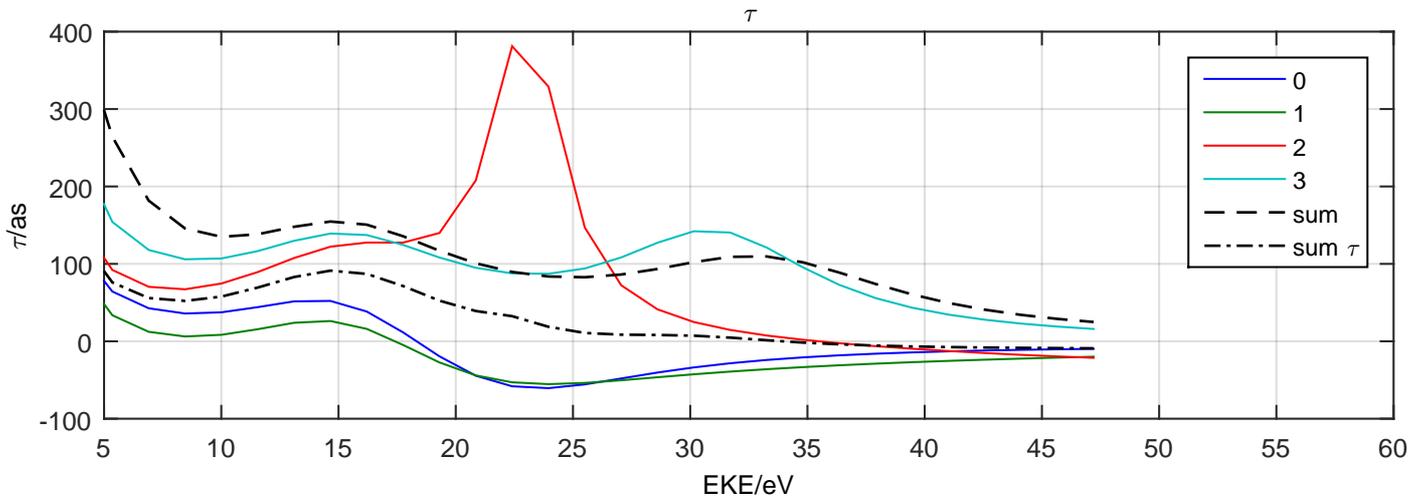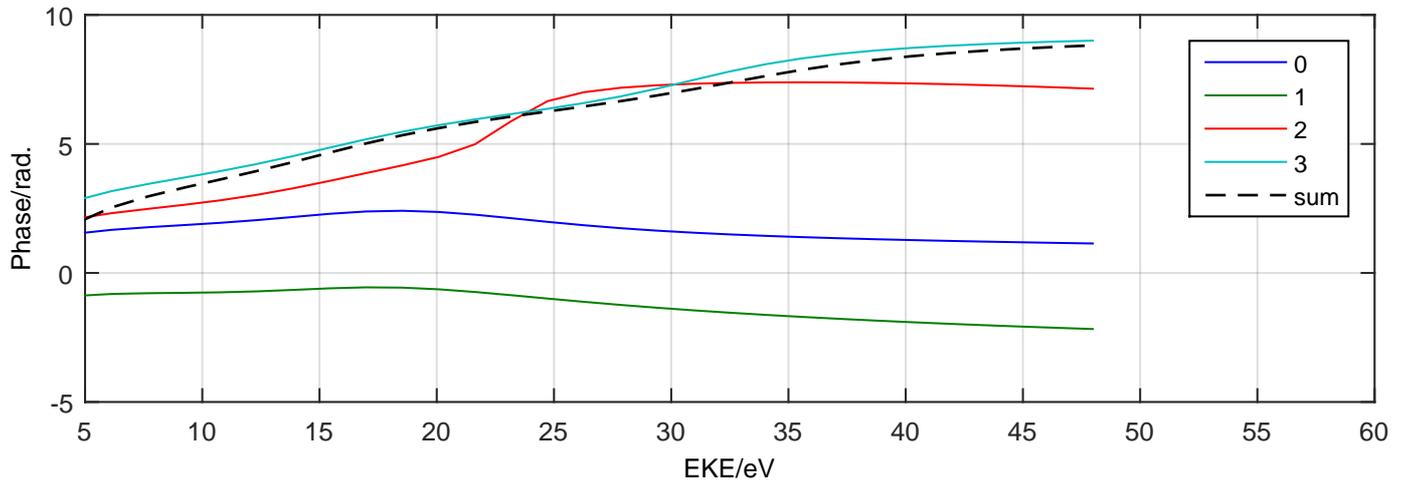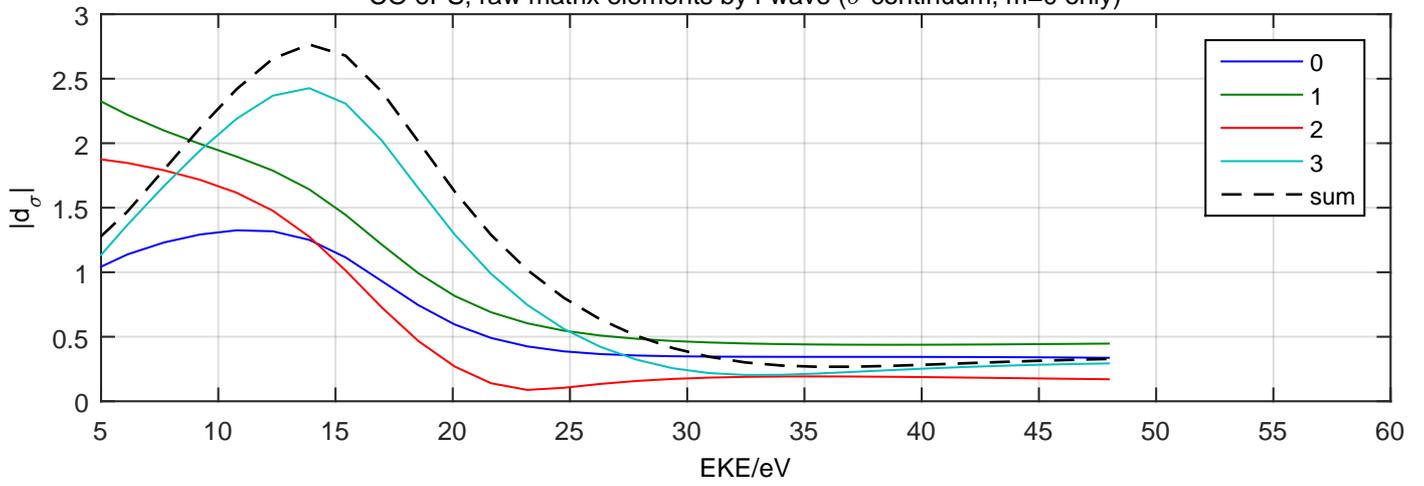
CO ePS, raw matrix elements by l-wave (π continuum, |m|=1 only)
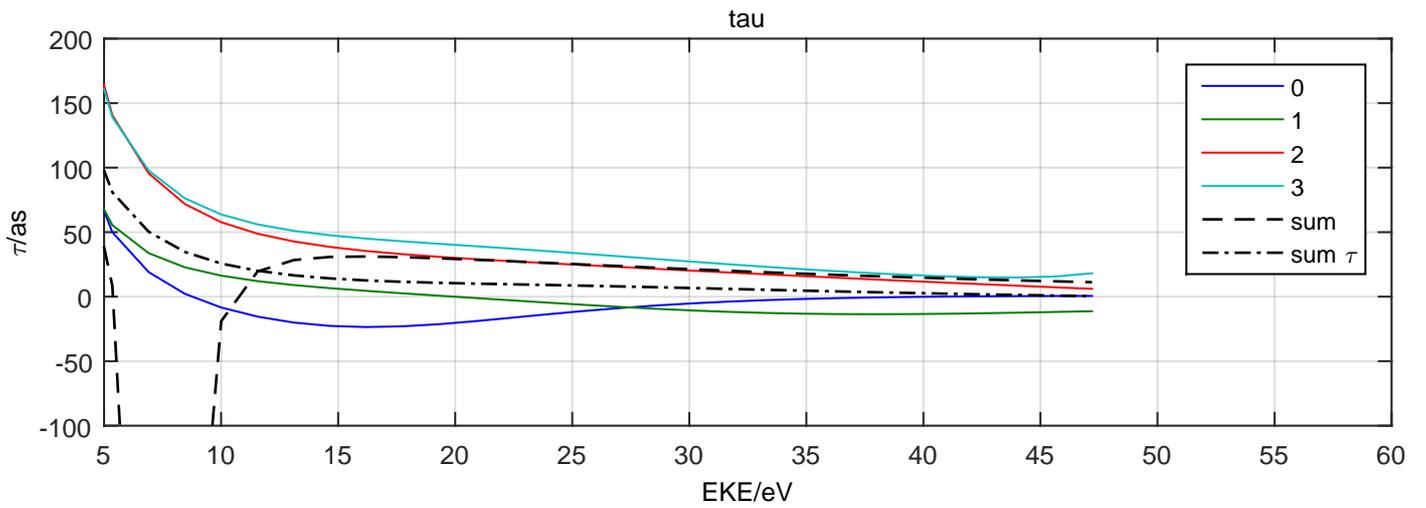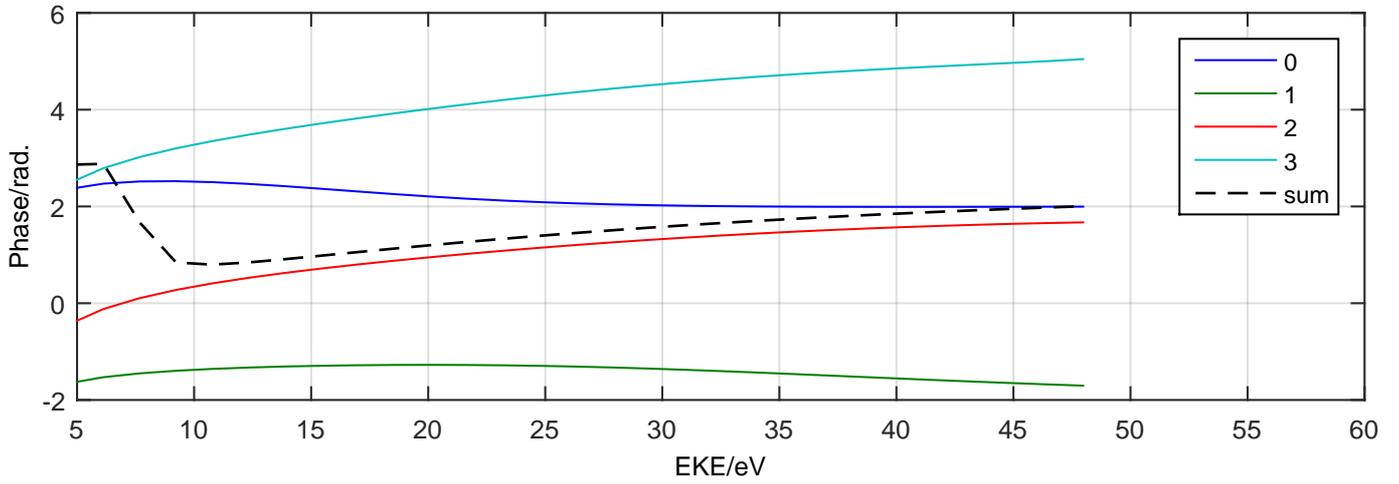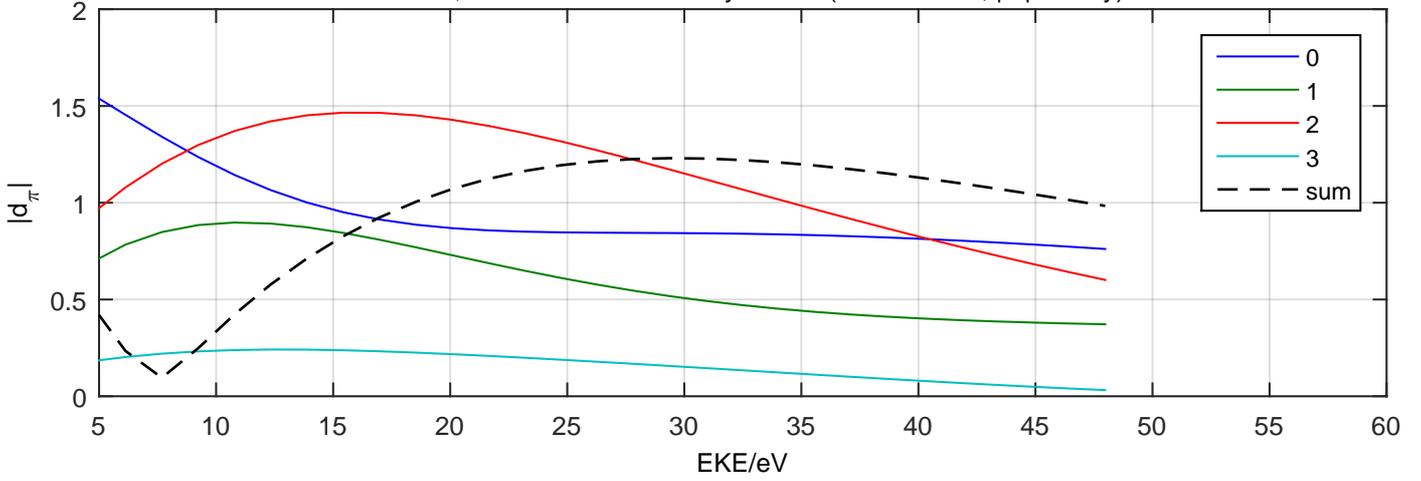
Angular line-outs, X-sect and Wigner delay

N$_2$, parallel (σ_u continuum)

N$_2$, perpendicular (π_g continuum)
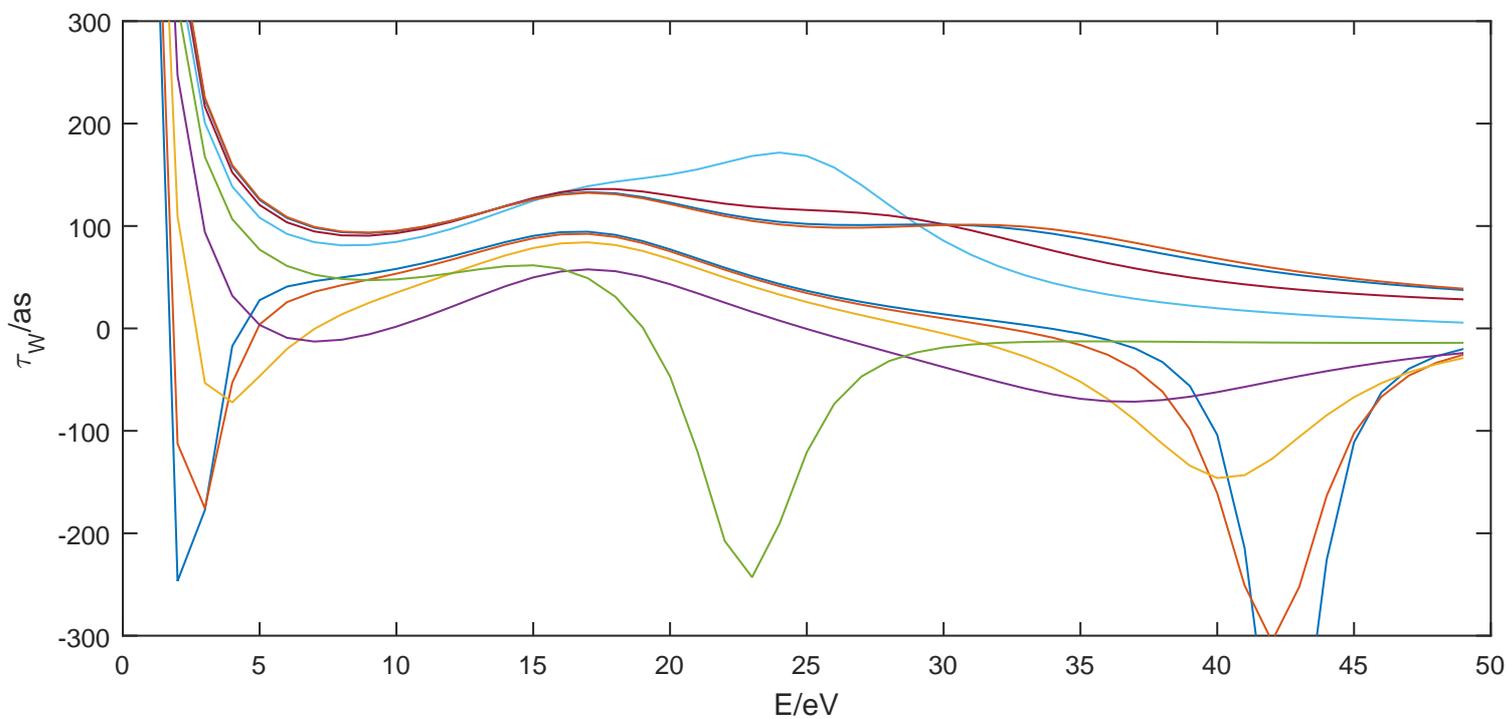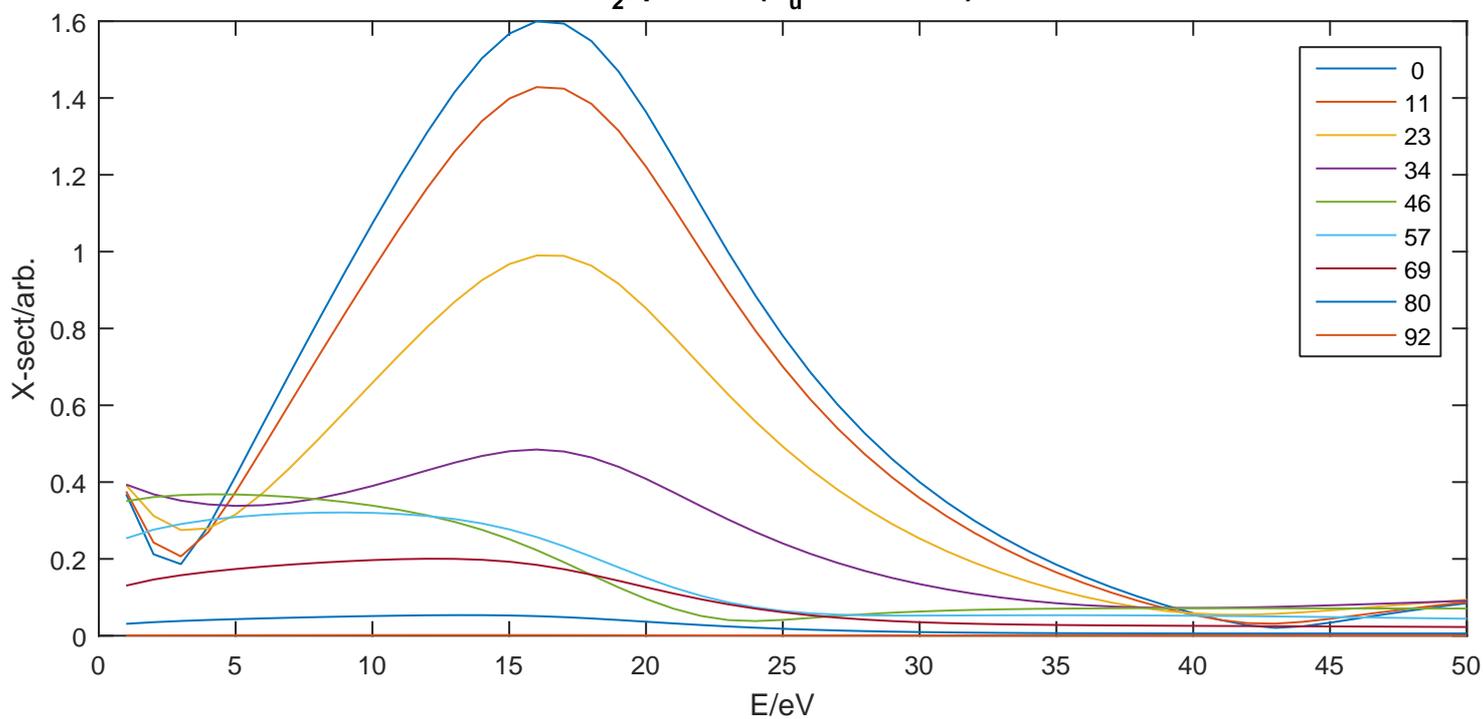
CO, parallel (σ continuum)

CO, perpendicular (π continuum)

Legend:
- 0
- 23
- 46
- 69
- 92
- 115
- 138
- 160
- 183