Electronic Supplementary Material (ESI) for Faraday Discussions.

This supplementary material of the paper ``Time-resolving the UV-initiated photodissociation dynamics of OCS'' by Evangelos T. Karamatskos, Suresh Yarlagadda, Serguei Patchkovskii, Marc J. J. Vrakking, Ralph Welsch, Jochen Küpper, and Arnaud Rouzée contains movies depicting the calculated wavepacket dynamics as contour plots of the time-dependent probability density in the 1 ^{1}A" and 2 ^{1}A' states, see section III of the manuscript for details.

1A'' R-r.mp4 – 2D probability density for (R. r) in the 1 ^{1}A" state

1A'' R-theta.mp4 – 2D probability density for (R, θ) in the 1 ^{1}A" state

2A' R-rR.mp4 – 2D probability density for (R, r) in the 2 ^{1}A' state

2A' R-theta.mp4 – 2D probability density for (R, θ) in the 2 ^{1}A' state

r, R, and θ are Jacobi coordinates, describing the CO bond length, the distance of sulphur to the centre-of-mass of CO and the angle (modulo π) between the centre-of-mass of CO and S, respectively.

The displayed range of the coordinates is

$1.8 < r < 2.8$

$3 < R < 50$

$0 < \theta < \pi$

Note that R is shown on a logarithmic scale, whereas r and θ on linear scales.

The time evolution of the probability densities is propagated over 600 fs, shown here in time steps of 2 fs, where t = 0.0 fs corresponds to the time of UV excitation, at which the rovibronic ground-state density is projected onto the 1 ^{1}A" and 2 ^{1}A' potential energy surfaces.

For more details, see section III of the manuscript.