

Supplementary information: Comparing the electronic relaxation dynamics of aniline and d₇-aniline following excitation at 272-238 nm

Oliver M. Kirkby,^a Matthieu Sala,^b Garikoitz Balerdi,^c Rebeca de Nalda,^d Luis Bañares,^c Stéphane Guérin,^b and Helen H. Fielding,^{*a}

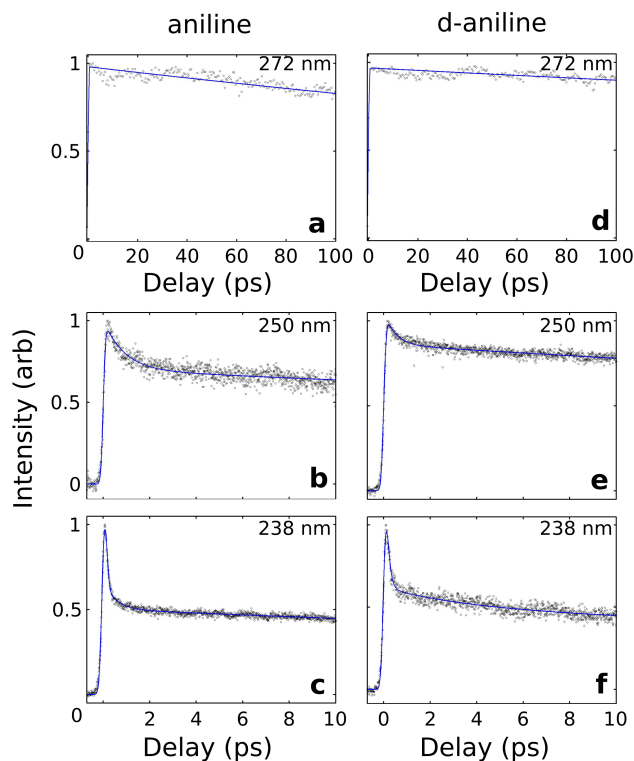


Fig. S1 Fits to the total integrated photoelectron signal decay in aniline (a-c) and d₇-aniline (d-f) used to obtain τ_1 time constants.

^a Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, U.K.; E-mail: h.h.fielding@ucl.ac.uk

^b Laboratoire Interdisciplinaire Carnot de Bourgogne UMR 5209 CNRS, Université de Bourgogne, BP 47870, F-21078 Dijon, France.

^c Departamento de Química Física I (Unidad Asociada I+D+i al CSIC), Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain.

^d Instituto de Química Física Rocasolano, CSIC, C/Serrano 119, 28006 Madrid, Spain.

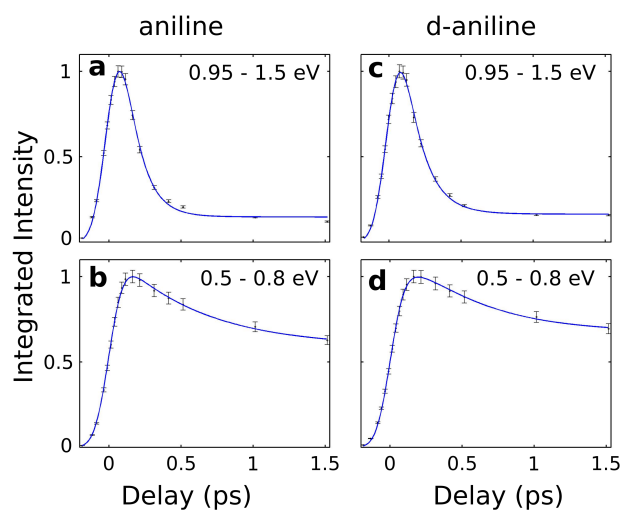


Fig. S2 Fits to the 250 nm photoelectron spectra integrated over 0.95 – 1.5 eV and 0.5 – 0.8 eV to determine τ_3 and τ_2 time constants, respectively. Error bars are two standard deviations in photoelectron intensity over the integrated regions.

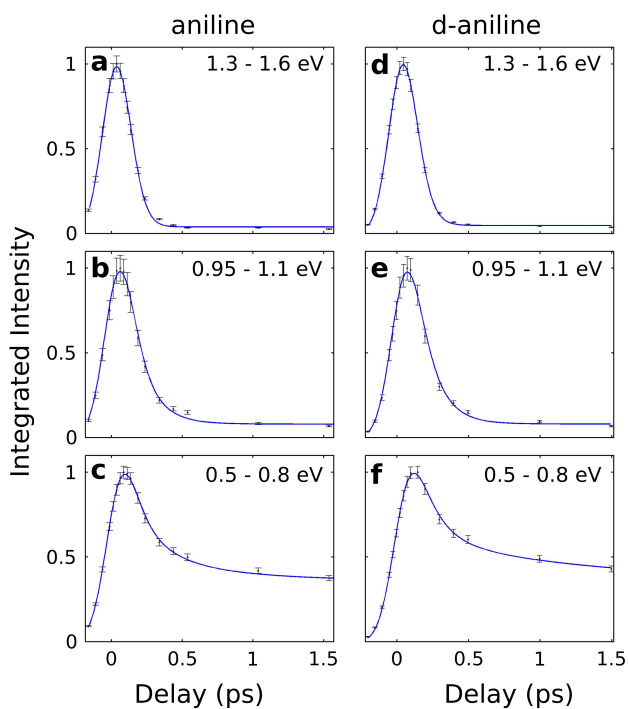


Fig. S3 Fits to the 238 nm photoelectron spectra integrated over 1.3 – 1.6 eV, 0.95 – 1.1 eV and 0.5 – 0.8 eV to determine τ_4 , τ_3 and τ_2 time constants, respectively. Error bars are two standard deviations in photoelectron intensity over the integrated regions.

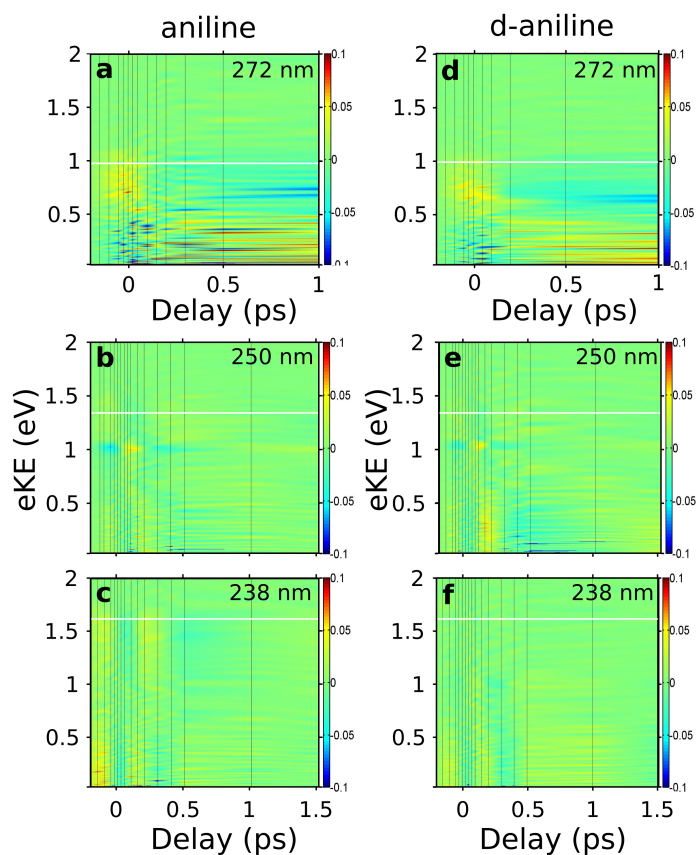


Fig. S4 Residuals of the photoelectron spectra fitted to eq. (2) in the paper subtracted from the experimental photoelectron spectra. The intensity scales are relative to the normalised intensities, the shading was smoothed using bilinear interpolation and the vertical black lines mark the pump-probe delays at which photoelectron spectra were recorded. Horizontal white lines mark the maximum eKE possible from $1 + 1'$ ionisation, calculated using the central wavelengths of the pump and probe laser pulses and the adiabatic ionisation potential of 7.72 eV.¹

References

- 1 M. A. Smith, J. W. Hager and S. C. Wallace, *J. Chem. Phys.*, 1984, **80**, 3097–3105.