
Contribution ID: **107** Type: **Contributed talk**

# Excited state dynamics of azanaphthalenes

*Tuesday, June 24, 2025 12:25 PM (20 minutes)*

Azanaphthalenes are nitrogen containing heterocycles, which have systematic variations of the nitrogen heteroatom centres within a bicyclic aromatic structure. With relevance to biological and chemical systems, understanding the underlying ultrafast dynamics upon photoexcitation in these molecules may lead to opportunities for rational design of photoactive molecules. Here, we use quantum chemical calculations undertaken at the SCS-ADC(2) level of theory to explore the photorelaxation processes occurring in six azanaphthalenes in order to rationalise observations from ultrafast transient absorption spectroscopy (TAS) experiments [1]. Our results indicate substantial differences in the propensity for intersystem crossing vs. internal conversion across these molecules, significantly affecting the photorelaxation rates. We explain this behaviour in terms of spin-orbit coupling effects and barriers on the potential energy surfaces.

[1] M. Garrow, L. Bertram, A. Winter, A. W. Prentice, S. W. Crane, P. D. Lane, S. J. Greaves, M. J. Paterson, A. Kirrander, D. Townsend, Commun. Chem., 2025, 8, 1-11.

**Authors:** KIRRANDER, Adam (University of Oxford); TOWNSEND, Dave (Heriot-Watt University); BERTRAM, Lauren (University of Oxford); GARROW, Malcom (Heriot-Watt University)

**Presenter:** BERTRAM, Lauren (University of Oxford)

**Session Classification:** Session 6 - Chirality II