There is intense current interest in the photophysical properties of metalloporphyrins due to their potential applications in many key chemical areas including biomimetic and optoelectronic systems. In this project, we will study how the structural features of isolated metalloporphyrins influence their intrinsic electronic spectra, to provide an improved fundamental understanding of the nature of the excited states. We will investigate the effect of the metal centre, alkylation of the porphyrin rings and annelation of the porphyrin rings on the position, width and intensity of absorption bands in the key “Soret” and Q band regions. Further experiments will focus on metalloporphyrin-aromatic molecule clusters to probe the effect of direct axial coordination to the metal centre on the electronic spectrum. The proposed studies will be performed in a novel custom-adapted laser-interfaced commercial mass spectrometer, which has now been shown to allow the routine acquisition of gas-phase UV spectra of electrosprayed ions, along with determination of photoproducts. The proposed research has the potential to dramatically improve the current fundamental understanding of metalloporphyrin excited states, in both the gas-phase and solution, and hence make a critical contribution to inform the rational design of new metalloporphyrin materials.

The project will provide very broad training opportunities in a range of highly-transferrable skills including mass spectrometry, (soft ionization techniques, CID, and mass spectral analysis), and laser spectroscopy (use of class 4 laser systems). Training will also be offered in computational chemistry techniques (ab initio and DFT) to support the interpretation of experimental results. The Dessent research group fosters a lively scientific environment for students, with regular group meetings, directed literature reading, close links to the other internal and external research groups, rapid publication of post-graduate results and attendance at external UK and international scientific meetings.

**Project title:** Laser Photochemistry of Metalloporphyrins and their Coordination Complexes

**Supervisor Name(s):** Dr Caroline Dessent

**Supervisor(s) Contact details:** caroline.dessent@york.ac.uk

Vanadyl (IV) meso-tetraphenyl-porphine, an example of a petroporphyrin.

The Department of Chemistry holds an Athena SWAN Gold Award and is committed to supporting equality and diversity for all staff and students.