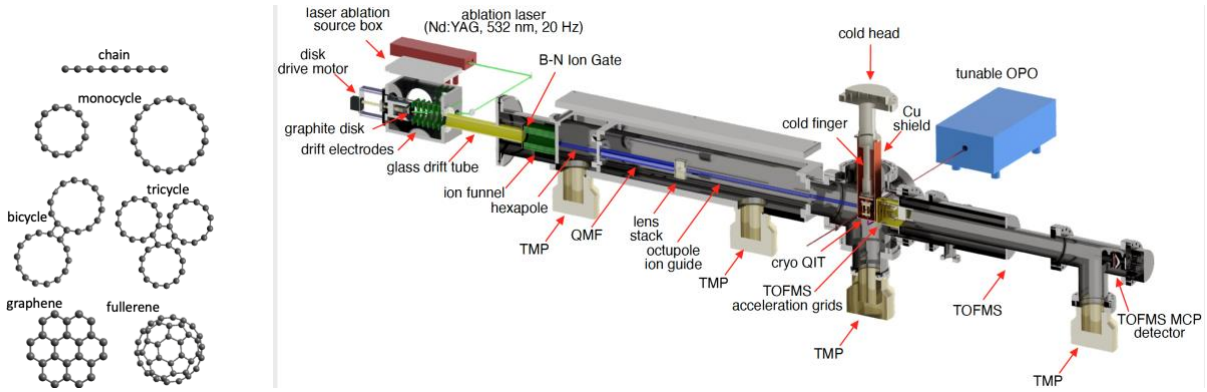
Electronic Spectra of Isomer-Selected Carbon Cluster Cations in a Cryogenic Ion Trap

Buntine, J. T., Marlton, S. J. P., Liu, C., Watson, P. Carrascosa, E.; Bull, J. N.; Jacovella, U.; Cotter, M. I., Bieske, E.J.*
*presenter
[1]evanjb@unimelb.edu.au, School of Chemistry, University of Melbourne, Australia

The past 40 years have witnessed the discovery of new carbon structures, including fullerenes, nanotubes and graphene, which complement the familiar graphite, diamond and amorphous carbon allotropes. It is less well known that small aggregates of carbon possess other structures, such as those shown below, which include chains, rings, bi-rings, and tri-rings, whose spectroscopic properties have scarcely been explored. Crucially, for any particular cluster size there are usually several coexisting isomers potentially confounding attempts to measure electronic or vibrational spectra of a particular monocycle, bicycle, tricycle or fullerene isomer.



Here we present and discuss electronic spectra of bare and hydrogenated carbon clusters measured using 2-colour resonance enhanced photodissociation spectroscopy in a cryogenically cooled ion trap. A novel aspect of the experimental arrangement is that the clusters are pre-selected using a drift tube ion mobility spectrometer and quadrupole mass filter, allowing us to trap and probe clusters with a particular size and shape (chain, monocycle, bicycle).[1, 2] We show that C_{2n}^+ ($6 \leq n \leq 18$) monocycles exhibit electronic absorptions in the visible and NIR region, with a progressive shift of the strongest transition to longer wavelength with increasing cluster size. The $C_{2n+1}H^+$ ($3 \leq n \leq 10$) clusters possess linear and cyclic isomers, with the latter becoming the dominant form for larger clusters. The two isomers exhibit distinct electronic transitions, which, again in both cases, progressively shift to longer wavelength with increasing cluster size.

[1] Buntine, J. T.; Carrascosa, E.; Bull, J. N.; Jacovella, U.; Cotter, M. I.; Watkins, P.; Liu, C.; Scholz, M. S.; Adamson, B. D.; Marlton S.J.P.; Bieske, E. J. An ion mobility mass spectrometer coupled with a cryogenic ion trap for recording electronic spectra of charged, isomer-selected clusters. *Rev. Sci. Instr.* **2022**, *93*, 043201.

[2] Buntine,J. T.; Cotter, M. I.; Jacovella, U.; Liu, C.; Watkins, P.; Carrascosa, E.; Bull, J. N.; Weston, L.; Muller, G.; Scholz, M. S.; Bieske, E. J. Electronic spectra of positively charged carbon clusters - C_{2n}^+ (n=6-14) *J. Chem. Phys.* **2021**, *155*, 214302.