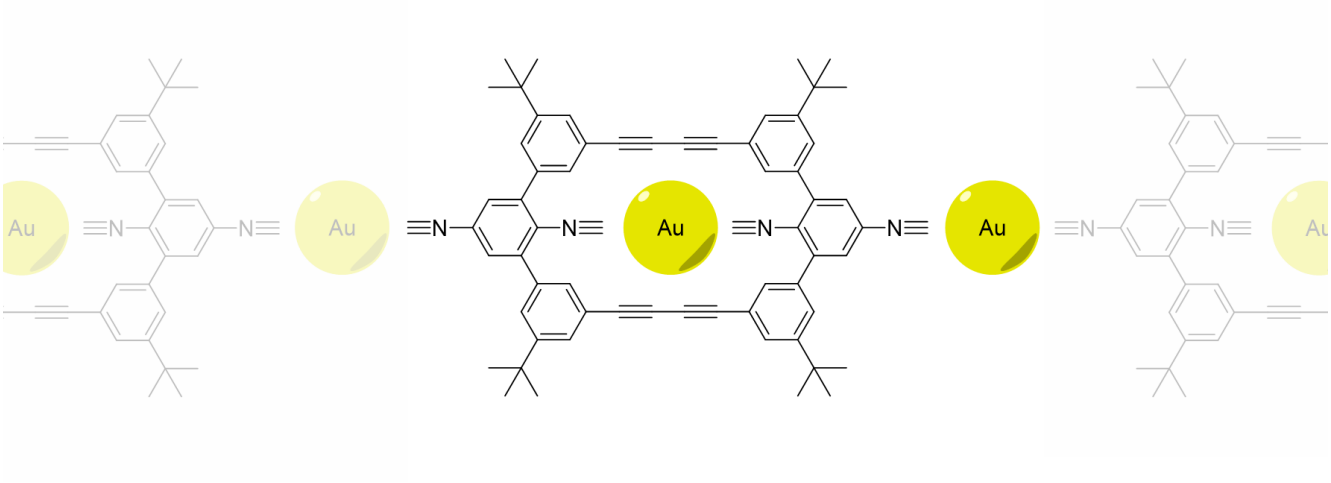
A Macrocyclic Au-Atom Acceptor

Charlotte Kress, Patrick Zwick and Marcel Mayor

University of Basel
charlotte.kress@stud.unibas.ch

Since the pioneering work of Aviram and Ratner,[1] the interest in single molecules for electrical devices significantly increased.[2] The physical properties of highly complex molecules are measured in a physical experimental set-up usually including two gold electrodes. The molecular anchoring requires a functional group with a high affinity to gold, an effective orbital hybridization, and a matching Fermi energy level.
Studies suggest, that the isocyanide-gold coordination bond is stronger than the thiol bond,[3] usually used as gold anchoring group. A recent study showed single molecule junction formation in an mechanically-controlable break junction (MCBJ) experiment of 99% of all traces with 1,4-benzenediisocyanide in a liquid environment. Further opening of the MCBJ resulted in the formation of a one-dimensional coordination polymer with respective conductance plateaus.[4] These findings motivated us to further investigate the isocyanide-gold interaction.
A macrocycle including the 1,4-benzene diisocyanide bridged by two diacetylenes was designed as a rigid bidentate ligand. Our efforts in the synthesis of this macrocyclic structure and promising results of a simplified test system will be presented at my poster.



[1] Aviram, A. & Ratner, M. A. Molecular rectifiers. *Chemical Physics Letters*, **1974**, *29*, 277–283.
[2] Zwick, P.; Weiland, K. J.; Malinčík, J.; Stefani, D.; Häussinger, D.; Zant, H. S. J.; Dulić, D.; Mayor, M., *The Journal of Organic Chemistry*, **2019**, accepted manuscript.
[3] Kiguchi, M., Miura, S., Hara, K., Sawamura, M. & Murakoshi, K., *Applied Physics Letters*, **2006**, 89, 213104.
[4] Vladyka, A., Perrin, M. L., Overbeck, J., Ferradas, R. R., Garcia-Suarez, V., Gantenbein, M., Brunner, J., Mayor, M., Ferrer, J., Calame, M., *Nature Communications*, **2019**, 10, 1–9.