Au(I) BIS-ACETYLIDES WITH DIPHOSPHINE BRIDGING LIGANDS AS MOLECULAR TWEEZERS FOR FULLERENES

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Fullerene recognition *via* supramolecular interactions is an extended area of Supramolecular Chemistry due to the unique electronic properties of the adducts formed between fullerenes and an adequate host, such as molecules containing non-planar polycyclic aromatic hydrocarbon (PAH) substituents [1].

In this work, a set of molecular tweezers based on dinuclear phosphine-bridged gold(I) acetylides with corannulene substituents have been designed and synthesized (Figure 1). Phosphines with different properties, such as geometry and flexibility, have been employed to determine how these properties affect the capability of the tweezers formed to bind fullerenes. The ability of these tweezers to host fullerenes has been studied by ¹H NMR titration experiments. Moreover, Au(I) atoms can establish aurophilic interactions favouring a tweezer-like pre-arrangement and, therefore, the cooperativity between these two features to host fullerenes is being evaluated by experimental and computational studies.

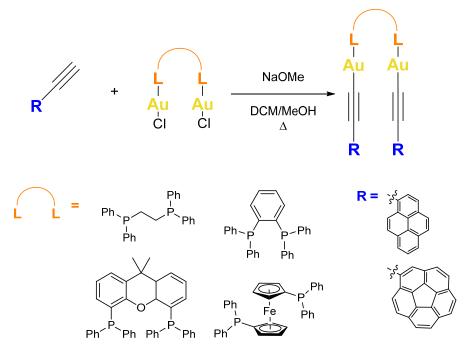


Figure 1. Synthesis scheme and compounds prepared in this work.

^{[1] (}a) Sygula, A. *Synlett* **2016**, 27 (14), 2070–2080. (b) Sacristán-Martín, A.; Miguel, D.; Diez-Varga, A.; Barbero, H.; Álvarez, C. M. *J. Org. Chem.* **2022**, 87 (24), 16691–16706.