

Corannulene-based reversible bistable molecular machines for fullerene recognition

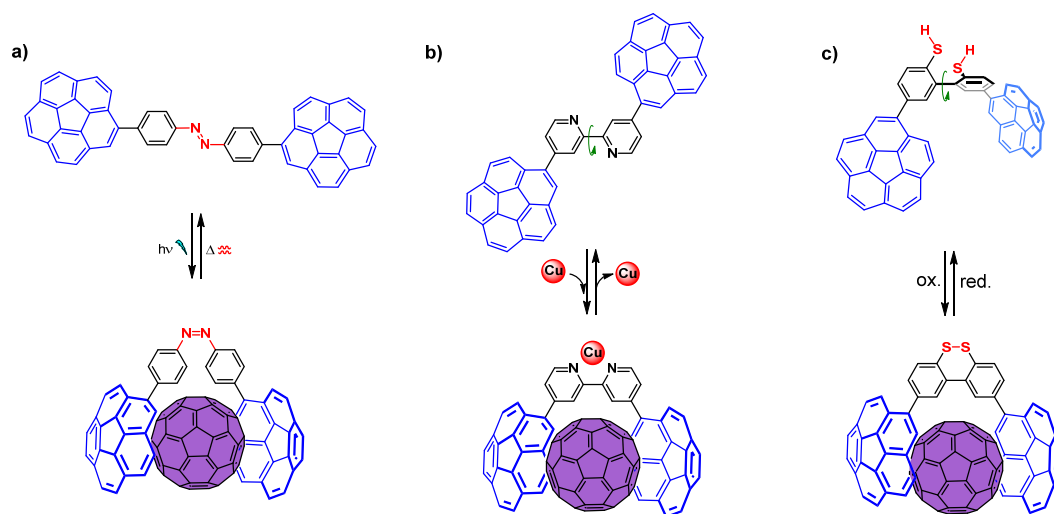
H. Barbero,^{a,*} A. Sacristán-Martín,^a S. Ferrero,^a D. Miguel,^a L. Álvarez-Miguel,^b P. Gómez-Iglesias,^a R. García-Rodríguez^a and C. M. Álvarez^{a,*}

^aGIR MIOMeT, IU CINQUIMA/Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid, Spain

^bUniversidad de Alcalá, Grupo SOSCATCOM, Departamento de Química Orgánica y Química Inorgánica, Facultad de Farmacia, 28871 Alcalá de Henares, Madrid, Spain

*hector.barbero@uva.es, cedonio.alvarez@uva.es

A molecular machine refers to a multistable chemical system capable of reversibly modify its structure by a relative movement of its constituent parts as a response to an external stimulus producing observable work.¹ They are actually key functional elements that support life itself in all living beings. In this talk we will focus on artificial molecular machines which switch their structure between two well-defined conformers/configurational isomers by photoisomerization,² metal coordination/decoordination,³ and redox process.⁴ (Scheme 1). All the species presented bear two units of corannulene ($C_{20}H_{10}$), a geodesic polyarene capable of establishing attractive interactions with fullerenes through concave-convex π - π interactions. The operational principle relies on the formation or disruption of a molecular tweezer by placing two corannulene units in the right location to establish a cavity for fullerene recognition. Their switching properties, especially the in-situ reversibility, and the impact produced onto their ability to recognize fullerenes (C_{60} , C_{70}) will be shown and discussed.



Scheme 1. Examples of switchable molecular tweezers bearing corannulene groups (in blue) operated by photoisomerization (a), metal coordination (b) and oxidation (c) showing their ability to bind fullerenes (in purple) in one state. Key atoms responsible for the isomerizations are highlighted in red.

References

1. Aprahamian, I. *ACS Cent. Sci.* **2020**, *6*, 347–358.
2. Barbero, H.; Ferrero, S.; Álvarez-Miguel, L.; Gómez-Iglesias, P.; Miguel, D.; Álvarez, C. M. *Chem. Commun.* **2016**, *52*, 12964–12967.
3. Sacristán-Martín, A.; Barbero, H.; Ferrero, S.; Miguel, D.; García-Rodríguez, R.; Álvarez, C. M. *Chem. Commun.* **2021**, *57*, 11013–11016.
4. Sacristán-Martín, A.; Miguel, D.; Barbero, H.; Álvarez, C. M. *Org. Lett.* **2022**, *24*, 5879–5883.