

The intriguing class of *altan*-molecules

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As a result of a theoretical investigation on additive patterns in polycyclic systems,¹ we have introduced the *altan*-molecules, which are formed from parent totally fused neutral polycyclics upon substitution of outgoing C–H bonds with C–C bonds pointing towards alternant carbon atoms only of an outer annulene. The latter turns out to be a $[4n]$ annulene, and is expected to host a paratropic current.^{1b} The computational investigation of the altanisation process has led to the design of a paramagnetic closed-shell molecule ([12,5]coronene, or equivalently *altan*-[12]annulene)², and of aromatic anionic bowl-shaped molecules, e.g. *altan*-corannulene hexaanion.³ The latter molecule, with three concentric loops of alternating tropicities which reverse changing the charge, actually forms half a cage of many C₈₀ endohedral fullerenes, and could be a reasonable synthetic target. The altanisation design has been recently challenged as it has been shown to lead to a diatropic outer loop not only in *altan*-kekulene^{1b}, but also in *altan*-[10,5]-coronene.⁴ We have recently unraveled this anomalous behaviour of the altanisation process, and we have found that several *altan*-molecules could be well added to the gamut of molecules, which are nowadays under intense experimental and theoretical scrutiny for the development of organic semiconductor devices.⁶

1. (a) Monaco, G.; Zanasi, R. *J. Chem. Phys.* **2009**, *131* (4), 044126; (b) Monaco, G.; Memoli, M.; Zanasi, R. *J. Phys. Org. Chem.* **2013**, *26* (2), 109–114.
2. Monaco, G.; Fowler, P. W.; Lillington, M.; Zanasi, R. *Angew. Chem. Int. Ed.* **2007**, *46* (11), 1889–1892.
3. Monaco, G.; Zanasi, R. *J. Phys. Org. Chem.* **2013**, *26* (9), 730–736.
4. Dickens, T. K.; Mallion, R. B. *Chem. Commun.* **2015**, *51* (10), 1819–1822.
5. Monaco, G. *Chem. Commun.* to be submitted.
6. Sun, Z.; Ye, Q.; Chi, C.; Wu, J. *Chem. Soc. Rev.* **2012**, *41* (23), 7857.