

Uncommon Polycyclic Open-Shell Structures: Cross-Conjugated Dianions and Mechano-Made Biradicals

J. Casado

¹Department of Physical Chemistry, University of Málaga, Málaga, Spain

E-mail: casado@uma.es

Significant advances in any field of research often come from unexpected experimental results. There are plenty of examples where the realization of uncommon behaviors in the long run trigger new applications. Examples of these in the field of organic electronics are the discovery of conductivity in PA or the serendipitous finding of PCBM as electron acceptor in bulk heterojunction solar cells, etc. The two findings I will describe here are not obviously of comparable relevance but allow me to introduce the reader in the topic of the talk [1-3]. The two stories deal with biradical or diradicals, or pairs of unpaired electrons in singlet ground electronic state configurations which allow a series of interesting properties as small singlet-triplet gaps, thermally activated intersystem crossing, magnetic hysteresis in pure organics, etc. The first case concerns with the properties of dianions of oligothiophenes which are stabilized in cross-conjugation forms (versus typical linear conjugations). This structure allows each anion to weakly interact each other thus forming the singlet open-shell and promoting the small gap with the triplet. The second case is about neutral biradicals generated after pressure application of a closed-shell molecule which provokes the rupture of one π -bond and generation of trapped, kinetically persistent biradicals. Their understanding and implications are discussed.

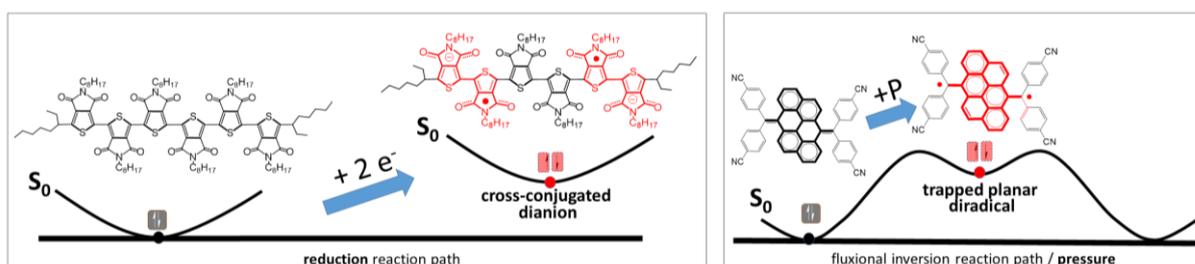


Figure 1: Cross-conjugated dianions and mechano-made biradicals.

References

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