2D-Delocalized vs Confined Diradicals

Juan Casado

Department of Physical Chemistry, Faculty of Science, University of Málaga Andalucía-Tech, 29071 Málaga, Spain (casado@uma.es)

Diradicals are beautiful chemical objects where the more basic and intricate aspects of the chemical bonding are revealed.¹ Not this being important enough, nowadays, diradical-based substrates are becoming very appealing for new organic electronic applications. We focus here in π -conjugated organic diradicals formed by competition between non-aromatic quinoidal structures and their canonical aromatic forms. How this quinoidal(closed-shell)-vs-aromatic(open-shell) energetic balance producing the diradical is affected by several situations has been our objective in the last few years.² Now, we focusses on how the properties of diradicals are influenced when several diradical canonical forms are available in such a way that create a 2D (i.e., bidimensional) π -electron delocalization surface in which the diradical substructures are in cross-conjugation mode producing the curious effect of diradical confinement.³



Herein, the diradical molecular properties of compound **1** in Figure 1 will be discussed in connection with 2D delocalization, cross-conjugation and π -surface confinement.

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