Reversible Oxidation of 40π Antiaromatic Expanded Isophlorins into a Polaron Pair

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 30π and 40π isophlorins are higher analogues of 20π isophlorins;^[1] and are the simplest example of expanded isophlorins having planar and ring inverted structures.^[2] The expanded derivatives of isophlorins provide number of examples for Huckel's (4n+2) π aromatic and $4n\pi$ anti-aromatic systems. In contrast to the aromatic expanded isophlorins, the $4n\pi$ antiaromatic systems differ in their optical and electrochemical properties. The large and planar expanded isophlorins exhibit reversible two-electron oxidation in comparison to their smaller analogues. A 40π conjugated macrocycle with eight furan rings was yielded by acid-catalyzed condensation of furan and pentafluorobenzaldehyde;^[3] and oxidized with trifluoroacetic acid or [Et₃O+SbCl₆] or NOBF₄.^[4] The oxidized product was identified as polaron pair. Single-crystal X-ray diffraction analysis confirmed a planar structure of the oxidized product and the free base.



References:

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