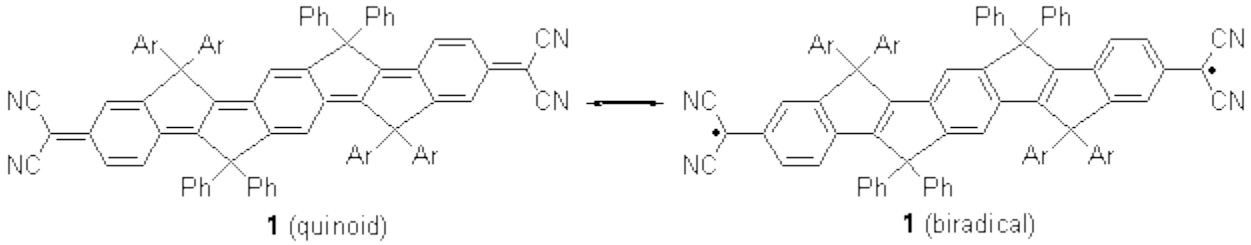
TRI-*P*-QUINODIMETHANE

Tsuji and Nakamura have prepared the tri-*p*-quinodimethane **1**.[1] Quinodimethanes are of interest because of their possible diradical character. This new example is most interesting. It is stable as a solid in air and ambient light for 6 months, or 2 months in solution. Its ESR shows fine structure, with a spin-spin distance estimated to be 14.6 Å, very close to the distance between the terminal carbons. The ground state is a singlet, with the triplet lying 2.12 kcal mol^{-1} higher in energy.



Ar = 4-octylphenyl

UB3LYP/6-31G** computations (lacking the aryl and phenyl sidechains) indicate a ground state singlet (with sizable spin contamination) and a gap to the triplet of 1.83 kcal mol^{-1}.

The computed geometry is shown in Figure 1.

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Figure 1. UB3LYP/6-31G** optimized geometry of **1**.

The analog having just two quinodimethane units showed no ESR signal and the computed singlet-triplet energy gap is 5.68 kcal mol^{-1}.

It would have been interesting to have computed the NICS values for the 6-member rings – as a measure of aromatic *vs.* non aromatic character to further support the participation of the biradical resonance structure contribution to **1**.

Source: http://comporgchem.com/blog/?p=1927