Bis-dibenzo[a,i]fluorenylidene, does it exist as stable 1,2-diradical?

The geometries, energies, and electronic properties of the two possible configurations of bis-[dibenzo[a,i]fluorenylidene] were investigated theoretically by density functional theory DFT B3LYP at the UB3LYP/6-311 + G(2d,p) // UB3LYP/6-31 + G(d,p) level of theory. According to the performed calculations, it was found that the singlet is 3.4 kcal mol\(^{-1}\) lower in energy compared to triplet state at room temperature. This gap is compared with those of other alkenes like ethylene, (61.9 kcal mol\(^{-1}\)) tetra-tert-butylenylene, (6.4 kcal mol\(^{-1}\)) and bis-fluorenylidene (19.5 kcal mol\(^{-1}\)). These results confirm the experimental findings of the paramagnetic properties determined by Franzen and Joschek. The low singlet-triplet gap in the case of bis-[dibenzo[a,i]fluorenylidene] is the result of a steric destabilization of the singlet due to strain and stabilization of the triplet electronic state by delocalization of each free electron within each aromatic moiety. This correlates with the special electronic structure of the triplet state of this compound, where facial interaction of two hydrogen atoms lying close to the lobes of each p-orbital occupied with a single electron at the distorted double bond in the triplet electronic state.