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Title:	Controlling Conformational Preferences of Didehydro-2,2',6,6'-tetrafluorobiphenyl biradicals Towards Designing High Spin Systems
Authors:	Somani, Ankit (/jspui/browse?type=author&value=Somani%2C+Ankit)
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Abstract:	<p>According to IUPAC Gold Book, a molecular entity possessing an unpaired electron is called free radical. The resulting species are highly reactive and these intermediates constitutes one of the important classes in organic chemistry. They play essential roles in organic synthesis, polymer chemistry, atmospheric chemistry and biochemistry. Radical chemistry is not just limited to free radicals; it is extended to biradical, triradical and even polyradicals. Such di- and polyradicals are significant in material chemistry, particularly in constructing molecular magnets that shows potential applications in data storage. In this regard, several strategies have been reported for constructing high spin organic molecular based magnets Through a computational investigation, we attempted to answer questions related to the spin-spin interactions and changes in the singlet-triplet energy gap in a conformationally flexible biradicals toward devising a new strategy to high spin systems. In this regard, design and DFT computations on the electronic structure, stability and singlet-triplet gap along with conformational preferences of biaryl based biradicals have been considered. As a preliminary system, didehydro-2,2',6,6'-tetrafluorobiphenyl biradicals with three possible isomers have been chosen, in which the two radicals are located at two different phenyl rings (3,3', 3,4' and 4,4'). Conformational preferences showed that the two radical centres were stationed in near orthogonal positions due to ortho-substituents. The minimal energy conformers were found to have a dihedral angle ranging between 54 and 65 o depending upon levels of theory. Based on the AIM analysis, we found out that F...F interaction as the major reason for this conformation. From the electronic structural calculations corresponding to the minimal energy conformers revealed that the stability of triplet states are more stable than the corresponding singlet states in all isomeric biradicals. Furthermore, BDE calculations also confirmed the stability order. Higher spin densities at the radical centers, and no spin-spin interactions were observed based on the computations. The effect of other ortho substituents revealed that triplet state is not only stabilized by this but also the minimal energy conformers were attaining an orthogonality. Based on these investigations, we confirmed that not only the orthogonality prevents the spin-spin coupling, but also favours a high spin triplet ground state.</p>
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