Stabilization of open-shell states in purely organic molecules

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Purely organic materials displaying a high-spin electronic state as the ground state, have deserved enormous attention in the last decades.[ref1, ref2] In general terms, most synthetic strategies aiming to obtain these materials deal with one of the following processes; either the synthesis of a precursor that after treatment yields the desired magnetic centers[ref1, ref3] or the use of a building block that is already a stable radical and later extended in 1, 2 or 3 dimensions[ref4, ref5]. In this talk I will present a joint research on the synthesis, characterization and theoretical analysis of the 2,6-dimethyl-4-nitrophenylthiazol-2-imine molecule appearing as a different approach for obtaining purely organic materials displaying a high-spin ground state, using as building blocks simple and neutral molecules. The molecules under study exhibit experimental fingerprints associated with a diradical species, such as EPR signal or reaction with TEMPO. This arises from the stabilization of the unpaired electrons resulting from the rupture of a double bond and a concomitant structural change, as an aggregation-induced phenomenon.[ref6] Moreover, other molecules showing the structural pattern that facilitates the aggregation-induced population of the triplet state, may be thought to exhibit the same properties.

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LOGOS (if required)