

Ferrocene-based diradicals of imino nitroxide, nitronyl nitroxide and verdazyl, and their cations are possible SMM: A quantum chemical study

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Abstract

Six diradicals designed from imino nitroxide, verdazyl and nitronyl nitroxide monoradicals coupled via the ferrocene moiety and the corresponding triradical cations are quantum chemically investigated. The transoid conformation is employed for considerations of general stability. All biradicals are found as very weakly and antiferromagnetically coupled. This agrees with experiment. The cations have strong antiferromagnetic spin-coupling. The charge and spin population distributions, spin alternation pattern, and the disjoint nature of SOMOs can be used to explain the nature and extent of magnetic interaction. Calculated EPR characteristics identify the neutral species as well as their cations as single molecule magnets.

