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以杂环为铁磁耦合单元的双中心双自由基高自旋有机分子的理论设计

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摘要 利用－·N－S－为自旋中心（SC），苯为端基（EG），苯、吡啶、哒嗪、嘧啶 、吡嗪、三嗪为耦合单元（FC），设计三种不同排列方式的新型稳定高自旋分子。 由于自旋密度在杂环（FC）和－·N－S－（SC）组成的体系中自由基双中心的部分 离域，导致－·N-S－自由基的特殊稳定性。三种不同的排列方式中，其三重态的 稳定性随主要SC（－N－）原子间距离的增大而降低。从三个系统八个体系三重态 的稳定性来看，FC上的杂原子位于取代基的间位能提高体系的铁磁耦合作用，而位 于邻位和对位则不利于铁磁耦合作用。

关键词 杂环化合物 游离基 苯 吡啶 哒嗪 嘧啶 耦合 三重态

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Theoretical Design of Biradical High Spin Organic Molecules with Two-center Spin Source and Heterocycles as Ferromagnetic Coupling Units

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Abstract Novel stable high spin molecules possessing three differently arranged fashions are designed using -·N- S- as spin-containing (SC) fragment, phenylene as end groups and various aromatic, such as benzene (1), 2,6-pyridine (2), 3,5-pyridine (3), pyridazine (4), 4,6- pyrimidine (5), 2,6-pyrimidine (6), pyrazine (7), triazine (8) as a ferromagnetic coupling (FC) unit. The effect of the different coupling units on the spin multiplicities of the ground states and their stabilities was investigated by means of AM1-CI approach. It is found that the spin densities on the two atoms of the SC are different from delocalization results in the specific stability of -·N-S-. In these molecules, the stabilities of the triplet states decrease when the distance between the atoms of central SC (-N-) increases. It is shown that nitrogen-containing aromatic rings as coupling unit influence the stabilities of high-spin ground states.

Key words HETEROCYCLIC COMPOUNDS FREE RADICAL BENZENE PYRIDINE PYRIDAZINE PYRIMIDINE PYRIMIDINE TRIPLET

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