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Full Papers

以-•N-N-作自旋中心杂环作端基的高自旋有机分子的理论研究

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摘要 本文设计了三种新颖的具有不同排列方式的高自旋有机分子，它们是-•N-N-作自旋中心、苯作铁磁耦合单元、杂环（如苯、吡啶、哒嗪、嘧啶、吡嗪、三嗪）作端基得到的。通过AM1-CI方法计算可知不同的端基对体系的高自旋基态的稳定性影响不同，同时发现由苯(FC)、杂环(EG)和-•N-N- (SC)组成的双自由基体系由于自旋密度在双中心的部分离域，导致-•N-N-自由基的特殊稳定性.而且由于SC三种不同的排列方式，导致其三重态的稳定性随主要SC(-N-)
原子间距离的增大而降低。从三种体系的三重态稳定性顺序可知以杂环作端基的三重态的稳定性高于以苯作端基的三重态的稳定性，而且在杂环中，以三嗪作端基的三重态的稳定性最高，嘧啶和吡嗪次之，吡啶和哒嗪最低。

关键词 杂环,端基,双自由基,高自旋,AM1-CI

分类号

Theoretical Design of High-spin Organic Molecules with —•N—N— as a Spin-containing Fragment and Heterocycles as an End Group

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Abstract Novel stable high spin molecules possessing three different arranged fashions are designed with —•N—N＜ as a spin-containing (SC) fragment, various aromatic, such as benzene (**1**), pyridine (**2**), pyridazine (**3**), pyrimidine (**4**), pyrazine (**5**), triazine (**6**) as end groups (EG) and phenyl as a ferromagnetic coupling (FC) unit. The effects of a different end groups on the spin multiplicities of the ground states and their stabilities were investigated by means of AM1-CI approach. It has been found that the spin densities on the two atoms of the SC fragment are different from delocalization resulting in the specific stability of —•N—N＜. In these molecules, the stabilities of the triplet states decrease when the distance between the atoms of central SC (—N—) increases. The orders of the stability of triplet states for **1a***n*, **1b***n*, **1c***n* [They are isomers in which SC is connected with FC in different way (**1a***n*, N_1NNN_1; **1b***n*, $N_1N\ N_1N$; **1c***n*, NN_1N_1N) and six heterocycles are EG] show that the stability of triplet states with heterocycles as end groups is higher than that with phenyl as end groups, and in the order: triazine (EG)＞pyrimidine, pyrazine＞pyridine, pyridazine.

Key words heterocycle end group biradical high-spin AM1-CI

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