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研究论文

具有光控功能的两种氮氧自由基体系磁偶合作用的理论研究

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摘要 采用密度泛函结合对称性破损态(DFT-BS)方法,
通过计算具有光控磁性分子开关功能的二氮氧自由基二芳基乙烯化合物的磁偶合常数,
合理解释了其分子结构发生开环和闭环变化时,
分子磁性发生的改变. 同时设计了二氮氧自由基二甲基二氢化芘分子光控开环和闭环模型,
并用同样的方法计算了模型分子的磁偶合常数,
发现这些模型分子的磁行为类似于二氮氧自由基二芳基乙烯化合物, 有可能也具有光控磁性分子开关功能.

关键词 氮氧自由基 二芳基乙烯 二甲基二氢化芘 磁偶合 密度泛函方法

分类号

Theoretical Study on Magnetic Coupling of Two Nitronyl Nitroxide Systems with Photoswitching Performance

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Abstract The magnetic coupling of a diarylethene with two nitronyl nitroxide compounds, which exhibits excellent photoswitching performance, was investigated by means of the density functional theory combined with broken-symmetry approach (DFT-BS) method. The calculated results verify that the magnetic coupling is changed with opening and closure of the ring. The same method was used to study model molecules of dimethyl dihydro pyrene with two nitronyl nitroxides. It was also found that the magnetic behavior of the open structures is different from that of close structure for the model molecules, hence the designed model molecules may also have the photoswitching performance.

Key words nitronyl nitroxide diarylethene dimethyl dihydro pyrene magnetic coupling density functional theory

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