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# 1，2，5-噻重氮和1，4-二正戊氧基苯环化的自由四氮杂卟啉及其金属镁配合物的结构和性质：密度泛函理论计算(英文)

# Structures and Properties of Porphyrazine with Annulated 1,2,5-thiadiazole and 1,4-diamyloxybenzene and Its Magnesium Complex: Density Functional Theory Calculations



中文关键词：四氮杂卟啉；　光谱；　密度泛函理论计算

英文关键词：porphyrazine; spectroscopy; density functional theory calculations

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中文摘要：

用DFT方法计算分析了1，2，5-噻重氮和1，4-二正戊氧基苯环化的自由四氮杂卟啉及其金属镁配合物的分子和电子结构，理论计算的键参数和单晶结构测定结果一致。进一步对1，2，5-噻重氮和1，4-二正戊氧基苯环化的自由四氮杂卟啉的红外光谱进行了正则坐标分析和光谱模拟，以及用TD-DFT方法对1，2，5-噻重氮和1，4-二正戊氧基苯环化的四氮杂卟啉金属镁配合物的电子吸收光谱进行了分析和谱峰归属，比较了四氮杂卟啉环上取代基的电子性质对四氮杂卟啉衍生物光谱性质的影响。

英文摘要：

Density functional theory (DFT) calculations were carried out to describe the molecular structure, atomic charges, molecular orbital energy gaps, HOMO orbital map, and infrared (IR) spectrum of metal-free porphyrazine with annulated 1,2,5-thiadiazole and 1,4-diamyloxybenzene groups (cis-$S_2A_2$)$PzH_2$ (A=the annulated 1,4-diamyloxybenzene ring, S=the 1,2,5-thiadiazole ring) in the peripheral position of the porphyrazine macr-ocycle. The calculated structure and IR spectrum of ($S_2A_2$)$PzH_2$ are in good consistency with the experimental results. It has been found that the electron-withdrawing 1,2,5-thiadiazole groups and the electron-donating 1,4-diamyloxybenzene groups at the peripheral positions of porphyrazine ring add obviously different effect to different pyrrole and pyrrolenine rings. In addition, time dependent-DFT (TD-DFT) calculations were also performed on the electronic absorption spectrum of ($S_2A_2$Pz)Mg, the nature of the main transitions have been assigned accordingly. With the assistance of animated pictures produced on the basis of the normal coordinates, the vibration modes in the IR spectrum of ($S_2A_2$)$PzH_2$ have also been identified.



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