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研究论文

两种槲皮素-Zn配合物的抗氧化活性及其结构的量子化学研究

蒋柳云*，刘玉明

(四川大学化学学院 成都 610064)

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摘要 按照不同比例合成了两种槲皮素-Zn配合物, 采用邻苯三酚自氧化法测定了其抗氧化活性, 然后对其结构在HF/LanL2DZ基组水平上进行了量子化学计算, 讨论了它们的几何构型、电荷分布、原子轨道对前沿分子轨道贡献、分子轨道能量及振动频率. 实验和理论分析都表明, 两种槲皮素-Zn配合物都具有较高的结构稳定性和不同程度的催化超氧阴离子的抗氧化活性.

关键词 配合物 抗氧化活性 量子化学计算

分类号

Study on Antioxidative Activities and Quantum Chemistry Calculation of Two Quercetin-zinc Complexes

JIANG Liu-Yun*, LIU Yu-Ming

(*College of Chemistry, Sichuan University, Chengdu 610064*)

Abstract Two quercetin-zinc complexes were synthesized according to different ratio reactants, and their biological activities were measured by means of pyrogallol autoxidation. The result shows that they have different level antioxidative activities. Quantum chemistry calculations were performed by using Gaussian 98 program at HF/LanL2DZ basis set. The geometry structures, charges, atomic orbital contribution to frontier molecular orbitals, molecular orbital energies and vibrational frequency were discussed. It indicates that they have good stabilities and relatively high different level antioxidative activities, which is consistent with the experimental result.

Key words complex antioxidative activity quantum chemistry calculation

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通讯作者 蒋柳云 jlytxg@sina.com.cn