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Full Papers

a,a,a,b-ZnT(*o*-BocThr)APP对咪唑衍生物和氨基酸酯的分子识别研究

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摘要 本文采用UV-Vis光谱滴定法、核磁、圆而色光谱、构象分析和量化计算等方法研究了手性主体a,a,a,b－四－[邻（叔丁氧羰苏氨酸）氨基苯基]卟啉锌，a,a,a,b-ZnT(*o*-BocThr)APP **1**，
对手性氨基酸酯类和咪唑类客体的分子识别。采用UV-Vis光谱滴定法测得了主客体之间的缔合常数和热力学参数。^{1}H NMR研究表明，与主体键合的客体的质子化学位移均向高场移动。圆二色光谱的研究表明，主体**1**
分别与*L*型和*D*型氨基酸酯缔合表现出完全对称的圆二色谱图。构象分析的研究表明，
缔合常数大的主客体配合物具有更稳定的构象，
主体与*D*型氨基酸酯的配合物的构象比*L*型的稳定。量化计算的结果从分子层次上对识别作用机制给出了合理的解释。

关键词 手性卟啉, 分子识别, 圆二色光谱, 构象分析, 量子化学计算
分类号

Study on the Molecular Recognition of *α,α,α,β*-ZnT(*o*-BocThr)APP toward Imidazole Derivatives and Amino Acid Esters

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Abstract Molecular Recognition of *α,α,α,β*-ZnT(*o*-BocThr)APP (**1**) toward a series of imidazole derivatives and amino acid esters was investigated. Association constants were determined in chloroform by means of UV-Vis titration method. The association constants of **1** with imidazole derivatives are larger than those of **1** with amino acid esters. ^{1}H NMR spectra were investigated to describe the binding mode of the recognition system, showing that all the protons of the guests were shifted to upfield. The circular dichroism spectra of **1**-*L*-/*D*-ValOMe showed a split cotton effect in Soret region, while those of **1**-*L*-/*D*-PheOMe showed no split cotton effect. Molecular modeling was performed to understand chiral recognition on a molecular level. Quantum chemical calculation was carried out based on the stable conformations of these recognition systems, which gave a reasonable explanation for the behavior of molecular recognition. The results indicated that the conformation of **1**-*D*-ValOMe was more stable than that of **1**-*L*-ValOMe.

Key words chiral porphyrin molecular recognition circular dichroism spectra configuration analysis quantum chemistry calculation

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