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研究论文

新型手性双核**Salen Zn(II)**配合物的分子识别研究

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摘要 采用新型Salen中间体合成了新型Salen Zn(II)配合物. 用紫外-可见光谱滴定法研究了主体双核Salen Zn(II)与咪唑、二胺类等含氮小分子的分子识别行为, 测定了它们的缔合常数. 对咪唑类客体的缔合常数顺序为K^{θ}(Im)＞K^{θ}(2-MeIm)＞K^{θ}(EMeIm); 对二胺类客体缔合常数顺序为K^{θ}(DAP)＞K^{θ}(DAE). 主体与咪唑类和二胺类客体的配位数分别是2和1. 主体与这些客体的识别过程为放热、熵减的焓驱动反应. 利用圆二色光谱研究了识别过程的Cotton效应. 用分子力学方法研究了主客体体系的最低能量构型, 通过量化计算对实验事实做了进一步解释.

关键词 新型手性Salen中间体 新型手性Salen Zn(II)配合物 分子识别 圆二色光谱 理论计算

分类号

Study on Molecular Recognition of New Dinuclear Chiral Salen Zn(II) Complex

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Abstract A new chiral dinuclear Salen Zn(II) complex was synthesized from a new chiral salen intermediate. The chiral molecular recognition of imidazoles and diamines was studied by the chiral salen Zn(II), and associative constants of host with guest were measured. The sequence of such constants of the host with imidazoles is K^{θ}(Im)＞K^{θ}(2-MeIm)＞K^{θ}(EMeIm), and that with diamines isK^{θ}(DAP)＞K^{θ}(DAE). The coordination numbers of the host with imidazoles are 2, while those with diamines are 1. It was found that the molecular recognition process was driven by decrease of enthalpy. CD spectra of host-guest recognition behavior were also studied. The minimal energy configurations of host-guest complexes were obtained by simulated annealing, and based on that, quantum chemical calculation was performed to explain the experimental results.

Key words new chiral salen intermediate dinuclear chiral Salen Zn(II) complex molecular recognition CD spectra quantum chemical calculation

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