

研究论文

CH/π, CH/O弱氢键在2,6-二(α-苯基苄基)-1,5-萘二酚主体分子包结物构筑中的作用

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摘要 设计、合成了一种新的主体分子2,6-二(α-苯基苄基)-1,5-萘二酚 (**1**).

它可与许多有机小分子形成配位包合物. 用IR和¹H NMR表征了配位包结物, 并测定了主客体分子的摩尔比:

1•DMF (1: 1), **1**•DMSO (1: 2), **1**•吡啶 (1: 1), **1**•喹啉(1: 2), **1**•N-甲基吡咯烷酮(1: 1).

用单晶X衍射分析了包结物 (**1**)•DMF的晶体结构, 属三斜晶系, 晶胞参数为*P*-1, *a*=0.9085(9) nm, *b*=0.9501(6) nm,

c=2.0995(6) nm, $\alpha=99.59(3)^\circ$, $\beta=90.13(4)^\circ$, $\gamma=96.20(7)^\circ$, *V*=1.776(2) nm³, *D*_c=1.898 g•cm⁻³. 结果表明,

主体分子间的CH/π弱氢键在决定主体分子的层状框架结构和客体分子在层间的填充方式中发挥了重要作用;

两种不等效的客体分子与主体分子的作用方式是不同的, 一种客体分子是通过CH/π,

CH/O弱氢键与同层的不同主体分子相互作用, 另一种是通过CH/π,

CH/O弱氢键与相邻层的不同主体分子相互作用.

关键词 [包结化合物](#) [2,6-二\(α-苯基苄基\)-1,5-萘二酚](#) [X射线衍射分析](#) [弱氢键相互作用](#)

分类号

Role of CH/π, CH/O Weak Hydrogen Bonds in Constructing Inclusion Compounds of 2,6-Bis(α-phenylbenzyl)-1,5-naphthalenediol

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Abstract A new kind of host molecule 2,6-bis(α-phenylbenzyl)-1,5-naphthalenediol (**1**) was designed and synthesized. It exhibits strong inclusion property with various small organic molecules. The inclusion compounds were characterized by IR and ¹H NMR. The molar ratios of host and guest are **1**•DMF (1: 1), **1**•DMSO (1: 2), **1**•pyridine (1: 1), **1**•quinoline (1: 2) and **1**•N-methyl-2-pyrrolidone (1: 1), respectively. The structure of inclusion compound of **1** with DMF was determined by single crystal X-ray diffraction with parameters of triclinic symmetry, *P*-1, *a*=0.9085(9) nm, *b*=0.9501(6) nm, *c*=2.0995(6) nm, $\alpha=99.59(3)^\circ$, $\beta=90.13(4)^\circ$, $\gamma=96.20(7)^\circ$, *V*=1.776(2) nm³, *D*_c=1.898 g•cm⁻³. The result showed that CH...π weak hydrogen bonding plays a very important role in constructing the layer host framework and guest molecule packing pattern. The contacts between two inequivalent guests DMF with host are different, and one is through CH...π and CH...O weak hydrogen bonding to the host molecules in the same layer, while the other is through the same interaction in the neighbor layer.

Key words [inclusion compound](#) [2,6-bis\(α-phenylbenzyl\)-1,5-naphthalenediol](#) [X-ray diffraction analysis](#) [weak hydrogen bonding interaction](#)

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