

超分子体系中轴-轮状D.D.主体分子的立体异构现象

郭文生,郭放,刘祁涛

辽宁大学化学科学与工程学院

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摘要 组装了轴-轮状主体分子1,1,6,6-四基乙-2,4-二炔-1,6-二醇(1)与天然主物异补骨脂素(2)。茴香醚(3)形成的两种超分子异构体的包结物晶体,它们的主客体分子摩尔比分别为1:2和2:1

单晶X射线衍射分析了游离主体分子以及超分子包结物晶体的结构,结果表明在主客体分子摩尔比1:2的晶体中,主体分子与异补骨脂素形成氢键,主体分子采取对位交叉式构象;在主客体分子摩尔比为2:1的晶体中,主体分子这间形成氢键,主体分子采取邻位交叉式构,

主体分子所取的构象取决于客体分子的性质,当客体分子为氢键好的受体时,可与主体分子生成1:2的包结物;当客体分子为氢键差的受体时,生成2:1有包结物,

本文还对三种晶体是的主体分子的立体构苯环两面角, C(1)和C(6)所连基团的夹角和能量变化规律进行了比较和分析。

关键词 [包结物](#) [立体异构](#) [四苯基己二炔二醇](#) [异补骨脂素](#) [茴香醚](#) [X射线衍射分析](#)

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## Stereoisomerism of a wheel -axle shaped D.D. host in supramolecular entties

Guo Wensheng,Guo Fang,Liu Qitao

**Abstract** Two types of supramolecular stereoisomers formed from a wheel -and - axle shaped host molecular 1,1,6,6-tetraphenylhexa - 2,4- diyne -1,6- diol(1) and isopsoralen (2) or anthole (3) were assembled with the host /guest molar ratio being 1:2 and 2:1 respectively. The single crystal structures of the free host and its two inclusion compounds were determined by X ray diffraction analysis. The results show that in the ctystal with host/guest molar ratio being 1:2, the host bound to isopsoralen (2) by hydrogen bond adopts in antiperipar conformation, while in the 2:1 crystal, the host is in a gauche conformation due ti the hydrogen bonding within the hosts. The observed of crystallization and molecular conformation of the host (1) were found to be primarily dependent on the nature of the guest environment. An antiperipar conformation of the host(1) is formed in the gust environment with goodH-bond donors, while a guche conformation is favored in a relatively poor H-bond donor guest. The regularity of thre changes in the dihedral angles of phenyl groups, the angles between the groups attached to C (1) and C(6) as ewll as the energy of the host compound in the three ctystals are also presented.

**Key words** [STEREOISOMERISM](#) [METHYL PHENYL ETHER](#) [X-RAY DIFFRACTION ANALYSIS](#)

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