

## $\alpha$ , $\alpha'$ -顺式二取代环十二酮的构象

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**摘要** 利用分子力学计算,  $^1\text{H}$  NMR,  $(^{13}\text{C})$  NMR和单晶X射线衍射分析技术研究了 $\alpha$ - $\alpha'$ -顺式二表明, 它们的优势构象骨架仍是[3333]-2-酮, 在晶体和溶液中, 它们的优势构象均为。 $\alpha$ -角顺,  $\alpha'$ -边外构象。在溶液中, 相同取代基的 $\alpha$ ,  $\alpha'$ -顺式二取代环十二酮存在两种互为镜象的[3333]-2-酮对映体构象, 平衡之中; 不同取代基的 $\alpha$ ,  $\alpha'$ -顺式二取代环十二酮存在在体积较大的基团为边外取代的[3333]-2-酮和角顺取代的[3333]-2-酮两种构象, 两种构象也处于动力学平衡之中, 以较大基团为边外取代的[3333]-2-酮构象占优势。

**关键词** [环十二酮](#) [构象](#) [分子力学](#) [X射线衍射分析](#) [质子磁共振谱法](#) [碳十三核磁共振谱法](#)

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## Conformation of $\alpha$ , $\alpha'$ -cis-Bissubstituted Cyclododecanones

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**Abstract** The conformation of  $\alpha$ ,  $\alpha'$ -cis-bissubstituted Cyclododecanones has been studied by means of molecular dynamics computations,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and X-ray diffraction analysis. The results indicate that the ring skeleton of their preferred conformation is still [3333]-2-one conformation. Both in crystal and solution, the preferred conformation of  $\alpha$ ,  $\alpha'$ -cis-bissubstituted Cyclododecanones is  $\alpha$ -corner-syn-,  $\alpha'$ -side-eso-bissubstituted [3333]-2-one conformation. In solution, the  $\alpha$ ,  $\alpha'$ -cis-bissubstituted Cyclododecanones with the same substituted groups may adopt two conformations, which are mirror image to each other and exist in a dynamic equilibrium, while the  $\alpha$ ,  $\alpha'$ -cis-bissubstituted Cyclododecanones with the different substituted groups may adopt two different [3333]-2-one conformations: one with the bigger group present in the  $\alpha$ -side-exo position, and the other with the bigger group present in the  $\alpha$ -corner-syn position, which also exist in a dynamic equilibrium and the former is much more preferred.

**Key words** [cyclododecanone](#) [CONFORMATION](#) [MOLECULAR MECHANICS](#) [XRD](#)  [\$^1\text{H}\$ NMR](#)  [\$^{13}\text{C}\$ NMR](#)

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