水溶液中甘氨酰-缬氨酸与稀土配位作用及其配合物构象的NMR研究

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摘要 本文测定了在三种不同稀土离子(镧La^3^+、钬Ho^3^+和镱Yb^3^+)的水溶液中甘氨酰-缬氨酸的^1H的^1^3C稀土诱导位移。计算了Ho、Yb与甘氨酰-缬氨酸配合物的稳定常数, 讨论了稀土与该配体的配位作用及对配合物构象进行了研究,发现配位后的甘氨酰-

缬氨酸以一种空间位阻较小的伸展构象存在。

关键词水溶液核磁共振谱法稳定常数钬络合物镱络合物镧络合物构象配位甘氨酸 P诱导位移缬氨酸 P

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NMR Studies on the coordination of rare earths with Glycyl-DL-Valine and the conformation of their complex in aqueous solution

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Abstract Lanthanide-induced shifts were measured for 13C and 1H nuclei of glycyl-DL-valine in the presence of three lanthanide cations (La3+, Ho3+ and Yb3+) in aqueous solution The stability constants of the coordination compounds of rare earths (Ho, Yb) with glycyl-DL-valine were calculated The coordination of rare earths with the ligand is discussed. The simulation for conformation of lanthanide coordination compounds with glycyl-DL-valine shows that the ligand is coordinated to lanthanide ion through oxygen atoms of carboxyl group and the bond length of Ln-O is 0.226 nm. In the coordination compounds, glycyl-DL-valine is in extended state with minimal steric hindrance.

 Key words
 AQUEOUS SOLUTION
 NMR SPECTROMETRY
 STABILITY CONSTANT
 HOLMIUM

 COMPLEX
 YTTERBIUM COMPLEX
 LANTHANUM COMPLEX
 CONFORMATION
 COORDINATION

 GLYCINE P
 COMPLEX
 CONFORMATION
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