Synthesis and Crystal Structure of Rare Earth Complex with Ciprofloxacin

Pin YANG¹*, Jia Bin LI¹, Yan Ni TIAN¹, Kai Bei YU²

¹Institute of molecular Science, Shanxi University, Taiyuan 030006 ²Analysis and Test Center, Chinese Academy of Sciences, Chengdu 610041

Abstract: The complex of rare earth with ciprofloxacin has been synthesized and characterized by means of x-ray single crystal diffraction. The structure features of the complex are decribed.

Keywords: Rare earth, ciprofloxacin, complex of cerium.

Ciprofloxacin(LH) was considered the best of the quinolone-group antibacterials¹ of the third generation, but low solubility and bioavailability were its shortcomings. Rare earth compounds can perform the function of antibacterial and anti-inflammation²⁻⁵. This thesis intends to combine ciprofloxacin with rare earth metal ion with the aim to improve the antibacterial activity.

Preparation

Pyridine was slowly added to a solution of ciprofloxacin hydrochloride (1.5 mmol) in 1 mole/L HCl (15 ml) until ciprofloxacin was entirely dissolved (Solution A). A 4 ml aqueous solution of $CeCl_3$ '7H₂O (0.75 mmol) was added to solution A under stirring and about 20 ml ethanol was added, too. Upon storage at room temperature, crystals of good quality were obtained.

A crystal of dimensions $0.54 \times 0.54 \times 0.54$ mm sealed in a glass capillary was used for X-ray diffraction data collection with MoK α radiation ($\alpha = 0.71073$ Å) on a Siemens P₄ four-circle diffractometer equipped with graphite crystals and incident beam monochromator. A total of 8227 independent reflections were collected in the range of $1.99 < \theta < 24.57^{\circ}$ by ω scan technique at 290(2)K.

The crystal is triclinic, space group Pī , with a=13.856(2) Å, b=13.899(3) Å, c=16.505(2) Å, α =92.730(10)° , β =114.390(10)° , γ =115.550(10)° ,V=2511.3(7) Å³, Z=2, Dc=1.294 Mg/m³, μ =1.025mm⁻¹, F(000)=1000, R₁=0.0449, wR₂=0.1354.

The structure was solved using direct method (SHELXTL 5.03) and data collection refined by using the XSCANS program. Hydrogen atoms, except H_2O of crystallization and coordination, were calculated theoretically.

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The structure features of complex are shown in **Figure 1**. The Ce⁺³ ion is coordinated by eight oxygens which belong to two ligands ions each acting as bidentate through oxygen of carboxyl and oxygen of carbonyl and four H₂O. It can be seen that the structure shown in **Figure 1**. is a coordinated ion of positive valence.

Figure 1. The structure of $[L_2Ce(H_2O)_4]^+$



It is the character of dissolution in water that improves the solubility and bioavailability of ciprofloxacin. Preliminary experiment has indicated that the antibacterial activity of ciprofloxacin complex with rare earth is inclined to increase.

Acknowledgments

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References and Notes

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