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# $[Gd(C_{10}H_0N_2O_4)(C_{10}H_8N_2O_4)(H_2O)_3]_2$ ·phen·4H<sub>2</sub>O的晶体结构和生物活性

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摘要 在水乙醇混合溶剂中,首次得到了2-羰基丙酸水杨酰腙、1,10-菲啰啉与硝酸钆形成的配合物[Gd  $(C_{10}H_9N_2O_4)(C_{10}H_8N_2O_4)(H_2O)_3$ ]2·phen·4 $H_2$ O,并测试了其单晶结构。该配合物属三斜晶系,空间群为P-I。每个配合物分子中有两个九配位的钆的结构单元,每个钆离子与两个三齿配体2-羰基丙酸水杨酰腙(分别以负一价和负二价形式)

和三个水分子配位。每个钆单元在空间呈扭曲的单帽四方反棱柱。同时还有一个游离的1,10-菲啰啉存在于晶格中,通过氢键与配位水作用。生物活性试验表明该配合物对三种病原菌有一定的抑菌活性。 关键词 <u>钆配合物,2-羰基丙酸水杨酰腙,1,10-菲啰啉,晶体结构,生物活性</u> 分类号

# Crystal Structure and Bioactivity of Complex $[Gd(C_{10}H_9N_2O_4)(C_{10}H_8N_2O_4)(H_2O)_3]$ \_\*phen\*4H\_2O

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**Abstract** A novel gadolinium(III) complex with N-(2-propionic acid)-salicyloyl hydrazone ( $C_{10}H_{10}N_2O_4$ ,  $H_3L$ ) and 1,10-phenanthroline ( $C_{12}H_8N_2$ , phen) was prepared and characterized. The crystal structure of  $[Gd(H_2L)(HL)-(H_2O)_3]$  2-phen-4 $H_2O$  was determined by X-ray single crystal diffractometry. The crystal complex crystallizes in the triclinic system with space group P-1. There are two 9-coordinated structure units in every complex molecule, in which Gd(III) is coordinated by two tridentate ligands ( $H_2L$  and HL forms) and three water molecules and both the structural units take a distorted monocapped square antiprism. There is a free 1,10-phenanthroline connecting with coordinated water by hydrogen bonds in the crystal. The bioactivity tests indicate that the complex is an inhibitor against three bacteria.

 Key words
 gadolinium(III) complex
 N-(2-propionic acid)-salicyloyl hydrazone
 1
 10-phenanthroline
 crystal

 structure
 bioactivity

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