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[Co(3,3-tri)(ibn)Cl]^2^+异构体的2DNMR及其分布规律的研究

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摘要 利用-维及二维核磁共振谱，如gCOSY和NOESY，对合成的5个[Co(3,3-tri)(ibn)Cl]^2^+几何异构体在溶液中的结构进行了解析，
与柱色层方法分离出的五带配合物对照的结果是：b1=m4;b2=m2;b3=m1;b4=m3
及b5=f3。利用量子化学从头算方法，从能量角度解释了配合物异构体的分布规律。

关键词 钴络合物 胺 P 二维核磁共振 从头计算法 分布规律 异构体

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Study on 2D NMR spectra and product distribution of the geometric isomers in [Co(3, 3-tri)(ibn)Cl]^2^+ system

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Abstract The configurations of the four geometric mer-isomers in a new [Co(3, 3-tri)(ibn)Cl]^2^+(3, 3-tri=N-(3-aminoethyl)-1, 3-propanediamine; ibn=1, 2-diamino-2-methylpropane) system were assigned by using 2D NMR techniques such as gCOSY and NOESY. Solvent used was Me~2So=d~6 with the central peak of the CD~3 septet as the reference (^1^3C, δ39.37; ^1H, δ2.49 relative to SiMe~4). Comparing to the eluates from the chromatographic column, cation exchange media used was Dowex 50 W×2 (H^+ form, 200～400 mesh; Biorad), the first band contains the m2, the second band contains the m4, the third band contains the m1, the fourth band contains the m3 and the last band contains the f3. An ab initio computational result (RHF/LANL2DZ level) suggests why the facial isomer has been isolated and the distribution of the four mer-isomers is not different from those of [Co(2, 2-tri)(diamine)Cl]^2^+.

Key words COBALT COMPLEX OXAZOLE P AB INITIO CALCULATION REGULARITIES OF DISTRIBUTION ISOMER

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