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Full Papers

顺铂化合物与鸟嘌呤异构体相互作用的理论研究

章志强, 周立新*, 和芹

[1]暨南大学化学系，广州，510632

[2]福州大学化学系，福州350002

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摘要 使用量子化学MPW1PW方法，优化了顺铂键连到DNA碱基-鸟嘌呤及互变异构体N7形成的配合物的构型，同时用MP2方法计算其能量，
以研究顺铂对鸟嘌呤互变异构作用的影响。结果表明：顺铂的键连引起了互变平衡的变化，但是各互变异构体之间的相对稳定性顺序并没有改变。氢原子在N1和N9上的（1，9）形式异构体总是最稳定的构型，但是别的异构体也可能共存于水中。同时，
各互变异构体可能经过同一中间体。

关键词 顺铂, 鸟嘌呤, 互变异构体

分类号

Interaction of Cisplatin Adducts with Guanine Tautomers: A Theoretical Study of Metalated Tautomeric Forms

ZHANG Zhi-Qiang[1,2],ZHOU Li-Xin*[,1], HE Qin[1,2]

[1] Department of Chemistry, Jinan University, Guangzhou, Guangdong 510632,China

[2] Department of Chemistry,Fuzhou University, Fuzhou, Fujian 350002, China

Abstract The influence of binding of cisplatin adducts on tautomeric equilibrium of guanine was investigated using quantum chemical method. The monoaqua adduct $[Pt(NH_3)_2Cl(H_2O)]^+$ and the diaqua adduct $[Pt(NH_3)_2(H_2O)_2]^{2+}$ were chosen for coordination to the N(7) site of guanine tautomers. The results demonstrate that the platinum adducts influence moderately on tautomeric equilibrium, but do not change the relative stability of tautomers whether in gas phase or in aqueous solution. The keto form having H atom at N(1) and N(9) was always the predominant structure when cisplatin adducts were bound to guanine. However, other forms could coexist in water. Meanwhile, our calculations suggest that the tautomeric equilibrium should be via the same intermediate.

Key words cisplatin guanine tautomer

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通讯作者 周立新 tlzhou@jnu.edul.cn