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研究论文

氧氟沙星的核磁共振波谱性质研究

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摘要 结合^{1}H, ^{13}C NMR, DEPT, COSY, HSQC, HMBC谱和碳氟偶合裂分行为, 对酸性及碱性溶液中氧氟沙星(Ofloxacin, OFL)的^{1}H和^{13}C谱分别进行归属, 研究了哌嗪环亚甲基构成的AA'BB'复杂自旋体系中各H的化学位移. 发现噁嗪环上的甲基处于直立键; 5H在酸性溶液中化学位移移向低场, 这可能与形成C—H...O弱氢键有关; 在碱性溶液中, OFL的羧基变为羧酸根, 造成羧基和羰基周围碳原子上π电子重新分布, 导致相应C的化学位移和碳氟偶合常数发生明显变化.

关键词 喹诺酮 氧氟沙星 核磁共振 哌嗪环

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Studies on NMR Behavior of Ofloxacin in Different pH Environment

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Abstract Systematic NMR spectroscopic investigation on ofloxacin in both acidic and alkaline solutions was carried out *via* ^{1}H, ^{13}C NMR, DEPT, COSY, HSQC spectra together with HMBC techniques. Complete assignment on ^{1}H and ^{13}C NMR of ofloxacin was obtained in different pH environments where the coupling constant between ^{13}C and ^{19}F was found to be very helpful for the assignment of aromatic ^{13}C NMR signals. Additionally, the chemical shifts of ^{1}H from the complex spin systems such as AA'BB' were obtained using HSQC technique. Comparisons were made among the NMR spectra in acidic solution and those in alkaline solution, which demonstrate that: (1) deprivation of H^+ from COOH in alkaline solution destroys the hydrogen bond between COOH and carbonyl group in ofloxacin. This brings about the redistribution of π elelctrons around the carboxyl and carbonyl groups so that significant variations of ^{13}C NMR chemical shift and coupling constant J_{FC} are observed. (2) In the alkaline solution, the removal of proton from N4 in piperazine ring induces considerable variation of chemical shift of methylene groups and causes remarkable changes of dynamic behavior of the piperazine ring.

Key words Quinolone Ofloxacin NMR Piperazine ring

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