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两个有抗惊活性的取代吡唑烷酮分子结构

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摘要 用X射线衍射方法测得两个有抗惊活性的3-吡唑烷酮化合物(1:1-丁基-5-对氟苯基-3-吡唑烷酮, 2:1-丙基-5-对甲基苯基-3-吡唑烷酮)的分子结构, 并用CNDO/2方法计算了它们的原子净电荷。结果表明R^1取代基的推电子能力影响3-吡唑烷酮主体分子骨架五元环中共轭酰胺体系的C-N和C-O键长以及电子云分布。增大R^1的推电子能力有利于抗惊活性的增加。而R^5取代基主要影响分子的疏水性及分子形状。

关键词 分子结构 X射线衍射分析 吡唑酮 P 微分重叠全忽略近似 取代基效应 抗惊活性

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Molecular structures of two 3-pyrazolidone compounds with potent anticonvulsant activity

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Abstract The crystal and molecular structures of two potent anticonvulsant compounds: 1-(n-butyl)-5-(p-fluorophenyl)-3-pyrazolidone (1) and 1-(n-propyl)-5-(p-methylphenyl)-3-pyrazolidone (2) were determined by X-ray diffraction method. The atomic net charges were calculated by CNDO/2 method. It is shown that the bond lengths of C-N and C-O of the conjugated amido groups and the atomic net charges in the five membered rings of 3-pyrazolidones are affected by the electronreleasing capabilities of R^1 groups. It is considered that a substituent being more electron-releasing at position 1 of the five membered ring of 3-pyrazolidone is favorable on enhancement of the anticonvulsant activity, and the substituent at position 5 might mainly affect the molecular steric shape and the hydrophobic property.

Key words MOLECULAR STRUCTURE X-RAY DIFFRACTION ANALYSIS PYRAZOLONE P CNDO APPROXIMATION SUBSTITUENT EFFECT

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