2- 芳基 -4- 苯基 -2, 3- 二氢 -1, 5- 苯并二氮杂卓与重氮乙酸乙酯反应机 理和 立体化学的研究 王洪钟,淳炯,金声

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摘要 2-芳基-4-苯基-2,3-二氢-1,5-苯并二氮杂卓与重氮乙酸乙酯在铜粉催化下反应, 得到环加成产物吖丙啶并苯并二氮杂卓I外,

还得到一个非预期的五员环产物吡咯并苯并二氮杂卓II。改变反应条件可以使化合物II的收率达到50%。通过研究反应过程中分离出的副产物反丁烯酸二乙酯III和4,5-二氢吡唑-3,4,5-三羧酸乙酯IV,初步提出了反应经过乙氧羰基甲基化苯并二氮杂卓翁中间体V再发生环加成反应的机制。通过X-射线单晶衍射分析和NMR分析研究了它们的立体化学,发现为立体专一性反应。

关键词 <u>苯并二氮杂卓</u> <u>乙酸乙酯P</u> <u>重氮化合物</u> <u>铜</u> <u>X射线衍射分析</u> <u>核磁共振谱法</u> <u>立体化学</u> 分类号 0621

Studies on the mechanism and stereochemistry of the reaction of 2- phenyl-4- aryl-2,3-dihydro-1, 5-benzodiazepine with ethyl diazoacetate

Wang Hongzhong, Chun Jiong, Jin Sheng

Abstract The reaction of 2-phenyl -4- aryl -2,3 -dihydro- 1,5- benzodiazepine with ethyl diazoacetate using power Cu as a catlyst gives a normal cycloaddition product, azirino-benzodiazepine (I), and an unprecedent product pyrro - benzodiazepine (II). The yield of (II) was increased to 50% under the optimum condition. From the reaction mechanism, which involved formation of benzodiazepinium ethoxycarbonylmethylate (V), the reaction mechanism, which involved formation of benzodiazepinium ethoxycarbonyl- methylate (V) followed by cycloaddition reaction, was tentatively proposed. The reaction was proved to be stereospecific based on the analysis of X - ray and NMR spectra.

Key wordsDIAZEPAMETHYL ACETATE PDIAZO COMPOUNDSCOPPERX-RAY DIFFRACTIONANALYSISNMR SPECTROMETRYSTEREOCHEMISTRY

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