

1, 3-双磷(膦)酰基丙烯类化合物的¹H、³¹P NMR研究

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摘要 本文报道了标题类化合物中十个化合物的¹H和³¹P NMR的研究结果。其中分别运用了2DJ分解谱以及异核COSY谱等多种技术,解析了它们的¹H和³¹P图谱,

从而证实了合成反应的区域选择性和立体选择性。文章中,讨论了手性中心或其它因素而表现出的不等性;

讨论了影响 δ_{P} 和 $J_{\text{P-H}}$ 数值的各种因素;还报道了比较少见的³¹P-³¹P之间的远程偶合。其中,

顺式产物的 $J_{\text{P-P}}$ 数值(约9Hz)大于反式产物的 $J_{\text{P-P}}$ (约7Hz)。

关键词 [烯类化合物](#) [丙烯](#) [磷酰基](#) [核磁共振](#) [谱图](#) [COSY谱](#) [区域选择性](#) [偶合反应](#) [顺式](#) [反式](#)

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¹H and ³¹P NMR studies of 1, 3-diphosphorylpropenes

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Abstract The ¹H and ³¹P NMR spectra of 1, 3-diphosphorylpropenes prepared by a new reaction were studied. Homo 2DJ and hetero 2D COSY have been employed in distinguishing J(HH) and J(PH), and the signals of the isomeric mixtures. ³J(HH) of vinyl groups confirmed the regioselectivity, showing the trans form to be the main products (~95%). In compounds except 1, 2 and 7, different positions of double bond give rise to the existence of two isomers, A and B, with the latter ~10% in excess. In 1 and 2, four identical R groups were divided in to two groups because of the presence of a double bond, and the same groups attached to the different achiral P atom are non-equivalent as well. These are confirmed by the spectra of hydrogenation products. However, δ_{P} of the two P atoms show different behavior with -P(O)Ph(OR) at the lowest field. $J_{\text{P-P}}$ among these compounds were obtained, $J_{\text{cis}}(9\text{Hz}) > J_{\text{trans}}(7\text{Hz})$. The reduced values from those of hydrogenation products confirm the enhancement of P-P coupling by π electrons.

Key words [PROPENE](#) [PHOSPHORYL](#) [NUCLEAR MAGNETIC RESONANCE](#) [REGIOSELECTIVITY](#) [COUPLING REACTION](#) [CIS-FORM](#) [TRANSFORM](#)

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