

磷酸化组氨酸形成六配位磷中间体的理论研究

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摘要

用MNDO方法对磷酸化组氨酸磷上酯交换反应侧链咪唑基所参与的六配位磷机理进行了研究。六配位磷中间体形成后,使咪唑基对面的异丙氧基反应活性提高。当磷上酯交换反应发生时,异丙氧基离去和另一分子醇进攻磷,从咪唑基的对面发生,在能量上和空间上都是有利的。六配位磷机理较好地解释了咪唑的催化作用。

关键词 [组氨酸](#) [磷酸化](#) [磷络合物](#) [MNDO](#) [咪唑](#) [催化反应](#) [酯交换](#)

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A theoretical study on the hexa-coordinate phosphorus intermediate of N-phosphorylhistidine

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Abstract The ester exchange reaction on phosphorus of N-phosphorylhistidine with primary alcohol has been studied by MNDO method. Due to the participation of imidazole group, a hexa-coordinate phosphorus intermediate was formed, in which the isopropoxyl group opposite to the imidazole was more labile than the others and much easier to leave because the activation energy was lowered by $64\text{kJ}\cdot\text{mol}^{-1}$. When this iso-propoxyl left, to a new form penta-coordinate phosphorus intermediate which then was to be attacked by an alcohol from the direction opposite to the imidazole group. The mechanism of hexa-coordinate phosphorus intermediate explains the catalytic effect of imidazole.

Key words [HISTIDINE](#) [PHOSPHORYLATION](#) [PHOSPHORUS COMPLEX](#) [IMIDAZOLE](#) [CATALYTIC REACTION](#) [TRANSESTERIFICATION](#)

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