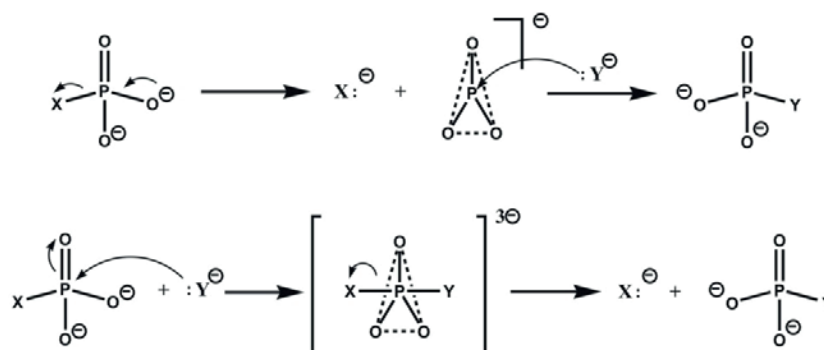


Mechanism of enzymatic phosphate ester hydrolysis: interplay of theory and experiment

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Enzymatic phosphate ester hydrolysis plays a crucial role in life processes. An especially important class is phosphoryl transfer, which belongs to the most important molecular reactions in living systems. Three different types of reaction paths can be considered both for the enzymatic and non-enzymatic processes (see Figure). Dissociative (top), associative (bottom, the structure in square brackets represents an



energetically locally stable intermediate), and concerted S_N2-type (bottom, the structure in square brackets represents a transition state). Experimental evidence supports the concerted mechanism for the non-enzymatic hydrolysis of phosphate monoesters, while sophisticated calculations on adequate enzyme models and some X-ray diffraction studies call for the possibility of both associative and dissociative mechanisms. I will present some examples for both mechanisms and stress the importance of the effect of protein environment, especially metal ions located in the active site.