

## Structure of a 1,3-diphosphaallyllithium

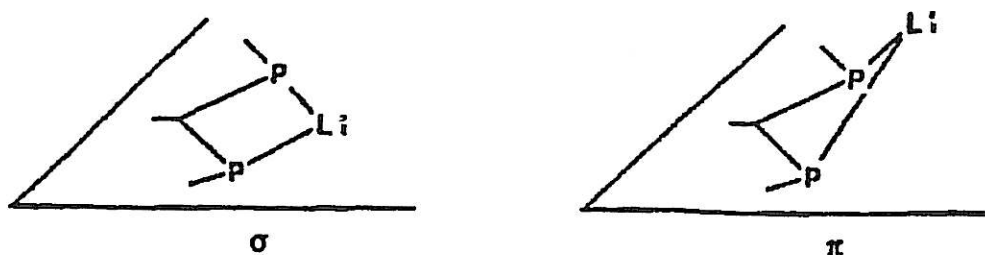
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For allyllithium compounds, the theoretical calculations, performed by R.v. Schleyer, indicate two possible structures : a  $\sigma$  structure with a more covalent character and a  $\pi$  structure with a more ionic character. According to these two calculated allyllithium structures, the  $\pi$ -allyl system appears more stable than the  $\sigma$  allyl system. Similar results have been obtained by Bachrach for the calculated 1,3-diphosphaallyllithium structures. Moreover, this author considers the  $\pi$ -diphosphaallyllithium as an intermediate in the 1,3-diphosphaallene formation.



We have recently determined the X-ray structure of 1,3-diphosphaallyllithium ( $\text{ArP}=\text{C}(\text{Me})\text{-PAr}^{\ominus}(\text{Li} \cdot 2 \text{Et}_2\text{O})^{\oplus}$ ). The position of Li atom in the PCP plane ( $d_{\text{PLi}}=2.80 \text{ \AA}$ ) involves a  $\sigma$  structure. Taking into account the rotation barrier around P-C bonds, we will discuss the mechanism of 1,3-diphosphaallene formation.

