

# Crystal and Molecular Structure of $\text{P}(\text{C}_6\text{H}_5)_5 \cdot 0.5 \text{ THF}$

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*Dedicated to Professor Hubert Schmidbaur on the occasion of his 70<sup>th</sup> birthday*

Pentaphenylphosphorus crystallizes from tetrahydrofuran (THF) as  $\text{P}(\text{C}_6\text{H}_5)_5 \cdot 0.5 \text{ THF}$  (triclinic space group:  $P\bar{1}$ ,  $a = 10.095(4)$ ,  $b = 10.252(3)$ ,  $c = 12.725(3)$  Å,  $\alpha = 71.21(1)$ ,  $\beta = 76.98(3)$ ,  $\gamma = 87.12(1)^\circ$ ,  $Z = 2$ ). Its molecular structure is an almost perfect trigonal bipyramid with significantly longer axial than equatorial P-C<sub>Ph</sub> bonds (P-C<sub>ax</sub> 1.982(2)/1.979(2), P-C<sub>eq</sub> 1.853(2)/1.845(2)/1.847(2) Å). It differs from the well established structure of solvent-free  $\text{P}(\text{C}_6\text{H}_5)_5$  (P. J. Wheatley, J. Chem. Soc. 2206 (1964)) in the relative orientation of the phenyl rings with respect to each other (axial rings) and with respect to the equatorial PC<sub>3</sub> plane (equatorial rings) but not in the trigonal-bipyramidal (tbp) geometry at phosphorus. Differences in the geometry around the central atom had been found previously for  $\text{Sb}(\text{C}_6\text{H}_5)_5$  (square pyramid) and  $\text{Sb}(\text{C}_6\text{H}_5)_5 \cdot 0.5 \text{C}_6\text{H}_{12}$  (tbp) but not in  $\text{As}(\text{C}_6\text{H}_5)_5$  and  $\text{As}(\text{C}_6\text{H}_5)_5 \cdot 0.5 \text{C}_6\text{H}_{12}$  (both tbp).

**Key words:** Phosphorus, Structural Chemistry, Pentacoordination, Structure Determination