The Crystal and Molecular Structure of *NN*-Dimethyldiphenylphosphinamide, Ph_2PONMe_2

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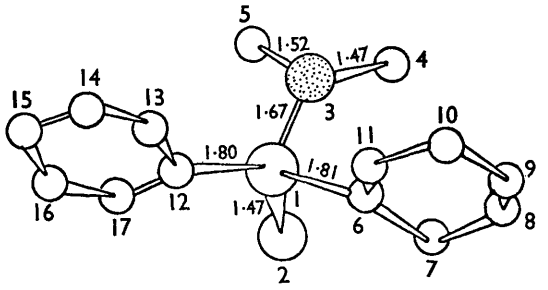
STRUCTURAL studies of organic phosphorus compounds are of importance in understanding bonding and reactions at phosphorus, as in the biochemistry of organic phosphorus compounds and mechanisms of their reactions.[1] Thus, we have determined the structure of *NN*-dimethyldiphenylphosphinamide. Crystals were furnished by Dr. Paul Haake, University of California.

The crystals are orthorhombic with lattice dimensions, $a = 7{\cdot}670$, $b = 11{\cdot}141$, $c = 15{\cdot}644$ Å. The space group is $P2_12_12_1$ and there are four molecules per unit cell. Intensity data was collected on a General Electric XRD-5 diffractometer with a single-crystal orienter using a scintillation counter for detector. Zirconium-filtered Mo-radiation was used. Intensities were

measured with a theta-two theta scan, counting background on both sides of the peak. The intensities of 863 independent reflections were above background.



FIGURE

The structure was solved from the Patterson and one Fourier analysis; refinement using Busing, Martin, and Levy's least squares programme has brought the final R to 6·4% refining positional and individual anisotropic temperature factors. The structure with pertinent bond distances is seen in the Figure. The phosphorus bond angles are close to tetrahedral ranging between 104·3 and 117·6° and the nitrogen, phosphorus, and two methyl carbons are nonplanar.

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[1] R. F. Hudson, "Structure and Mechanism in Organo-phosphorus Chemistry", Academic Press, 1965.