The Structure of 2,2,4,4-Tetrafluoro-1,3-dimethyl-2,4-diphenyl-1,3-diaza-2,4-diphosphacyclobutane, $(MeNPF_2Ph)_2$

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THE active interest in five-co-ordination[1] and the recent publication by two groups[2,3] of the structure of 2,2,2,4,4,4-hexachloro-1,3-dimethyl-1,3-diaza-2,4-diphosphacyclobutane, (*N*-methyltrichlorophosphinimine dimer) have prompted us to report structural studies on a closely related molecule.

Crystals of 2,2,4,4-tetrafluoro-1,3-dimethyl-2,4-diphenyl-1,3-diaza-2,4-diphosphacyclobutane, $(MeNPF_2Ph)_2$, were furnished by Dr. Reinhard Schmutzler.[4] The compound crystallizes in the orthorhombic crystal system with $a = 11{\cdot}11$, $b = 7{\cdot}64$, and $c = 18{\cdot}36$ Å. Systematic absences

TABLE

Bond distances and interatomic angles in $(MeNPF_2Ph)_2$.

Bond	Distance (Å)*	Atoms	Angle
P–N	1·64	N–P–N′	80·6°
P–N′	1·78	C(1)–P–N′	97·9
P–F(1)	1·57	F(1)–P–N′	91·7
P–F(2)	1·62	F(2)–P–N	92·5
P–C(1)	1·79	F(2)–P–C(1)	91·8
		F(2)–P–F(1)	87·0
N–C(7)	1·44		
		N–P–F(1)	128
C(1)–C(2)	1·42	N–P–C(1)	122
C(2)–C(3)	1·39	F(1)–P–C(1)	109
C(3)–C(4)	1·39		
C(4)–C(5)	1·40	P–N–P′	99·4
C(5)–C(6)	1·40	P–N–C(7)	134
C(6)–C(1)	1·39	P′–N–C(7)	125
		C(6)–C(1)–C(2)	119
		C(1)–C(2)–C(3)	120
		C(2)–C(3)–C(4)	118
		C(3)–C(4)–C(5)	123
		C(4)–C(5)–C(6)	119
		C(5)–C(6)–C(1)	119

* Estimated standard deviations of all bond distances involving P atoms are less than 0·02 Å.

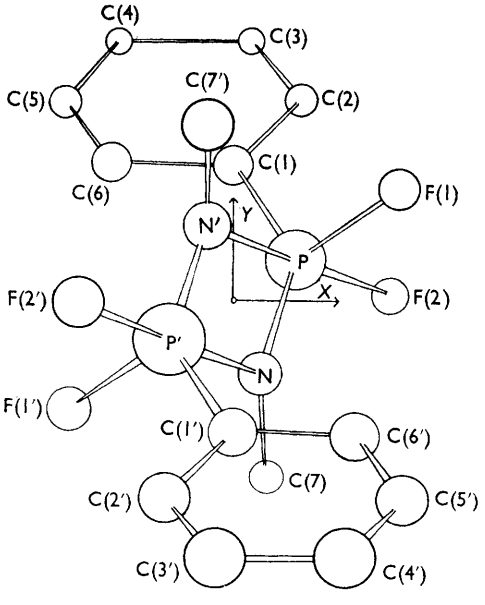

FIGURE. *The molecular configuration of* $(MeNPF_2Ph)_2$.

indicate the unique space group *Pbca*. The molecules possess a crystallographic centre of symmetry since the unit cell contains 4 molecules of $(MeNPF_2Ph)_2$ while the space group has eight-fold general positions. The structure, based on 676 visually estimated diffraction maxima, has been refined to an unweighted discrepancy index $R_1 = 10{\cdot}9\%$

The principle features of the molecule are shown in the Figure. The Table lists bond distances and interatomic bond angles. The $(NP)_2$ ring system is planar; the co-ordination environment of each phosphorus atom is approximately trigonal bipyramidal. The phosphorus trigonal plane contains one nitrogen, one fluorine, and a carbon of the phenyl ring. The two axial positions are occupied by a fluorine and the second nitrogen of the $(NP)_2$ ring. As expected the different N–P and P–F bonds exhibit longer bond-distances in axial positions of the trigonal bipyramid than in equatorial positions.

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