Molecular Structures of Non-geminally Substituted Phosphazenes. Part VI.[1] Crystal Structure of 2,*cis*-4,*trans*-6,*trans*-8-Tetrachloro-2,4,6,8-tetraphenylcyclotetraphosphazatetraene

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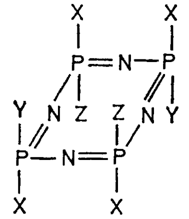
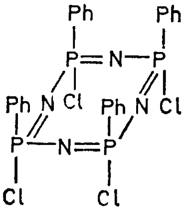
Crystals of the title compound (Ia) are triclinic, $a = 11{\cdot}47$, $b = 9{\cdot}31$, $c = 8{\cdot}14$ (all $\pm0{\cdot}02$) Å, $\alpha = 114{\cdot}2$, $\beta = 115{\cdot}2$, $\gamma = 89{\cdot}3°$ (all $\pm0{\cdot}3°$), space group $P\bar{1}$, $Z = 1$. The structure was solved by Patterson and superposition methods from visually estimated photographic *X*-ray intensity data and refined by full-matrix least-squares to *R* 0·081 for 1890 reflexions. The molecule occupies a crystallographic centre of symmetry and the eight-membered phosphazene ring has a chair conformation with P–N–P angles of 132·9 and 137·9°. Mean bond lengths (P–N 1·572, P–Cl 2·044, P–C 1·796, and C–C 1·38 Å) are similar to those in the 2,*cis*-4,*cis*-6,*cis*-8-isomer. The phosphazene ring shape is very similar to that in three other chlorotetraphosphazenes but is less puckered than that in its derivative $N_4P_4(NHMe)_4Ph_4$.

ONE of the aims of this series of papers is to study differences in configuration and conformation of the phosphazene ring in isomeric or otherwise closely related compounds. 2,*cis*-4,*trans*-6,*trans*-8-Tetrachloro-2,4,6,8-tetraphenylcyclotetraphosphazatetraene [β-*trans*-$N_4P_4Cl_4Ph_4$,† (Ia)], one of the first non-geminally substituted tetrameric phosphazenes to be prepared,[2] is isomeric with *cis*-$N_4P_4Cl_4Ph_4$,† (II), and is the precursor of β-*trans*-$N_4P_4(NHMe)_4Ph_4$ (Ib) whose molecular structures were described in Parts II [3] and I.[4] Although our full description of the crystal structure of (Ia) is only now being presented, an approximate determination of the structure had been achieved prior to the crystallographic work on these other phosphazenes and a summary of the results was published.[5] The β-*trans*-configuration was first assigned to this isomer of $N_4P_4Cl_4Ph_4$ [reported m.p.: 248 °C (ref. 2); 260—263 °C (ref. 6)] by Grushkin *et al.*[6] by use of proton n.m.r. and dielectric constant measurements.



(I) a; X = Cl, Y = Z = Ph
b; X = NHMe, Y = Z = Ph
c; X = Y = Cl, Z = NMe_2
d; X = Y = NMe_2, Z = Cl



(II)

EXPERIMENTAL

Crystal Data.—$C_{24}H_{20}Cl_4N_4P_4$, $M = 629{\cdot}7$, Triclinic, $a = 11{\cdot}47$, $b = 9{\cdot}31$, $c = 8{\cdot}14$ Å (all $\pm0{\cdot}02$ Å), $\alpha = 114{\cdot}2$, $\beta = 115{\cdot}2$, $\gamma = 89{\cdot}3°$ (all $\pm0{\cdot}3°$), $U = 703$ Å^3, $D_m = 1{\cdot}50$ (by flotation), $Z = 1$, $D_c = 1{\cdot}49$, $F(000) = 320$. Cu-K_α radiation, $\lambda = 1{\cdot}5418$ Å; μ(Cu-K_α) $= 61{\cdot}2$ cm^{-1}. Space group $P\bar{1}$ (No. 2).

The crystals, which were grown from a solution in benzene, are tabular with {100} best developed. The unit cell defined above was used in preference to the Delaunay-reduced cell ($a = 10{\cdot}88$, $b = 9{\cdot}53$, $c = 8{\cdot}14$ Å, $\alpha = 117{\cdot}0$, $\beta = 107{\cdot}4$, $\gamma = 91{\cdot}8°$) primarily to avoid the larger α value of the latter. Lattice parameters were determined by methods based on the $\alpha_1 - \alpha_2$ spot separation.[7,8]

X-Ray intensities were measured from equi-inclination Weissenberg photographs of the layers *hk*0—3 and 0—5*kl* recorded with Cu-K_α radiation. Out of a possible 2256 reflexions, 1890 with intensities equal to or above the minimum observable were obtained from a crystal of dimensions *ca.* 0·20 × 0·18 × 0·17 mm. The intensities were corrected for Lorentz and polarisation effects but not for absorption.

Least-squares refinement was carried out initially at the Atlas Computer Laboratory, Chilton, using the '*X*-ray '63' program package and subsequently on the University of Essex PDP 10 computer with a program written by Dr. G. M. Sheldrick. Atomic scattering factors were calculated by the analytic function $f = C + \sum_{i=1}^{4} A_i \exp(-B_i \sin^2\theta/\lambda^2)$, the parameters *A*, *B*, and *C* being taken from ref. 9 for chlorine, phosphorus, nitrogen, and carbon, and from ref. 10 for hydrogen.

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† β-*trans* = 2,*cis*-4,*trans*-6,*trans*-8-, and *cis* = 2,*cis*-4,*cis*-6,*cis*-8-.

[1] Part V, G. J. Bullen and P. E. Dann, *J.C.S. Dalton*, 1974, 705.

[2] R. A. Shaw and C. Stratton, *Chem. and Ind.*, 1959, 52; *J. Chem. Soc.*, 1962, 5004.

[3] Part II, G. J. Bullen and P. A. Tucker, *J.C.S. Dalton*, 1972, 1651.

[4] Part I, G. J. Bullen and P. R. Mallinson, *J.C.S. Dalton*, 1972, 1412.

[5] G. J. Bullen, P. R. Mallinson, and A. H. Burr, *Chem. Comm.*, 1969, 691.

[6] B. Grushkin, A. J. Berlin, J. L. McClanahan, and R. G. Rice, *Inorg. Chem.*, 1966, **5**, 172.

[7] P. Main and M. M. Woolfson, *Acta Cryst.*, 1963, **16**, 731.

[8] N. W. Alcock and G. M. Sheldrick, *Acta Cryst.*, 1967, **23**, 35.

[9] D. T. Cromer and J. T. Waber, *Acta Cryst.*, 1965, **18**, 104.

[10] J. B. Forsyth and M. Wells, *Acta Cryst.*, 1959, **12**, 412

Structure Determination.—A centrosymmetric structure (and hence space group $P\bar{1}$) is indicated by (i) the result of a zero moment $[N(z)]$ test[11] on the full set of 2256 intensities, and (ii) the number of large peaks in the sharpened Patterson function. The unit cell contains four chlorine and four phosphorus atoms. There are 24 intense peaks and 8 moderate peaks in the Patterson function (excluding the origin peak). A centrosymmetric arrangement of the eight heavy atoms would produce 24 double- and 8 single-weight vectors, whereas a non-centrosymmetric arrangement would produce 56 vectors of similar (single) weight. An image of the structure was recovered from the Patterson function by use of Buerger's minimum function superposition technique.[12] The nitrogen atoms and 5 of the 12 carbon atoms in the asymmetric unit were identified from this image, and the positions of the remaining carbon atoms were obtained from a Fourier synthesis. Atomic positions were refined by Fourier and full-matrix least-squares techniques, anisotropic temperature factors being introduced when R was 0·19. Hydrogen atoms were placed at calculated positions, assuming C–H 1·05 Å, and they were assigned isotropic temperature factors $(\overline{u^2})$ of 0·10 Å^2. Their parameters were not refined. The weighting scheme used was $w = (A/|F_o|)^2$ if $|F_o| > A$ but otherwise $w = 1$, the value of A being adjusted (final value 9 on an absolute scale) until the average $w\Delta^2$ for groups of reflexions ($\Delta = |F_o| - |F_c|$) was almost constant over the whole range of $|F_o|$ and $\sin\theta/\lambda$. The final R is 0·081 for 1890 reflexions and R' $[= \Sigma w^{\frac{1}{2}}\Delta/\Sigma w^{\frac{1}{2}}|F_o|]$ is 0·090. In the last cycle of refinement all parameter shifts were $<0{\cdot}1\sigma$.

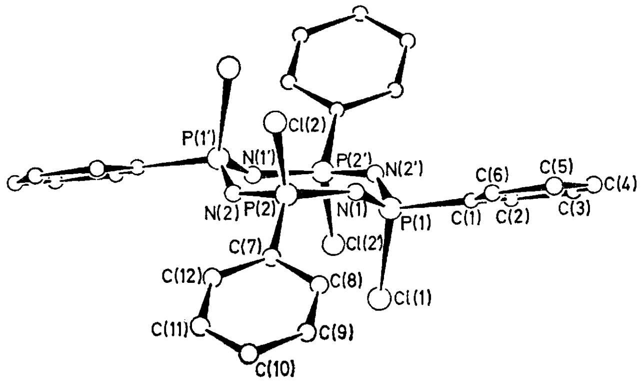

FIGURE 1 Molecular shape of β-*trans*-$N_4P_4Cl_4Ph_4$, (Ia), and numbering of the atoms. A primed atom is related to the corresponding unprimed atom by inversion through the molecular centre, at $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

RESULTS AND DISCUSSION

The shape of the molecule and the numbering of the atoms are shown in Figure 1. Final atomic co-ordinates and thermal parameters are given in Tables 1—3. Observed and calculated structure factors are listed in Supplementary Publication No. SUP 21005 (11 pp., 1 microfiche).* Bond lengths are given in Table 4 and bond angles in Table 5.

TABLE 1

Fractional atomic co-ordinates (× 10^4), with estimated standard deviations in parentheses

	x/a	y/b	z/c
Cl(1)	3697(2)	4642(2)	7410(3)
Cl(2)	3327(2)	2256(2)	−383(3)
P(1)	3395(1)	5479(2)	5329(3)
P(2)	3905(1)	2727(2)	2563(3)
N(1)	3086(4)	4013(6)	3254(10)
N(2)	5444(4)	3085(6)	3703(8)
C(1)	1922(5)	6268(7)	5014(10)
C(2)	1996(5)	7771(7)	6452(12)
C(3)	862(6)	8398(9)	6199(13)
C(4)	−310(6)	7529(9)	4524(13)
C(5)	−377(6)	6053(9)	3114(13)
C(6)	732(5)	5412(8)	3335(12)
C(7)	3341(6)	828(7)	2326(10)
C(8)	2093(7)	467(9)	2130(15)
C(9)	1683(10)	−1004(11)	1918(19)
C(10)	2464(11)	−2131(11)	1908(14)
C(11)	3693(10)	−1796(9)	2082(15)
C(12)	4131(7)	−300(8)	2314(13)

TABLE 2

Fractional co-ordinates (× 10^3) assigned to hydrogen atoms. Each atom is numbered according to the carbon atom to which it is attached

	x/a	y/b	z/c		x/a	y/b	z/c
H(2)	290	843	772	H(8)	147	130	214
H(3)	89	953	728	H(9)	74	−127	176
H(4)	−117	800	432	H(10)	213	−324	178
H(5)	−129	541	186	H(11)	429	−266	204
H(6)	67	428	223	H(12)	507	−2	248

TABLE 3

Components U_{ij} of thermal vibration tensors (Å^2, × 10^3), with estimated standard deviations in parentheses

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl(1)	43·1(8)	83·7(12)	102·7(15)	58·7(11)	32·4(10)	17·2(7)
Cl(2)	56·1(9)	66·3(10)	66·1(10)	25·5(8)	19·6(9)	0·7(7)
P(1)	23·1(6)	41·6(7)	71·2(11)	21·7(7)	20·1(7)	8·5(5)
P(2)	25·2(6)	38·2(7)	61·3(10)	14·5(6)	18·0(7)	4·0(5)
N(1)	31(2)	53(3)	87(4)	7(3)	22(3)	12(2)
N(2)	31(2)	51(2)	73(3)	23(2)	27(3)	7(2)
C(1)	29(2)	49(3)	73(4)	27(3)	21(3)	10(2)
C(2)	34(3)	54(3)	81(5)	15(3)	19(3)	12(2)
C(3)	42(3)	75(4)	89(5)	19(4)	30(4)	21(3)
C(4)	33(3)	80(4)	91(5)	29(4)	30(4)	24(3)
C(5)	29(3)	73(4)	97(6)	20(4)	18(4)	6(3)
C(6)	33(3)	55(3)	86(5)	14(3)	20(3)	8(2)
C(7)	41(3)	46(3)	64(4)	14(3)	23(3)	−2(2)
C(8)	60(4)	61(4)	122(7)	21(4)	58(5)	−2(3)
C(9)	96(6)	75(5)	157(10)	32(6)	82(7)	−9(5)
C(10)	117(8)	70(5)	87(6)	27(4)	48(6)	−18(5)
C(11)	97(6)	59(4)	106(7)	41(4)	36(6)	11(4)
C(12)	66(4)	49(3)	92(5)	27(3)	30(4)	11(3)

TABLE 4

Bond lengths (Å), with estimated standard deviations in parentheses

P(1)–N(1)	1·566(6)	C(1)–C(2)	1·382(9)
P(2)–N(1)	1·583(5)	C(2)–C(3)	1·390(8)
P(2)–N(2)	1·568(4)	C(3)–C(4)	1·372(9)
P(1')–N(2)	1·571(5)	C(4)–C(5)	1·359(10)
Mean	1·572(3)	C(5)–C(6)	1·373(8)
		C(6)–C(1)	1·383(8)
P(1)–Cl(1)	2·044(3)	C(7)–C(8)	1·402(9)
P(2)–Cl(2)	2·043(3)	C(8)–C(9)	1·372(12)
Mean	2·044(3) *	C(9)–C(10)	1·372(14)
		C(10)–C(11)	1·381(14)
P(1)–C(1)	1·795(5)	C(11)–C(12)	1·397(11)
P(2)–C(7)	1·796(6)	C(12)–C(7)	1·379(9)
Mean	1·796(4)	Mean	1·380(12) †

* Standard deviation increased to allow for error in unit-cell parameters. † Standard deviation calculated from deviations of individual values from the mean.

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* See Notice to Authors No. 7 in *J.C.S. Dalton*, 1973, Index issue.

[11] E. R. Howells, D. C. Phillips, and D. Rogers, *Acta Cryst.*, 1950, **3**, 210.

[12] M. J. Buerger, *Acta Cryst.*, 1950, **3**, 87; 1951, **4**, 531.

TABLE 5

Bond angles (°), with estimated standard deviations in parentheses

N(1)–P(1)–N(2′)	119·6(3)	P(1)–C(1)–C(2)	119·0(4)
N(1)–P(2)–N(2)	121·7(3)	P(1)–C(1)–C(6)	120·8(5)
		P(2)–C(7)–C(8)	120·6(5)
P(1)–N(1)–P(2)	132·9(3)	P(2)–C(7)–C(12)	120·2(5)
P(1′)–N(2)–P(2)	137·9(3)		
		C(1)–C(2)–C(3)	119·2(5)
Cl(1)–P(1)–C(1)	104·4(3)	C(2)–C(3)–C(4)	119·8(6)
Cl(2)–P(2)–C(7)	102·6(2)	C(3)–C(4)–C(5)	120·8(5)
		C(4)–C(5)–C(6)	120·4(6)
Cl(1)–P(1)–N(1)	108·3(3)	C(5)–C(6)–C(1)	119·7(6)
Cl(1)–P(1)–N(2′)	108·3(3)	C(6)–C(1)–C(2)	120·2(5)
Cl(2)–P(2)–N(1)	103·9(3)	C(7)–C(8)–C(9)	119·2(8)
Cl(2)–P(2)–N(2)	108·1(2)	C(8)–C(9)–C(10)	121·9(9)
		C(9)–C(10)–C(11)	119·5(8)
N(1)–P(1)–C(1)	107·2(3)	C(10)–C(11)–C(12)	119·4(8)
N(2′)–P(1)–C(1)	108·0(3)	C(11)–C(12)–C(7)	120·7(8)
N(1)–P(2)–C(7)	111·2(3)	C(12)–C(7)–C(8)	119·2(6)
N(2)–P(2)–C(7)	107·6(3)		

The phosphazene ring in (Ia) has a chair conformation with strict crystallographic symmetry C_i ($\bar{1}$) like that in (Ib)[4] (Figure 2) but in contrast to the ring in (II) which has an irregular crown conformation.[3] Bond lengths and bond angles are compared with those of the *cis*-isomer in Table 6. The agreement of the P–N and P–Cl bond lengths is very good but the P–C bonds are 0·01—0·02 Å shorter in the *cis*-isomer. This discrepancy is however on the borderline of significance. The P–N–P angles show a greater spread in the *cis*-isomer.

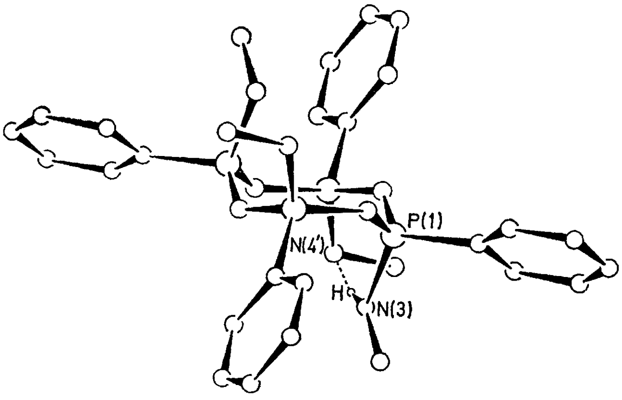

FIGURE 2 Molecular shape of β-*trans*-$N_4P_4(NHMe)_4Ph_4$, (Ib)

TABLE 8

Torsion angles (°) ($\tau_1 - \tau_4$, see Figure 3) and P–N–P angles in eight-membered phosphazene rings with approximate symmetry C_{2h}

	(Ib)[a]	(Ia)[b]	(Id)[c]	(Ic)[d]	*T*-$N_4P_4Cl_8$[e]	$N_4P_4F_4(NMe_2)_4$[f]
τ_1	95	75	76	77	76	66
τ_2	−53	−41	−44	−41	−45	−50[g]
τ_3	−21	−24	−19	−26	−20	−5[g]
τ_4	73	62	61	65	59	40
P–N–P	125,131	133,138	135,136	131,138	134,138	138,141

[a] Ref. 4. [b] This work. [c] Ref. 1. [d] Ref. 14. [e] Ref. 15. [f] By calculation from the atomic positions given in ref. 13. The torsion angles quoted in ref. 13 are incorrect. [g] For this compound the very large difference between τ_2 and τ_3 represents a considerable departure from C_{2h} symmetry.

In addition to being rigorously centrosymmetric, the phosphazene ring in (Ia) has the approximate symmetry $C_{2h}(2/m)$, six of the eight atoms in the ring being almost coplanar [see Table 7, plane (i)] while the other two atoms, P(1) and P(1′), lie 0·58 Å from the mean plane of these six. The torsion (dihedral) angles in the ring are shown in Figure 3 and they are compared in Table 8 with the torsion angles[1,4,13-15] in the other tetrameric phosphazenes known to have rings with approximate C_{2h} symmetry. The pattern of torsion angles is very similar in the four chlorophosphazenes but different in (Ib)[4] and $N_4P_4F_4(NMe_2)_4$[13] whose rings are respectively more and less puckered than in the chloro-derivatives. In so far as the degree of puckering depends on the size of the P–N–P angles in the ring, this difference is to be expected since the degree of delocalisation of the lone pairs on the cyclic nitrogen atoms will decrease in the sequence fluoro- > chloro- > other derivatives, owing to the differing abilities of the exocyclic ligands to

TABLE 6

Comparison of bond lengths (Å) and bond angles (°) in the *cis*- and β-*trans*-isomers of $N_4P_4Cl_4Ph_4$

	cis	β-*trans*
P–N	1·556—1·579	1·566—1·583
P–C	1·776—1·788	1·795, 1·796
P–Cl	2·036—2·045	2·043, 2·044
N–P–N	119·3—122·3	119·6, 121·7
P–N–P	133·1—142·0	132·9, 137·9
Cl–P–C	102·0—103·5	102·6, 104·4

TABLE 7

Equations of mean planes through sets of atoms and distances (Å) of the atoms from the plane (in square brackets). Co-ordinates in Å are referred to orthogonal axes *a′*, *b′*, and *c*, where *b′* lies in the *bc* plane

Plane (i): N(1), P(2), N(2), N(1′), P(2′), N(2′)
$-0{\cdot}007X + 0{\cdot}312Y - 0{\cdot}950Z = 1{\cdot}235$
[P(2) 0·029, N(1) −0·022, N(2) −0·023]

Plane (ii): C(1)—(6)
$0{\cdot}180X + 0{\cdot}394Y - 0{\cdot}901Z = 1{\cdot}621$
[C(1) −0·003, C(2) 0·002, C(3) −0·002, C(4) 0·001, C(5) −0·002, C(6) 0·002, P(1) 0·031]

Plane (iii): C(7)—(12)
$0{\cdot}390X + 0{\cdot}302Y + 0{\cdot}870Z = 1{\cdot}284$
[C(7) −0·001, C(8) 0·000, C(9) −0·002, C(10) 0·006, C(11) −0·007, C(12) 0·005, P(2) −0·027]

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[13] D. Millington, T. J. King, and D. B. Sowerby, *J.C.S. Dalton*, 1973, 396.

[14] Part IV, G. J. Bullen and P. E. Dann, *J.C.S. Dalton*, 1973, 1453.

[15] A. J. Wagner and A. Vos, *Acta Cryst.*, 1968, **B24**, 707.

withdraw electrons. Nevertheless it is perhaps surprising that the ring in (Ib) should be so much more puckered or indeed that its cyclic P–N–P angles (125, 131°) should be smaller than those in $N_4P_4(NMe_2)_8$ (133°) where there are eight strongly electron-donating groups attached to the ring. A possible explanation lies in the close contact (3·27 Å) between atoms N(3) and N(4′) in (Ib) (Figure 2). Since the hydrogen atom attached to N(3) must lie in the region between these two nitrogen atoms (see Figure 2; the hydrogen atom co-ordinates were not determined exactly) it seems very probable that the distance 3·27 Å indicates an NH · · · N intramolecular hydrogen bond (shown by the broken line in Figure 2).* The greater puckering of the ring would then result from the drawing-together of these two exocyclic nitrogen atoms.

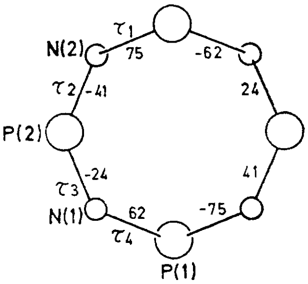
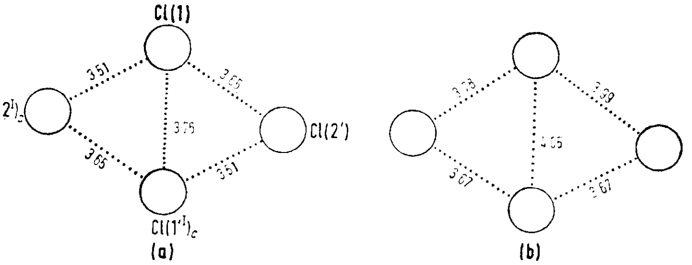


FIGURE 3 Torsion angles (°) in the phosphazene ring

The pattern of asymmetry in the torsion angles is also of interest. A ring with exact C_{2h} symmetry would have torsion angles $\tau_1 = \tau_4$ and $\tau_2 = \tau_3$. It is surprising to us that the form of the departure from this symmetry (the pattern of asymmetry) is so similar in the four chloro-derivatives. In the case of $N_4P_4Cl_8$ one would expect the isolated molecule to possess exact C_{2h} symmetry and it would be natural to attribute the observed asymmetry to crystal lattice forces. However it seems unlikely that crystal lattice forces would lead to such similar patterns of asymmetry in all four molecules. The observed asymmetry may indicate a tendency within the molecule for the axial chlorine atom to be closer to one exocyclic neighbour than to the other. For example, in $N_4P_4Cl_8$ the two Cl(ax) · · · Cl intramolecular non-bonded distances are 3·78 and 4·14 Å,[15] and in (Ia) the Cl(1) · · · Cl(2′) distance is 3·65 Å whereas the Cl(1) · · · C distances are 4·06 Å or more (one would expect van der Waals Cl · · · C and Cl · · · Cl distances to be similar). It is, however, difficult to decide which is cause and which is effect.



(a) (b)

FIGURE 5 Groups of non-bonded Cl · · · Cl contacts (with distances in Å) in (a) (Ia), and (b) (II). The four chlorine atoms are exactly coplanar in (a) but not quite in (b)

The phenyl groups in (Ia) are orientated so that their planes are almost perpendicular to the adjoining Cl–P–C plane, the Cl–P–C–C torsion angles being 79° at P(1) and 88° at P(2). A similar symmetrical orientation was found for three of the four phenyl groups in (II) and was attributed to equalisation of intramolecular chlorine–carbon repulsions at the two sides of the phenyl ring.[3] This symmetrical orientation does not usually occur in molecules which have two phenyl groups attached to the same phosphorus atom, such as gem-$N_3P_3Cl_2Ph_4$ [16] or gem-$N_4P_4Cl_4Ph_4$,[17] the planes of the phenyl groups being rotated (about the P–C bond) relative to each other.

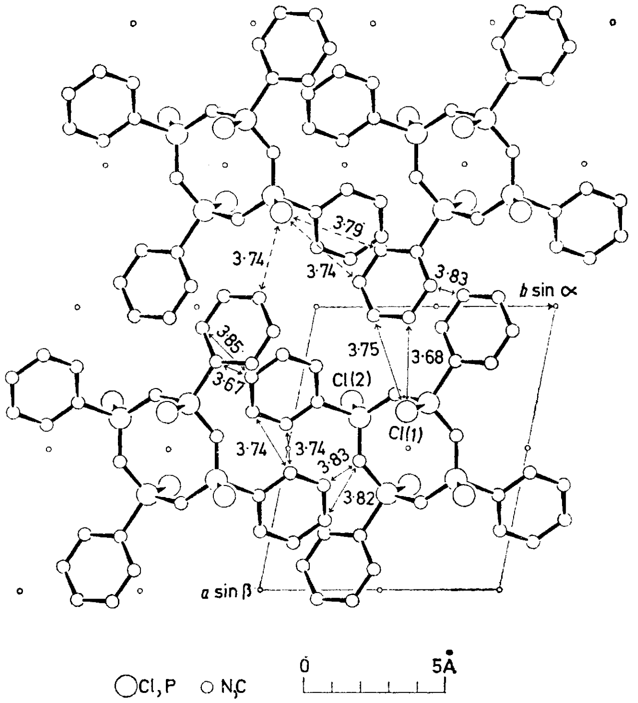


FIGURE 4 Projection of the structure down the c axis. Distances (Å) marked by full arrows are between molecules at the same z height and those marked by broken arrows are between molecules differing in height by one c lattice translation

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* This bond was not mentioned in ref. 4, where it was noted merely that there are no intermolecular hydrogen bonds in this structure.

[16] N. V. Mani, F. R. Ahmed, and W. H. Barnes, *Acta Cryst.*, 1966, **21**, 375.

[17] G. J. Bullen and P. E. Dann, unpublished results.

Intermolecular distances $\leqslant 3{\cdot}85$ Å are shown in Figure 4. The closest contacts of each type are Cl $\cdots$ CH 3·68, C $\cdots$ CH 3·67, and N $\cdots$ CH 3·82 Å. The closest intermolecular Cl $\cdots$ Cl contacts (not marked in Figure 4) are between molecules separated by one *c* lattice translation: Cl(1) $\cdots$ Cl(2^{I}) 3·51 and Cl(1) $\cdots$ Cl($1'^{\mathrm{I}}$) 3·76 Å (atoms with superscript I are at x, y, $1 + z$). There is also an intramolecular distance Cl(1) $\cdots$ Cl(2′) of 3·65 Å, so that Cl(1) makes non-bonded contact with three other chlorine atoms while Cl(2) makes contact with only two chlorine atoms, and a pair of molecules forms a group of five Cl $\cdots$ Cl contacts of similar length arranged as in Figure 5(a). It is of interest that a very similar spatial arrangement of five Cl $\cdots$ Cl non-bonded contacts occurs in the *cis*-isomer [Figure 5(b)], though in that case the contacts are all intramolecular. It would seem that in both structures the chlorine atoms in contact attempt to form a fragment of a hexagonal net. In the β-*trans*-isomer this influences the packing of the molecules while in the *cis*-isomer it influences their shape.

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