Table 2. *Hydrogen bonds in the title compound*

E.s.d.'s are given in parentheses and refer to the last decimal places.

X—H···Y	X···Y(Å)	XHY(°)
N(6)—H(6A)···N(1^{i})	2·903 (5)	163 (4)
N(6)—H(6B)···N(7^{ii})	3·080 (5)	175 (4)
N(1′)—H(1′)···N(3′^{iii})	2·831 (6)	158 (5)

Symmetry codes: (i) $-x, \frac{1}{2}+y, -\frac{1}{2}-z$; (ii) $-x, -\frac{1}{2}+y, -\frac{1}{2}-z$; (iii) $x, \frac{3}{2}-y, \frac{1}{2}+z$.

The crystal structure viewed along the *c* axis is shown in Fig. 2 and the geometry of the hydrogen bonds is listed in Table 2. The adenine moieties are arranged so as to form ribbons along the twofold screw axis through the N(6)H···N(7) and N(6)H···N(1) hydrogen bonds. Such a ribbon structure of adenines has often been found in crystals of adenine derivatives (*e.g.*, Takimoto, Takenaka & Sasada, 1981). The imidazolyl groups are connected to each other along the *c* axis by the N(1′)H···N(3′) hydrogen bonds. As seen from Fig. 2, a double molecular sheet is formed parallel to the *bc* plane. In the sheet, close contacts are C(4)···C(11) [3·720 (6) Å] and C(5)···C(11) [3·452 (6) Å] between the molecules related by the *c* glide. The double sheets are loosely packed, the shortest contact being 3·911 (8) Å for C(6′)···C(6′).

There are no direct interactions between the neutral imidazolyl group and the adenine moiety. This is in contrast with the stacking interaction between the protonated imidazolyl group and the adenine moiety in the crystal of 3-(9-adeninyl)propionhistamide hydrochloride. Such a difference in interaction patterns explains well the experiments in solution; the biological consequence of this has already been mentioned in a previous paper (Takenaka, Takimoto & Sasada, 1984).

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Structure of Tris(4-methoxyphenyl)phosphine

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Abstract. $C_{21}H_{21}O_3P$, $M_r = 352·37$, monoclinic, $P2_1/c$, $a = 9·881$ (3), $b = 9·636$ (3), $c = 19·801$ (3) Å, $\beta = 91·83$ (2)°, $V = 1884·4$ Å^3, $Z = 4$, $D_m = 1·24$ (1), $D_x = 1·242$ Mg m^{-3}, λ(Cu $K\bar{\alpha}$) = 1·54178 Å (graphite monochromated), μ(Cu $K\alpha$) = 1·408 mm^{-1}, $F(000) = 744$, $T = 293$ K, final $R = 0·039$ for 1422 unique nonzero reflections. The geometry around P is pyramidal with C—P—C angles of 99·6 (2)–102·9 (2)° and P—C distances of 1·824 (4)–1·830 (4) Å. One of the phenyl rings is more distorted from planarity than

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the other two, and the P atom is further from this plane than from the other two. Each methoxy C atom is close to its phenyl plane. The title compound does not show the threefold symmetry found in the analogous tris-(4-methoxyphenyl)arsine.

Introduction. As part of a series of studies on complexes of various substituted phosphines with heavy post-transition metals, $Hg(ClO_4)_2$ complexes of the title compound have been prepared and investigated by X-ray diffraction (Allman, Goel & Beauchamp, 1986). The structure of the free ligand was determined for comparison purposes.

Experimental. Compound obtained as described earlier (Allman & Goel, 1982). Recrystallization from ethanol yielded colorless prisms. Crystal dimensions: 0·123 $(100\text{–}\bar{1}00)$ × 0·205 $(001\text{–}00\bar{1})$ × 0·195 mm $(11\bar{1}\text{–}\bar{1}\bar{1}1)$. D_m measured by flotation in aqueous NaCl.

Laue symmetry and space group determined from precession and cone-axis photographs. Unit-cell parameters accurately determined from 25 reflections $(12 < \theta < 20°)$ centered on an Enraf–Nonius CAD-4 diffractometer. Data collected as described elsewhere (Bélanger-Gariépy & Beauchamp, 1980). $2\theta_{max} = 120°$, range of *hkl*: $0 \le h \le 11$, $0 \le k \le 10$, $-22 \le l \le 22$. Standards (e.s.d.): 210 (1·2%), 002 (1·2%), $11\bar{4}$ (1·2%). 2794 unique reflections measured, 1422 observed, 1372 unobserved $[I < 3{\cdot}0\sigma(I)]$. Corrections for Lorentz effect, polarization and absorption (Gaussian integration, grid 8 × 8 × 8, transmission range: 0·71–0·86).

Structure solved by direct methods. P and two carbon rings found by *MULTAN* (Main, Woolfson, Lessinger, Germain & Declercq, 1974). Remaining atoms including all hydrogens located by standard Fourier techniques. Function $\sum w(|F_o| - |F_c|)^2$ minimized by full-matrix least squares. $w = 1/\sigma^2(F)$. Parameters refined: scale factor, coordinates (all atoms), temperature factors, anisotropic (non-hydrogen atoms) or isotropic (hydrogens). Final $wR = 0{\cdot}047$, $S = 1{\cdot}49$, shift/σ (max.) 0·09, (av.) 0·02. Residual electron density (e Å^{-3}) in final ΔF map: max. = 0·21, min. = −0·12 (both near P), general background $< \pm 0{\cdot}11$.

Scattering curves from Cromer & Waber (1965), except for H (Stewart, Davidson & Simpson, 1965). Anomalous-dispersion correction for P from Cromer (1965). Computer programs listed elsewhere (Authier-Martin & Beauchamp, 1977). Refined coordinates listed in Table 1.*

* A view of the unit cell and lists of structure factors, anisotropic thermal parameters, distances and angles involving H atoms and distances and angles in substituted triphenylphosphines have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42690 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. A view of the molecule is shown in Fig. 1. Interatomic distances and bond angles involving the non-hydrogen atoms are listed in Table 2.

The P—C distances [1·824 (4)–1·830 (4) Å] show no significant differences and their average value (1·827 Å) is similar to those found for other phosphines without bulky *ortho* substituents (Butters, Haller-Pauls & Winter, 1982; Daly, 1964; Cameron, Howlett & Miller, 1978; Sobolev, Bel'skii, Romm & Gur'yanova, 1983). There are significant differences, probably arising from packing effects, between the C—P—C angles [99·6 (2)–102·9 (2)°], but their average (101·5°) is similar to those observed for similar phosphines. This value, much lower than 109·5°, reflects the stereochemical effect of the P lone pair.

The C—C distances in the phenyl rings (Table 2) average 1·385 Å, and there is a slight tendency for the C_P—C_{ortho} distances (av. 1·392 Å) to be somewhat

Table 1. *Refined coordinates* (C, O $\times 10^4$, P $\times 10^5$, H $\times 10^3$) *and equivalent isotropic temperature factors* (Å$^2 \times 10^3$)

$$U_{eq} = \tfrac{1}{3}\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}†
P	68735 (12)	13445 (12)	65562 (5)	63
O(1)	906 (3)	1765 (3)	5907 (1)	76
O(2)	7173 (3)	1974 (3)	9570 (1)	72
O(3)	8222 (3)	−4715 (3)	6483 (1)	71
C(11)	5056 (4)	1434 (4)	6368 (2)	53
C(12)	4581 (4)	1493 (4)	5695 (2)	65
C(13)	3230 (4)	1607 (4)	5522 (2)	64
C(14)	2269 (4)	1670 (4)	6017 (2)	58
C(15)	2725 (4)	1623 (4)	6688 (2)	60
C(16)	4068 (4)	1499 (4)	6857 (2)	58
C(17)	388 (5)	1912 (6)	5236 (2)	103
C(21)	6950 (3)	1461 (4)	7478 (2)	52
C(22)	7212 (4)	2738 (4)	7783 (2)	55
C(23)	7281 (4)	2862 (4)	8478 (2)	55
C(24)	7082 (4)	1734 (4)	8888 (2)	51
C(25)	6821 (4)	453 (4)	8603 (2)	55
C(26)	6758 (4)	341 (4)	7904 (2)	59
C(27)	7050 (5)	831 (5)	10012 (2)	91
C(31)	7244 (4)	−503 (4)	6455 (2)	54
C(32)	8591 (4)	−899 (4)	6535 (2)	61
C(33)	8970 (4)	−2291 (5)	6547 (2)	63
C(34)	7981 (4)	−3310 (4)	6455 (2)	55
C(35)	6652 (3)	−2927 (4)	6350 (2)	54
C(36)	6293 (3)	−1544 (4)	6354 (2)	54
C(37)	9588 (5)	−5180 (5)	6578 (3)	97
H(12)	530 (3)	151 (3)	535 (2)	65 (10)
H(13)	291 (3)	166 (3)	506 (2)	83 (12)
H(15)	204 (3)	169 (3)	700 (2)	85 (12)
H(16)	436 (3)	149 (3)	732 (1)	60 (10)
H(17)	79 (4)	118 (4)	495 (2)	125 (16)
H(18)	−59 (4)	184 (4)	527 (2)	128 (15)
H(19)	78 (4)	274 (4)	506 (2)	132 (16)
H(22)	736 (3)	357 (3)	748 (2)	81 (11)
H(23)	744 (3)	371 (3)	867 (1)	36 (8)
H(25)	674 (3)	−32 (3)	887 (2)	66 (10)
H(26)	660 (3)	−47 (3)	772 (1)	48 (9)
H(27)	773 (4)	14 (4)	999 (2)	106 (14)
H(28)	712 (4)	119 (4)	1048 (2)	113 (15)
H(29)	604 (4)	41 (4)	997 (2)	118 (15)
H(32)	940 (3)	−15 (4)	663 (2)	97 (13)
H(33)	989 (3)	−255 (3)	663 (1)	67 (10)
H(35)	597 (3)	−357 (3)	627 (1)	64 (10)
H(36)	540 (3)	−126 (3)	628 (1)	53 (9)
H(37)	991 (4)	−490 (4)	701 (2)	131 (16)
H(38)	955 (4)	−621 (4)	666 (2)	138 (17)
H(39)	1006 (3)	−485 (3)	622 (2)	83 (12)

† U_{iso} for hydrogen atoms.

greater than the others (av. C_{ortho}—C_{meta} = 1·379 Å, C_{meta}—C_{para} = 1·383 Å). Some steric effect on P on the attached ring is indicated by the C_{ortho}—C_P—C_{ortho} angle being smaller (av. 116·7°) and the C_P—C_{ortho}—C_{meta} angles being greater (av. 121·9°) than the ideal value of 120°. The remaining angles are closer to ideal (av. C_{ortho}—C_{meta}—C_{para} = 120·2, C_{meta}—C_{para}—C_{meta} = 119·0°). Rings 1 and 2 are planar within 1·2σ (0·005 Å) and the P atom deviates by only 0·063 (1) Å from the plane of ring 1 and not at all from that of ring 2. Ring 3 is more distorted, with distances as large as 0·016 Å (4σ) between individual C atoms and the plane. The distance of P from this plane is also much greater [0·198 (1) Å].

The C—O and O—CH_3 distances, averaging 1·368 and 1·420 Å, respectively, are similar to those reported for methoxy-substituted phenyl rings (Alper, Einstein, Petrignani & Willis, 1983; Haagensen, 1978; Mootz, Poll, Wunderlich & Wussow, 1981; Sobolev & Belsky, 1981). The C_{para}—O—CH_3 angle (av. 118·5°) is also normal. The O atoms deviate from the planes of their respective rings by 0·023 (3) Å for O(1), 0·003 (3) Å for O(2) and 0·082 (3) Å for O(3), showing again steric effects for ring 3. The O—CH_3 bond is almost perfectly eclipsed with respect to an adjacent C_{para}—C_{meta} bond. The torsion angles are: C(13)—C(14)—O(1)—C(17) = −4·7 (6), C(25)—C(24)—O(2)—C(27) = 2·8 (3), C(33)—C(34)—O(3)—C(37) = −3·4 (5)°. The steric requirement of the methyl group is probably responsible for the C_{meta}—C_{para}—O angles oriented *cis* with respect to the methyl groups [125·9 (3), 124·1 (3), 124·7 (3)°] being ~8° greater than those *trans* to it [116·4 (3), 116·3 (3), 115·7 (3)°].

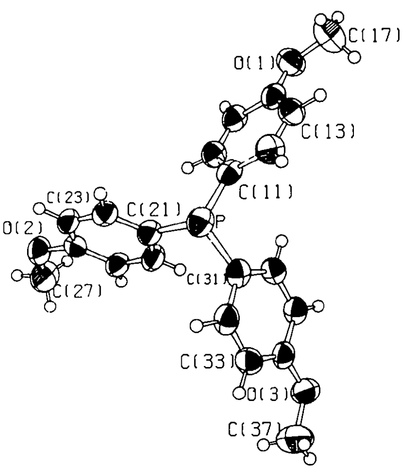

Fig. 1. View of the $P(C_6H_4OCH_3)_3$ molecule. The C atoms are assigned two-digit symbols: the first digit (1,2,3) is the ring number, the second corresponds to sequential numbering around the ring, position 1 being the C attached to P and 7 the methyl carbon. Ellipsoids correspond to 50% probability.

Table 2. *Interatomic distances* (Å) *and bond angles* (°)

P—C(11)	1·824 (4)	C(24)—C(25)	1·378 (5)
P—C(12)	1·828 (4)	C(25)—C(26)	1·388 (5)
P—C(13)	1·830 (4)	C(26)—C(21)	1·387 (5)
C(11)—C(12)	1·400 (5)	C(24)—O(2)	1·370 (4)
C(12)—C(13)	1·372 (6)	O(2)—C(27)	1·414 (5)
C(13)—C(14)	1·388 (5)	C(31)—C(32)	1·389 (5)
C(14)—C(15)	1·390 (5)	C(32)—C(33)	1·393 (6)
C(15)—C(16)	1·363 (5)	C(33)—C(34)	1·393 (5)
C(16)—C(11)	1·398 (5)	C(34)—C(35)	1·373 (5)
C(14)—O(1)	1·360 (5)	C(35)—C(36)	1·379 (6)
O(1)—C(17)	1·416 (5)	C(36)—C(31)	1·385 (5)
C(21)—C(22)	1·391 (5)	C(34)—O(3)	1·375 (5)
C(22)—C(23)	1·381 (5)	O(3)—C(37)	1·429 (5)
C(23)—C(24)	1·375 (5)		
C(11)—P—C(21)	102·1 (2)	C(22)—C(23)—C(24)	121·1 (3)
C(11)—P—C(31)	102·9 (2)	C(23)—C(24)—C(25)	119·7 (3)
C(21)—P—C(31)	99·6 (2)	C(24)—C(25)—C(26)	118·7 (3)
P—C(11)—C(12)	119·6 (3)	C(25)—C(26)—C(21)	122·9 (3)
P—C(11)—C(16)	124·4 (3)	C(23)—C(24)—O(2)	116·3 (3)
C(12)—C(11)—C(16)	115·9 (3)	C(25)—C(24)—O(2)	124·1 (3)
C(11)—C(12)—C(13)	122·3 (4)	C(24)—O(2)—C(27)	118·3 (3)
C(12)—C(13)—C(14)	120·6 (4)	P—C(31)—C(32)	116·7 (3)
C(13)—C(14)—C(15)	117·7 (3)	P—C(31)—C(36)	125·7 (3)
C(14)—C(15)—C(16)	121·4 (4)	C(32)—C(31)—C(36)	117·5 (3)
C(15)—C(16)—C(11)	122·0 (3)	C(31)—C(32)—C(33)	121·5 (4)
C(13)—C(14)—O(1)	125·9 (3)	C(32)—C(33)—C(34)	119·3 (3)
C(15)—C(14)—O(1)	116·4 (3)	C(33)—C(34)—C(35)	119·6 (3)
C(14)—O(1)—C(17)	118·9 (3)	C(34)—C(35)—C(36)	120·2 (3)
P—C(21)—C(22)	119·3 (3)	C(35)—C(36)—C(31)	121·8 (3)
P—C(21)—C(26)	123·9 (3)	C(33)—C(34)—O(3)	124·7 (3)
C(22)—C(21)—C(26)	116·8 (3)	C(35)—C(34)—O(3)	115·7 (3)
C(21)—C(22)—C(23)	120·8 (3)	C(34)—O(3)—C(37)	118·4 (3)

The analogous tris(4-methoxyphenyl)arsine molecule lies on a crystallographic threefold axis and the ring makes an angle of 42° with this axis (Sobolev & Belsky, 1981). In the present phosphine, departure from threefold symmetry arises mainly from the orientation of ring 2, which makes an angle of 31° with the pseudo threefold axis, whereas, for rings 1 and 3, the angles (46 and 48°, respectively) are closer to those found in the arsine derivative. The methoxy group of ring 2 is also flipped in the opposite direction from the other two.

The molecules interact by normal van der Waals contacts.

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Structure of *N,N'*-Diphenyl-2,4-hexadiyne-1,6-diamine

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Abstract. $C_{18}H_{16}N_2$, $M_r = 260{\cdot}3$, monoclinic, $P2_1/c$, $a = 8{\cdot}740$ (4), $b = 16{\cdot}858$ (9), $c = 9{\cdot}915$ (5) Å, $\beta = 99{\cdot}02$ (4)°, $V = 1443$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}198$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 0·8 cm^{-1}, $F(000) = 552$, $T = 150$ K, $R = 0{\cdot}067$ using 2603 independent observed reflections. The molecules have pseudo-*cis* configuration and are linked in the crystal *via* N—H···N hydrogen bonds to form infinite double chains. The absence of a stacking arrangement of the 1,3-butadiyne groups of neighbouring molecules is consistent with the observed inertness of the compound to solid-state polymerization.

Introduction. Some derivatives of diacetylene (1,3-butadiyne) exhibit a structurally determined ability to undergo solid-state polymerization (Wegner, 1977). As part of a study on the relation between crystal structure and solid-state reactivity of diacetylenes we carried out a single-crystal X-ray study of *N,N'*-diphenyl-2,4-hexadiyne-1,6-diamine, which is stable to UV and γ-radiation.

Experimental. Pale yellow prismatic crystal, dimensions 0·3 × 0·3 × 0·8 mm, used for measurement of unit-cell parameters (24 reflections with $25 \le 2\theta \le 28°$) and intensities of 3273 reflections ($-11 \le h \le 11$, $0 \le k \le 21$, $0 \le l \le 12$) with Syntex $P2_1$ diffractometer (Mo $K\alpha$, graphite monochromator, $\theta/2\theta$ scan, $2\theta_{max} = 55°$). No significant variation in intensities of 3 standard reflections (100, 020, 004) measured after every 100 reflections. No absorption and secondary-extinction corrections. Structure solved by direct methods, revealing all non-hydrogen atoms, and refined by full-matrix least squares with anisotropic thermal parameters for non-hydrogen atoms, using 2603 independent reflections with $I \ge 2\sigma(I)$ and minimizing $\sum w(|F_o| - |F_c|)^2$, $w = 1/[\sigma^2(F_o) + (F_c)^2]$. Scattering factors from *International Tables for X-ray Crystallography* (1974). Hydrogen atoms located by difference Fourier synthesis and refined isotropically. $R = 0{\cdot}067$, $wR = 0{\cdot}072$, $S = 5{\cdot}23$, max. (shift/σ) = 0·5, final electron-density fluctuations ±0·4 e Å^{-3}. All calculations carried out with an Eclipse S/200 computer using *INEXTL* programs (Gerr, Yanovsky & Struchkov, 1983).†

Discussion. The positional and thermal atomic parameters are listed in Table 1; the atom numbering, bond lengths and main bond angles are shown in Fig. 1. A full list of bond angles involving non-hydrogen atoms is given in Table 2.

The molecule has a non-symmetrical pseudo-*cis* configuration unusual for symmetrically substituted diacetylenes; the pseudo torsion angles N(1)C(1)-

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† Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42691 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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