FISCHER, N. H., OLIVIER, E. J. & FISCHER, H. D. (1979). *Fortschr. Chem. Org. Naturst.* **38**, 47–390.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
Nicolet Instrument Corporation (1986). *SHELXTL* for Desktop 30 (Microeclipse), PN269-1040340, April 1986. Nicolet XRD Corp., Madison, WI, USA.
WHITE, E. H. & WINTER, R. E. K. (1963). *Tetrahedron Lett.* pp. 137–139.

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Structure of Diphenyl(2-pyridyl)phosphine*

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Abstract. $C_{17}H_{14}NP$, $M_r = 263{\cdot}28$, monoclinic, $P2_1/n$, $a = 9{\cdot}9023\ (2)$, $b = 9{\cdot}8780\ (3)$, $c = 14{\cdot}8926\ (4)$ Å, $\beta = 92{\cdot}948\ (3)°$, $V = 1454{\cdot}8\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}202$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}70932$ Å, $\mu = 0{\cdot}17$ mm^{-1}, $F(000) = 552$, $T = 293$ K, $R = 0{\cdot}043$ for 1680 unique observed reflections. The phenyl and pyridyl rings are planar and make angles of 71·6 (1), 46·9 (1)° (phenyls) and 45·1 (1)° (pyridyl) with the basal plane of the PCCC pyramid.

Experimental. White crystal of $C_{17}H_{14}NP$ (Maisonnet, Far, Olmstead, Hunt & Balch, 1982) from diethyl ether–hexane at 273 K, 0·15 × 0·35 × 0·35 mm; Enraf–Nonius CAD-4 controlled by the NRCCAD software (Le Page, White & Gabe, 1986). Data collected in the θ–2θ mode up to $2\theta = 55°$, graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from a least-squares refinement of the setting angles of 100 reflections ($35 \le 2\theta \le 45°$); systematic absences ($h0l$, $h + l = 2n + 1$, $0k0$, $k = 2n + 1$) consistent with space group $P2_1/n$; no statistically significant change in the intensities of the three standard reflections monitored ($\bar{1}3\bar{1}$, 006, $\bar{3}13$). 3446 unique reflections ($-12 \le h \le 12$, $0 \le k \le 12$, $0 \le l \le 19$), 1680 with $I_{net} \ge 3\sigma(I_{net})$.

Corrections for Lorentz and polarization effects applied but not for absorption. Structure solved by direct methods and difference-map techniques. N atom differentiated from C atoms by refining on occupancies with the ring atoms being defined as C atoms at first and with the isotropic U values fixed at 0·04 Å^2. Positions of all the H atoms revealed by subsequent difference maps. Final refinement by full-matrix least squares on all atoms treating isotropically the H atoms and anisotropically all the others; $\sum w(|F_o| - |F_c|)^2$ was minimized with $w^{-1} = \sigma^2(F_o) + 0{\cdot}0002F_o^2$, $R = 0{\cdot}043$, $wR = 0{\cdot}041$, $S = 1{\cdot}5$ for 229 parameters and 1680 reflections ($R = 0{\cdot}094$, $wR = 0{\cdot}051$ for all 3446 reflections), $(\Delta/\sigma)_{max} = 0{\cdot}004$; in the final difference map, general background below 0·24 e Å^{-3}. All computations with *NRCVAX* system of programs (Gabe, Lee & Le Page, 1985); atom scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). Atomic positions are listed in Table 1, selected bond lengths and

Table 1. *Atomic parameters x, y, z and* B_{eq}

E.s.d.'s refer to the last digit printed.

	x	y	z	B_{eq}* (Å^2)
P	0·96935 (7)	0·15507 (7)	0·29975 (5)	4·13 (3)
N18	1·14047 (22)	0·3508 (3)	0·26210 (15)	5·88 (12)
C1	0·88855 (22)	0·1617 (3)	0·18700 (15)	3·74 (11)
C2	0·8969 (3)	0·0488 (3)	0·13287 (22)	4·87 (15)
C3	0·8419 (3)	0·0493 (5)	0·04591 (25)	6·23 (19)
C4	0·7799 (3)	0·1627 (5)	0·01216 (24)	6·64 (20)
C5	0·7704 (3)	0·2755 (4)	0·06388 (24)	6·16 (18)
C6	0·8242 (3)	0·2750 (3)	0·15106 (21)	4·87 (15)
C7	0·8292 (3)	0·1559 (3)	0·37458 (16)	4·05 (11)
C8	0·6937 (3)	0·1622 (3)	0·34783 (21)	4·98 (14)
C9	0·5956 (4)	0·1565 (4)	0·4115 (3)	6·78 (20)
C10	0·6321 (5)	0·1470 (4)	0·5007 (3)	7·32 (21)
C11	0·7649 (5)	0·1405 (4)	0·52758 (24)	7·27 (21)
C12	0·8625 (4)	0·1436 (3)	0·46535 (20)	5·61 (16)
C13	1·03095 (22)	0·3302 (3)	0·30983 (15)	3·86 (11)
C14	0·9775 (3)	0·4308 (3)	0·36097 (18)	4·35 (13)
C15	1·0372 (3)	0·5563 (4)	0·36375 (23)	5·77 (17)
C16	1·1475 (4)	0·5793 (4)	0·31469 (23)	6·55 (18)
C17	1·1944 (4)	0·4745 (5)	0·26558 (22)	7·33 (20)

* B_{eq} is the mean of the principal axes of the thermal ellipsoid.

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Table 2. *Selected bond lengths* (Å) *and angles* (°) *in* $C_{17}H_{14}NP$

Ring *A*		Ring *B*		Ring *C*	
P–C1	1·824 (2)	P–C7	1·824 (2)	P–C13	1·837 (3)
C1–C2	1·381 (4)	C7–C8	1·381 (4)	C13–C14	1·375 (4)
C2–C3	1·379 (5)	C8–C9	1·394 (4)	C14–C15	1·373 (5)
C3–C4	1·361 (7)	C9–C10	1·362 (7)	C15–C16	1·363 (5)
C4–C5	1·361 (6)	C10–C11	1·357 (7)	C16–C17	1·363 (6)
C5–C6	1·378 (5)	C11–C12	1·373 (5)	C17–N18	1·324 (5)
C6–C1	1·382 (4)	C12–C7	1·380 (4)	N18–C13	1·342 (3)
C1–C2–C3	120·9 (3)	C7–C8–C9	120·2 (3)	C13–C14–C15	119·5 (3)
C2–C3–C4	119·9 (3)	C8–C9–C10	120·5 (4)	C14–C15–C16	119·3 (3)
C3–C4–C5	120·5 (3)	C9–C10–C11	119·7 (3)	C15–C16–C17	117·7 (3)
C4–C5–C6	119·7 (4)	C10–C11–C12	120·3 (4)	C16–C17–N18	124·8 (3)
C5–C6–C1	121·1 (3)	C11–C12–C7	121·5 (4)	C17–N18–C13	116·8 (3)
C6–C1–C2	117·9 (3)	C12–C7–C8	117·8 (3)	N18–C13–C14	121·9 (3)
C2–C1–P	118·2 (2)	C8–C7–P	125·6 (2)	C14–C13–P	126·2 (2)
C6–C1–P	123·9 (2)	C12–C7–P	116·6 (2)	N18–C13–P	111·9 (2)
C1–P–C7	104·5 (1)	C7–P–C13	101·9 (1)	C13–P–C1	99·8 (1)

	Range	Average*
<C–H>	0·83 (3)–0·99 (3)	0·93[4]
<C–C–H>	115·7(2)–123·8(2)	120[3]

Shortest intermolecular contacts (excluding H···H)†

N18···C16′	3·627 (5)	N18···H16′	3·26 (3)

* Standard deviation on average value calculated as: $\sigma(\bar{x}) = [\sum_{i=1}^{n} (x_i - \bar{x})^2/(n-1)]^{1/2}$.

† Atom $X(x, y, z) \rightarrow$ atom X' $(\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z)$.

angles are given in Table 2.* The numbering scheme is given in Fig. 1.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51526 (29 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

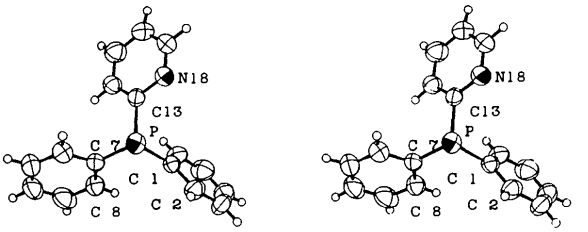

Fig. 1. Stereoview of $C_{17}H_{14}NP$ (50% boundary ellipses are shown).

Related literature. This study was aimed at providing structural data on the title compound, thus allowing for a comparison between the free ligand and its liganded states in which a Co/NO metallic fragment is attached to the N and/or P donor sites of the molecule (Roustan, Ansari & Ahmed, 1987).

References

GABE, E. J., LEE, F. L. & LE PAGE, Y. (1985). In *Crystallographic Computing* 3, edited by G. M. SHELDRICK, C. KRUGER & R. GODDARD. Oxford: Clarendon Press.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

LE PAGE, Y., WHITE, P. S. & GABE, E. J. (1986). Proc. Am. Crystallogr. Assoc. Meet., Hamilton, Ontario, Canada. Abstract PA 23.

MAISONNET, A., FAR, J. P., OLMSTEAD, M. M., HUNT, C. T. & BALCH, A. L. (1982). *Inorg. Chem.* **21**, 3961–3967.

ROUSTAN, J. L., ANSARI, N. & AHMED, F. (1987). *Inorg. Chim. Acta*, **129**, L11–L12.

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Structure of 5-Hydroxy-7,4′-dimethoxyflavanone

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Abstract. 5-Hydroxy-7-methoxy-2-(4-methoxyphenyl)chroman-4-one, $C_{17}H_{16}O_5$, $M_r = 300{\cdot}3$, monoclinic, $C2/c$, $a = 17{\cdot}38\ (2)$, $b = 5{\cdot}321\ (4)$, $c = 30{\cdot}74\ (3)$ Å, $\beta = 98{\cdot}27\ (7)°$, $V = 2814\ (4)$ Å^3, $Z = 8$, $D_x = 1{\cdot}42$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 0{\cdot}6$ cm^{-1}, $F(000) = 1264$, $T = 173$ K, $R = 0{\cdot}0696$ for 1024 observed reflections with $I > 2\sigma(I)$. Lattice sites are occupied randomly by 2*R* or 2*S* isomers leading to partial disorder. The pyranone ring has a sofa conformation and the dihedral angle between the aromatic *A* and *B* rings is 70·8 (2)°. The hydrogen of the 5-hydroxy group is intramolecularly hydrogen-bonded to the carbonyl group.

Experimental. White needle-shaped crystals, m.p. 391 K, from an earlier study (Miles & Main, 1985), recrystallized from methanol. Space group defined by precession photography as $C2/c$ or Cc, the former

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