

Fig. 2. Stereoview of the contents of the unit cell showing O...O close contacts.

molecules of the nitronorbornanol thus associate as hydrogen-bonded cyclic tetramers in which the hydroxy, but not the nitro, groups are involved. Fig. 2 shows unit-cell contents and the putative hydrogen-bonded cyclic tetramers.

**Related literature.** Other nitronorbornanols investigated in these laboratories show hydrogen bonding between hydroxy and nitro groups (Boeyens, Denner & Michael, 1984*a,b*).

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## 2,4,4,6-Tetraphenyl-3(4*H*)-pyridinone

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**Abstract.** C<sub>29</sub>H<sub>21</sub>NO, *M<sub>r</sub>* = 399.49, monoclinic, *P*2<sub>1</sub>/*a*, *a* = 21.713 (5), *b* = 13.524 (4), *c* = 7.259 (2) Å,  $\beta$  = 95.20 (2)°, *V* = 2123.0 (11) Å<sup>3</sup>, *Z* = 4, *D<sub>x</sub>* = 1.250 g cm<sup>-3</sup>,  $\lambda$ (Mo *K*α) = 0.71073 Å,  $\mu$  = 0.81 cm<sup>-1</sup>, *F*(000) = 840, *T* = 294 K, *R* = 0.055 for 2248 observed reflections. In the pyridine ring the C(5)=C(6)—N(1)=C(2) moiety is almost planar and forms a dihedral angle of 35.0 (2)° with the carbonyl plane of C(2), C(3), C(4) and O(7). The 2- and 6-phenyl groups are slightly rotated from the C(5)=C(6)—N(1)=C(2) plane: the dihedral angles are 10.3 (1) and 23.2 (2)° for the 2- and 6-positions, respectively.

**Experimental.** The title compound was synthesized by the method given by Maeda, Nakamura & Sakai (1983). Recrystallization from acetone–ethanol gave orange plate-like crystals of dimensions 0.5 × 0.2 × 0.1 mm; Rigaku AFC-4 diffractometer; cell parameters were determined from 20 independent 2θ values (25 < 2θ < 30°); intensity measurements were per-

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formed with graphite-monochromated Mo *K*α radiation up to 2θ = 50.0° (*h* = 29 → 29, *k* 0 → 18, *l* 0 → 10), ω–2θ scan technique, scan speed 4° min<sup>-1</sup> in θ, scan width (1.0 + 0.35tanθ)°; background 5 s before and after each scan; three standard reflections (961, 372, 234) were monitored every 50 reflections and showed no significant variation in intensities. 3743 unique reflections were measured, 2252 with  $|F_o| > 3\sigma(|F_o|)$  were used for structure determination; corrections for Lorentz and polarization effects, absorption ignored; direct methods (*MULTAN78*; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and full-matrix least-squares refinement (*SHELX76*; Sheldrick, 1976) with anisotropic thermal parameters for non-H atoms and isotropic ones for H atoms, minimizing the function  $\sum w(|F_o| - |F_c|)^2$ ,  $w = [\sigma^2(|F_o|) + 0.0040|F_o|^2]^{-1}$ ; some H atoms located on difference Fourier map, other H-atom positions determined geometrically and included in subsequent refinements; four intense reflections (110, 200, 011, 617) seemed to suffer from extinction and were not used in refinements; final *R* = 0.055 and *wR* = 0.065 for 2248 observed reflec-

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Table 1. Final atomic coordinates ( $\times 10^4$ ) with *e.s.d.'s* in parentheses and equivalent isotropic temperature factors,  $B_{\text{eq}}$  ( $\text{\AA}^2$ ), for non-hydrogen atoms

	$x$	$y$	$z$	$B_{\text{eq}}$
N(1)	9216 (1)	2897 (2)	2946 (4)	3.6
C(2)	9385 (2)	2190 (2)	1919 (5)	3.1
C(3)	9216 (2)	1136 (2)	2326 (5)	3.2
C(4)	8587 (1)	1013 (2)	3101 (4)	2.9
C(5)	8518 (2)	1851 (2)	4446 (5)	3.2
C(6)	8833 (2)	2697 (2)	4381 (5)	3.3
O(7)	9561 (1)	455 (2)	2110 (4)	4.6
C(8)	9769 (2)	2420 (2)	390 (5)	3.1
C(9)	9997 (2)	3372 (3)	215 (6)	4.6
C(10)	10320 (2)	3615 (3)	-1262 (7)	5.9
C(11)	10432 (2)	2921 (3)	-2569 (7)	5.6
C(12)	10218 (2)	1979 (3)	-2414 (6)	5.2
C(13)	9885 (2)	1726 (3)	-948 (5)	4.3
C(14)	8124 (1)	1107 (2)	1369 (4)	3.1
C(15)	7702 (2)	1883 (3)	1141 (5)	3.9
C(16)	7293 (2)	1943 (3)	-434 (6)	4.7
C(17)	7302 (2)	1237 (4)	-1790 (6)	5.1
C(18)	7720 (2)	476 (3)	-1605 (6)	4.9
C(19)	8133 (2)	413 (3)	-47 (5)	4.0
C(20)	8544 (1)	32 (2)	4133 (4)	2.9
C(21)	8063 (2)	-625 (3)	3804 (5)	3.6
C(22)	8037 (2)	-1490 (3)	4828 (6)	4.3
C(23)	8491 (2)	-1703 (3)	6211 (6)	4.6
C(24)	8975 (2)	-1044 (3)	6601 (5)	4.3
C(25)	9000 (2)	-188 (3)	5562 (5)	3.8
C(26)	8773 (2)	3523 (2)	5704 (5)	3.6
C(27)	8571 (2)	3358 (3)	7437 (5)	4.0
C(28)	8492 (2)	4138 (3)	8623 (6)	4.9
C(29)	8615 (2)	5082 (3)	8092 (7)	5.7
C(30)	8820 (3)	5248 (3)	6413 (8)	7.1
C(31)	8904 (3)	4484 (3)	5202 (7)	5.9

$$B_{\text{eq}} = (4/3) \sum_i \sum_j \beta_{ij} a_i \cdot a_j$$

Table 2. Selected bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) with *e.s.d.'s* in parentheses

N(1)—C(2)	1.287 (4)	C(4)—C(5)	1.512 (5)
N(1)—C(6)	1.417 (4)	C(4)—C(14)	1.543 (5)
C(2)—C(3)	1.508 (5)	C(4)—C(20)	1.531 (4)
C(2)—C(8)	1.480 (5)	C(5)—C(6)	1.337 (5)
C(3)—C(4)	1.532 (5)	C(6)—C(26)	1.486 (5)
C(3)—O(7)	1.207 (4)		
C(2)—N(1)—C(6)	120.1 (3)	C(3)—C(4)—C(20)	111.7 (3)
N(1)—C(2)—C(3)	120.1 (3)	C(5)—C(4)—C(14)	111.6 (3)
N(1)—C(2)—C(8)	119.2 (3)	C(5)—C(4)—C(20)	108.6 (3)
C(3)—C(2)—C(8)	120.6 (3)	C(14)—C(4)—C(20)	113.9 (3)
C(2)—C(3)—C(4)	114.6 (3)	C(4)—C(5)—C(6)	122.5 (3)
C(2)—C(3)—O(7)	122.0 (3)	N(1)—C(6)—C(5)	121.7 (3)
C(4)—C(3)—O(7)	123.4 (3)	N(1)—C(6)—C(26)	115.0 (3)
C(3)—C(4)—C(5)	107.5 (3)	C(5)—C(6)—C(26)	123.1 (3)
C(3)—C(4)—C(14)	103.2 (3)		

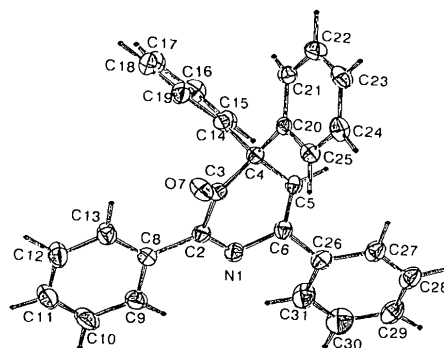


Fig. 1. ORTEP plot (Johnson, 1965) of the title compound with the atom numbering. The thermal ellipsoids enclose 30% probability.

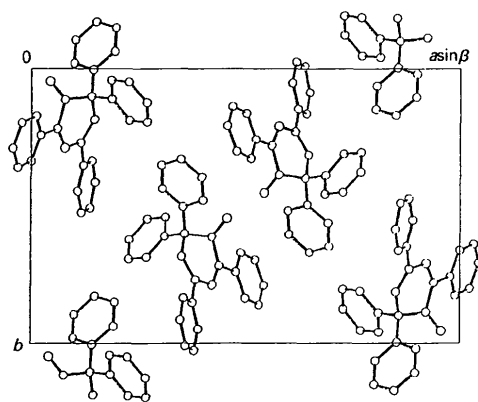


Fig. 2. Crystal structure viewed along the *c* axis.

tions and 364 refined parameters;  $(\Delta/\sigma)_{\text{max}} = 0.05$ ; final difference map showed  $-0.18 < \Delta\rho < 0.17 \text{ e \AA}^{-3}$ ; atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV); calculations carried out on an IBM 4381-R24 computer at Ochanomizu University. Final atomic coordinates are listed in Table 1,\* and selected bond distances and angles in Table 2. The molecule with the atom numbering is shown in Fig. 1, and the crystal structure in Fig. 2.

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\* Lists of anisotropic thermal parameters for non-H atoms, positional and thermal parameters for H atoms, bond distances and angles, equations of least-squares planes, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54377 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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