the arabinose chain C(2)—C(15)—C(16)—C(17)—C(18)—C(19) of, successively, −175·6 (1), 84·9 (1), 72·3 (1)°.

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Structures of Two *N*-Arylpyridones: 1-(*o*-Chlorophenyl)-3-methoxy-2-methyl-4-pyridone (1) and 3-Methoxy-2-methyl-1-(1-naphthyl)-4-pyridone (2)

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Abstract. Compound (1), $C_{13}H_{12}ClNO_2$, $M_r = 249{\cdot}7$, orthorhombic, *Pbca*, $a = 10{\cdot}889$ (5), $b = 12{\cdot}064$ (6), $c = 18{\cdot}663$ (8) Å, $V = 2451{\cdot}7$ (2) Å^3, $Z = 8$, $D_x = 1{\cdot}35$ g cm^{-3}, graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 2{\cdot}96$ cm^{-1}, $F(000) = 1040$, $T = 293$ K, $R = 0{\cdot}044$ for 1296 unique observed reflections [$I \geq 3\sigma(I)$]. Compound (2), $C_{17}H_{15}NO_2$, $M_r = 265{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 15{\cdot}207$ (4), $b = 11{\cdot}360$ (4), $c = 7{\cdot}897$ (3) Å, $V = 1364{\cdot}2$ (8) Å^3, $Z = 4$, $D_x = 1{\cdot}292$ g cm^{-3}, graphite-monochromated Cu $K\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å, $\mu = 6{\cdot}45$ cm^{-1}, $F(000) = 560$, $T = 293$ K, $R = 0{\cdot}067$ for 752 unique observed reflections [$I \geq 3\sigma(I)$]. The aryl and pyridone rings are twisted towards each other with dihedral angles between the two ring planes of 91·31 (9) (compound 1) and 85·5 (3)° (compound 2). Molecular packing is realized *via* C—H···O contacts through the pyridone oxygen with C···O distances of 3·247 (4), 3·269 (4), 3·359 (4) Å (1) and 3·26 (1), 3·32 (1) Å (2).

Introduction. Many biphenyls with bulky substituents in *ortho* positions exhibit an axial chirality due to the restricted rotation along the C—C bond; even their enantiomeric pairs can be resolved (Stoddart, 1982). *N*-Aryl-4-pyridones have been synthesized and barriers to partial rotation about the C—N bond studied (Mintas, Orhanović, Jakopčić, Koller, Stühler & Mannschreck, 1985). X-ray structure determination of two representatives of the series was performed in order to determine the angles of rotation along the C—N bond (Fig. 1). Perpendicular orientation of the pyridone and aryl rings (Fig. 4) stabilizes the particular enantiomer conformation and permits the enantiomer separation.

Experimental. Weissenberg photographs (Cu $K\alpha$ radiation) determined the space groups *Pbca* for (1) and $P2_12_12_1$ for (2). Both compounds exhibit axial chirality; the centrosymmetrical space group of (1) implies the presence of two enantiomers in a 1:1 ratio (Fig. 1). However, the quality of the crystals of (2) prevented the determination of the absolute configuration by X-ray structure analysis. Preliminary cell dimensions were from oscillation photographs; final ones from diffractometer measurements; 20 reflections ($6 < \theta < 13°$) for (1) and 16 ($7 < \theta < 12°$) for (2). Crystals used: 0·10 × 0·16 × 0·35 (1) and 0·12 × 0·15 × 0·25 mm (2); Philips PW 1100 computer-controlled four-circle diffractometer, ω-scan mode [scan width =

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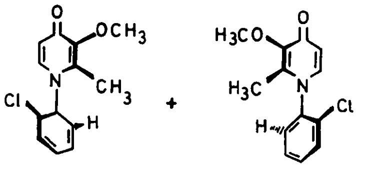
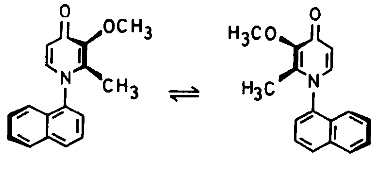
1·2° (θ) (1,2), scan speed 0·04 (1), 0·06° (θ) s^{-1} (2)], graphite-monochromated Mo $K\alpha$ radiation, 1330 recorded and 1296 observed reflections with $I \geq 3\sigma(I)$ in the range $3 < \theta < 30°$ for compound (1). Data collection for (2) was performed with Mo $K\alpha$ and Cu $K\alpha$ radiations. Structure-determination results presented in this paper are on the basis of Cu $K\alpha$ recorded intensities. 752 observed reflections in the range $3 < \theta < 68°$ were recorded. Lorentz and polarization corrections were applied. *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) gave the solution for (1) and (2) [based on 268 reflections having $|E| > 1{\cdot}22$ (1) and 230 with $|E| > 1{\cdot}20$ (2)]. Difference syntheses located the H atoms; refinement by full-matrix least squares minimizing $\sum w||F_o| - |F_c||^2$ with unit weights; a scale factor, atomic coordinates and anisotropic thermal parameters for the non-H atoms were refined; in structure (1) H-atom coordinates and isotropic thermal parameters were refined; in structure (2) H atoms were included in structure-factor calculation only. The highest peak in difference Fourier maps = 0·25 (1) and 0·5 e Å^{-3} (2), max. shift/e.s.d. = 0·4 (1) and 0·2 (2). Final R = 0·044 (1) and 0·067 (2); scattering factors from Cromer & Mann (1968) and (for H) Stewart, Davidson & Simpson (1965); anomalous-dispersion correction according to Cromer & Liberman (1970). Calculations were carried out on the Univac 1110 computer at the University Computing Centre in Zagreb with *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976). Final atomic coordinates of the non-H atoms and equivalent isotropic thermal parameters are given in Tables 1 and 2.*



Compound (1)



Compound (2)

Fig. 1. Axial chirality of *N*-aryl-4-pyridones.

Table 1. *Final atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (× 10^2) *for non*-H *atoms of* (1)

	x	y	z	U_{eq}* (Å^2)
Cl	8293 (1)	2225 (1)	2090 (1)	8·8 (1)
N(1)	9244 (2)	3786 (2)	986 (1)	4·7 (2)
C(2)	10082 (3)	4401 (2)	1378 (2)	4·4 (3)
C(3)	11306 (3)	4282 (3)	1232 (2)	4·4 (3)
O(3)	12131 (2)	4873 (2)	1646 (1)	5·5 (2)
C(4)	11770 (3)	3564 (3)	681 (2)	5·2 (3)
O(4)	12885 (2)	3473 (2)	546 (1)	6·5 (2)
C(5)	10831 (3)	2972 (3)	298 (2)	5·9 (3)
C(6)	9628 (3)	3100 (3)	454 (2)	5·4 (3)
C(7)	7938 (3)	3861 (3)	1132 (2)	4·6 (3)
C(8)	7409 (3)	3166 (3)	1626 (2)	5·3 (3)
C(9)	6151 (3)	3225 (3)	1752 (2)	6·8 (3)
C(10)	5454 (3)	3964 (4)	1371 (2)	7·5 (3)
C(11)	5989 (4)	4658 (4)	888 (2)	7·5 (4)
C(12)	7241 (3)	4621 (3)	765 (2)	6·2 (3)
C(13)	9591 (3)	5161 (3)	1934 (2)	6·2 (3)
C(14)	12638 (3)	5802 (3)	1283 (2)	6·7 (3)

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

Table 2. *Final atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (× 10^2) *for non*-H *atoms of* (2)

	x	y	z	U_{eq}* (Å^2)
N(1)	8565 (6)	1921 (6)	6412 (10)	4·2 (3)
C(2)	7846 (7)	1276 (8)	5787 (12)	4·1 (3)
C(3)	7951 (7)	99 (8)	5588 (12)	4·0 (4)
O(3)	7252 (5)	−516 (6)	4874 (8)	5·9 (3)
C(4)	8748 (7)	−530 (8)	6020 (14)	5·2 (4)
O(4)	8827 (5)	−1626 (6)	5820 (11)	7·5 (3)
C(5)	9421 (7)	191 (9)	6698 (14)	5·2 (4)
C(6)	9313 (7)	1362 (9)	6863 (13)	5·0 (4)
C(7)	8518 (7)	3190 (8)	6520 (13)	4·2 (4)
C(8)	8867 (6)	3865 (7)	5145 (13)	3·8 (3)
C(9)	8808 (7)	5103 (7)	5246 (15)	4·4 (4)
C(10)	8434 (7)	5625 (9)	6728 (15)	5·6 (4)
C(11)	8110 (7)	4947 (9)	8030 (15)	5·7 (5)
C(12)	8156 (6)	3724 (8)	7934 (14)	5·1 (5)
C(13)	7028 (7)	1931 (8)	5357 (15)	6·1 (5)
C(14)	6742 (7)	−1163 (11)	6102 (15)	7·6 (5)
C(15)	9232 (7)	3336 (8)	3694 (13)	4·6 (4)
C(16)	9524 (7)	4027 (9)	2388 (14)	6·0 (4)
C(17)	9457 (8)	5255 (10)	2490 (16)	6·5 (5)
C(18)	9124 (7)	5803 (9)	3898 (14)	5·3 (4)

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

Discussion. Bond lengths and angles for both compounds are listed in Table 3. Molecular packing with atom numbering is shown in Figs. 2 and 3 for compounds (1) and (2), respectively. Fig. 4 illustrates the twisted conformation along the C—N bonds of (1) and (2).

Bond lengths and angles (Table 3) correspond to the given atom type and hybridization with the exception of the C(10)—C(11) bond of 1·360 (6) Å in (1). These C atoms exhibit somewhat higher temperature movement with $U_{eq} = 7{\cdot}5 \times 10^{-2}$ Å^2 (Table 1). C(10) is involved in a C—H···O type of interaction [C(10)···O(4), 3·247 (4) Å, $x-1, y, z$]. In general, the geometry of the pyridone skeleton in (1) is in good agreement with the values observed in 1-(*o*-aminophenyl)-2,6-dimethyl-4-

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and C—H bond lengths have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51286 (29 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. *Interatomic distances* (Å) *and angles* (°)

	Compound (1)	Compound (2)
Cl–C(8)	1·722 (3)	—
N(1)–C(2)	1·386 (4)	1·41 (1)
N(1)–C(6)	1·359 (4)	1·35 (1)
N(1)–C(7)	1·450 (4)	1·44 (1)
C(2)–C(3)	1·367 (4)	1·36 (1)
C(2)–C(13)	1·484 (5)	1·49 (1)
C(3)–O(3)	1·383 (4)	1·39 (1)
C(3)–C(4)	1·436 (5)	1·45 (1)
O(3)–C(14)	1·420 (4)	1·44 (1)
C(4)–O(4)	1·245 (4)	1·26 (1)
C(4)–C(5)	1·437 (5)	1·42 (1)
C(5)–C(6)	1·351 (5)	1·35 (1)
C(7)–C(8)	1·373 (5)	1·43 (1)
C(7)–C(12)	1·373 (5)	1·38 (1)
C(8)–C(9)	1·392 (5)	1·41 (1)
C(9)–C(10)	1·371 (6)	1·43 (2)
C(10)–C(11)	1·360 (6)	1·38 (2)
C(11)–C(12)	1·384 (5)	1·39 (1)
C(8)–C(15)	—	1·41 (1)
C(9)–C(18)	—	1·41 (2)
C(15)–C(16)	—	1·37 (2)
C(16)–C(17)	—	1·40 (2)
C(17)–C(18)	—	1·37 (2)
C(2)–N(1)–C(6)	120·6 (3)	120·2 (7)
C(2)–N(1)–C(7)	120·9 (2)	120·1 (8)
C(6)–N(1)–C(7)	118·5 (3)	119·7 (8)
N(1)–C(2)–C(3)	118·7 (3)	117·6 (9)
N(1)–C(2)–C(13)	117·5 (3)	118·0 (8)
C(3)–C(2)–C(13)	123·8 (3)	124·4 (9)
C(2)–C(3)–O(3)	117·9 (3)	117·0 (9)
C(2)–C(3)–C(4)	123·3 (3)	123·9 (9)
O(3)–C(3)–C(4)	118·8 (3)	119·1 (8)
C(3)–O(3)–C(14)	113·2 (2)	113·2 (7)
C(3)–C(4)–C(5)	113·9 (3)	114·2 (8)
C(3)–C(4)–O(4)	122·8 (3)	122·6 (9)
O(4)–C(4)–C(5)	123·3 (3)	123 (1)
C(4)–C(5)–C(6)	121·7 (3)	121·3 (9)
N(1)–C(6)–C(5)	121·7 (3)	122·8 (9)
N(1)–C(7)–C(8)	120·0 (3)	118·1 (8)
N(1)–C(7)–C(12)	119·3 (3)	120·3 (9)
C(8)–C(7)–C(12)	120·7 (3)	121·7 (8)
Cl–C(8)–C(7)	120·4 (2)	—
Cl–C(8)–C(9)	119·9 (3)	—
C(7)–C(8)–C(9)	119·7 (3)	117·9 (9)
C(7)–C(8)–C(15)	—	122·4 (8)
C(9)–C(8)–C(15)	—	119·7 (9)
C(8)–C(9)–C(10)	119·3 (4)	119·0 (9)
C(8)–C(9)–C(18)	—	120 (1)
C(10)–C(9)–C(18)	—	121·2 (8)
C(9)–C(10)–C(11)	120·5 (3)	121·4 (9)
C(10)–C(11)–C(12)	120·8 (4)	120 (1)
C(7)–C(12)–C(11)	118·9 (3)	120 (1)
C(8)–C(15)–C(16)	—	119·8 (9)
C(15)–C(16)–C(17)	—	120 (1)
C(16)–C(17)–C(18)	—	122 (1)
C(9)–C(18)–C(17)	—	118·7 (9)

pyridone hemihydrate (Bailey, Cox, Falshaw, Fenton, Grundy, Haigh & Philips, 1983); the lengthening of N(1)—C(2), 1·386 (4) Å (1), is also observed in the quoted structure with a mean value of 1·382 (3) Å (two independent molecules). However, in both the structures presented in this paper the C—N bonds are asymmetrical [N(1)—C(2), 1·386 (4) and N(1)—C(6), 1·359 (4) Å (1); N(1)—C(2), 1·41 (1) and N(1)—C(6), 1·35 (1) Å (2)]. The pyridone and aryl rings are planar within the limits of experimental error. The pyridone and aryl [phenyl in (1) and naphthyl in (2)] rings are not coplanar; they are twisted with dihedral angles 91·31 (9) (1) and 85·5 (3)° (2). Almost perpendicular orientation of these two rings is observed in 1-(*o*-aminophenyl)-2,6-dimethyl-4-pyridone hemihydrate, 89·7 and 85·5° (two independent molecules). Molecular packing in both structures is realized through C—H···O contacts between the carbonyl O(4) of the pyridone ring and the aromatic ring: O(4)···C(6), 3·269 (4) $(\frac{1}{2}+x, \frac{1}{2}-y-1, -z)$, O(4)···C(10), 3·247 (4)

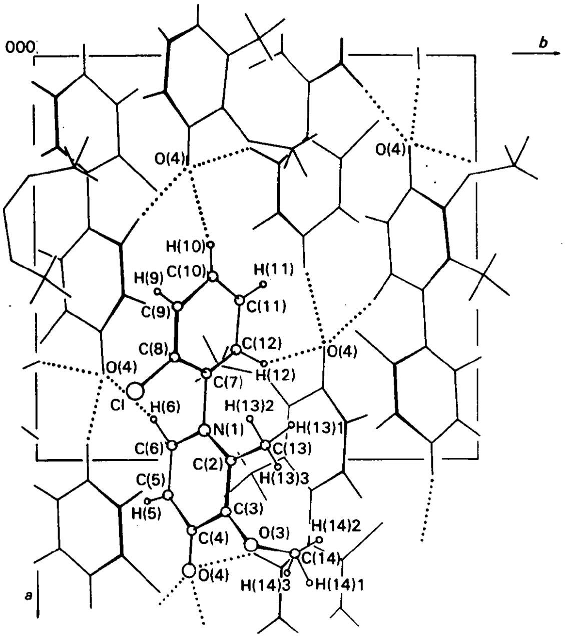


Fig. 2. Molecular packing of structure (1) viewed along **c**. The atom numbering is shown.

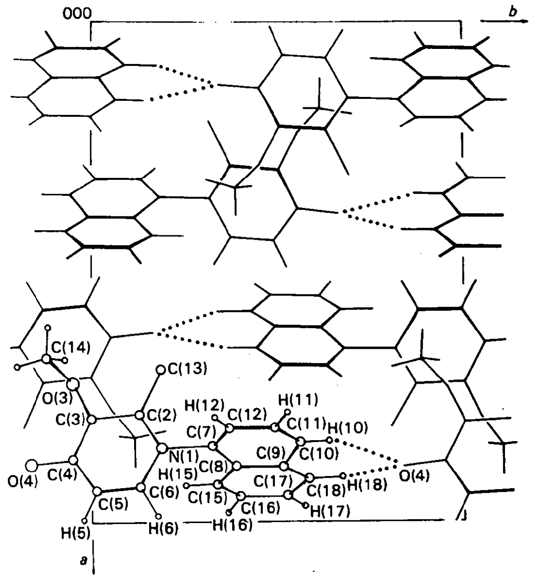
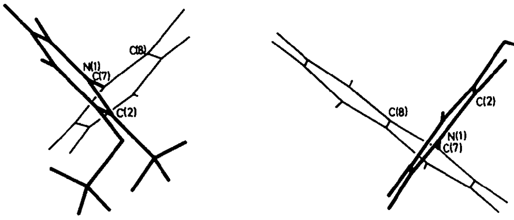


Fig. 3. Molecular packing of structure (2) viewed along **c** with the atom numbering.



Compound (1) Compound (2)

Fig. 4. Twisted conformation along C—N bonds of *N*-aryl-4-pyridones with torsion angles −89·4 (4) (1) and −95 (1)° (2) for the atom sequence C(2)—N(1)—C(7)—C(8).

(1+*x*, *y*, *z*), O(4)···C(12), 3·359 (4) Å (−*x*+2, *y*+1, −*z*) (1) (Fig. 2), and O(4)···C(10), 3·261 (1) (*x*, *y*−1, *z*), O(4)···C(18), 3·32 (1) Å (*x*, *y*−1, *z*) (2) (Fig. 3). Molecules connected by C—H···O interactions are joined into two-dimensional sheets at $c \simeq 0$ and 1 (Fig. 2). In (2) molecules are aligned into chains running in the **b** direction (Fig. 3).

The crystals used in this structure determination were prepared by Dr M. Mintas, Faculty of Technology, University of Zagreb. Support of this research by the Self-Management Council for Scientific Research of S. R. Croatia is gratefully acknowledged.

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Structure of Lamotrigine Methanol Solvate: 3,5-Diamino-6-(2,3-dichlorophenyl)-1,2,4-triazine–Methanol, a Novel Anticonvulsant Drug

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Abstract. $C_9H_7Cl_2N_5.CH_3OH$, $M_r = 288$, monoclinic, $P2_1/n$, $a = 15{\cdot}456$ (3), $b = 11{\cdot}736$ (2), $c = 7{\cdot}300$ (3) Å, $\beta = 94{\cdot}417$ (3)°, $V = 1320{\cdot}3$ (5) Å^3, $Z = 4$, $D_x = 1{\cdot}449$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 42{\cdot}52$ cm^{-1}, $F(000) = 592$, $T = 293$ K, $R = 0{\cdot}055$ for 2444 observed reflections. The phenyl and triazine aromatic rings make a dihedral angle of 80·6 (9)° with each other. The bond linking the two rings is 1·480 (3) Å. The structure is stabilized by a network of hydrogen bonds involving amino and ring N atoms, one of the Cl atoms and the methanol of crystallization.

Introduction. Lamotrigine [3,5-diamino-6-(2,3-dichlorophenyl)-1,2,4-triazine] (I) is a novel anticonvulsant chemically unrelated to current antiepileptic drugs. Studies (Lamb, Leach, Miller & Wheatley, 1985) suggest its usefulness for generalized seizures with a possible wider profile than current drugs of first choice (*i.e.* phenytoin and carbamazepine). It may also be useful for absence seizures (Jawad, Oxley, Yuen & Richens, 1985). Clinical studies on humans (Cohen, Ashby, Crowley & Peck, 1985) showed that lamotrigine produced no important side effects and indicated a more favourable central-nervous-system (CNS) side-effect profile than phenytoin. In addition to lamotrigine's potential therapeutic utility as an antiepileptic, it is also possible that the drug, by virtue of its ability to block the release of excitatory amino acids, may prove of therapeutic value in several CNS degenerative disorders possibly attributable to the neurotoxic action of such acids, *e.g.* brain ischaemia and stroke, Huntington's chorea and senile dementia (Meldrum, 1985). The structure analysis reported here was undertaken as part of a study of convulsant and

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