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1-(4-Decylphenyl)pyridin-4(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.129
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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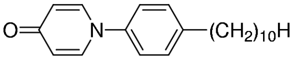
The title compound, $C_{21}H_{29}NO$, forms infinite one-dimensional molecular chains *via* weak C—H···O interactions. The hydrogen bonding may preclude the formation of π–π interactions.

Comment

Liquid crystals (LCs) with large birefringence are potential building blocks for incorporation into electro-optic devices including a number of different flat panel display configurations (Kuo & Suzuki, 2002). In addition, LCs are useful molecular units for applications utilizing polar order, such as photorefractivity (Marder *et al.*, 1997), pyroelectricity (Lang & Das-Gupta, 2000), and piezoelectricity (Pralle *et al.*, 2000) in thin organic films (TOFs); such films require non-centrosymmetric architectures. We are interested in developing TOFs with polar order through supramolecular self-assembly approaches (Dyer, Wolf *et al.*, 2003). With this goal in mind, hydrogen bonding (HB) emerges as an attractive building tool due to its robust binding strength, unique binding directionality, and dynamic reversibility. A series of molecules with the structure of HB–Donor···Linker···HB–Acceptor have already been designed and prepared (Landorf *et al.*, 2002), and their self-assembly and optical properties are under current investigations (Dyer, Li *et al.*, 2003). It has been shown that the HB strength and geometry will affect the ultimate microstructure and polar order in TOFs, thereby determining the corresponding macro-architecture and optical properties (Facchetti, Letizia *et al.*, 2004; Facchetti, Annoni *et al.*, 2004). A diverse range of HB units is therefore crucial for the design and optimization of such non-centrosymmetric HB–Donor···Linker···HB–Acceptor molecular structures. The compound 1-(4-decylphenyl)pyridin-4(1*H*)-one, (I), containing the highly polarizable 1*H*-pyridin-4-one heterocycle (hereafter referred to as C10A-pyridone), should exhibit highly anisotropic polarizability and calculations predict a large dipole moment (9.2 D). It is known that the 1*H*-pyridin-4-one heterocycle can participate in complex formation and intermolecular hydrogen bonding, therefore the pyridone moiety may prove useful in creating polar order in TOFs (Dyer *et al.*, 1997).



(I)

The pyridone ring is planar, the maximum deviation from its least-squares plane being 0.005 (2) Å (N1). The carbonyl O atom is coplanar with the pyridone ring, deviating from the ring plane by only −0.002 (2) Å. The benzene ring of the

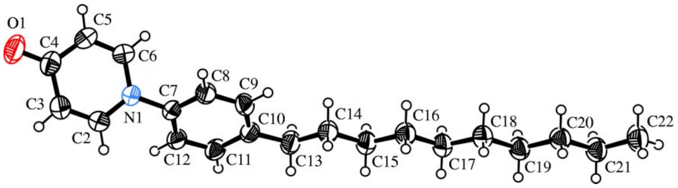


Figure 1
The molecular structure and atom-numbering scheme for (I), with displacement ellipsoids drawn at the 50% probability level.

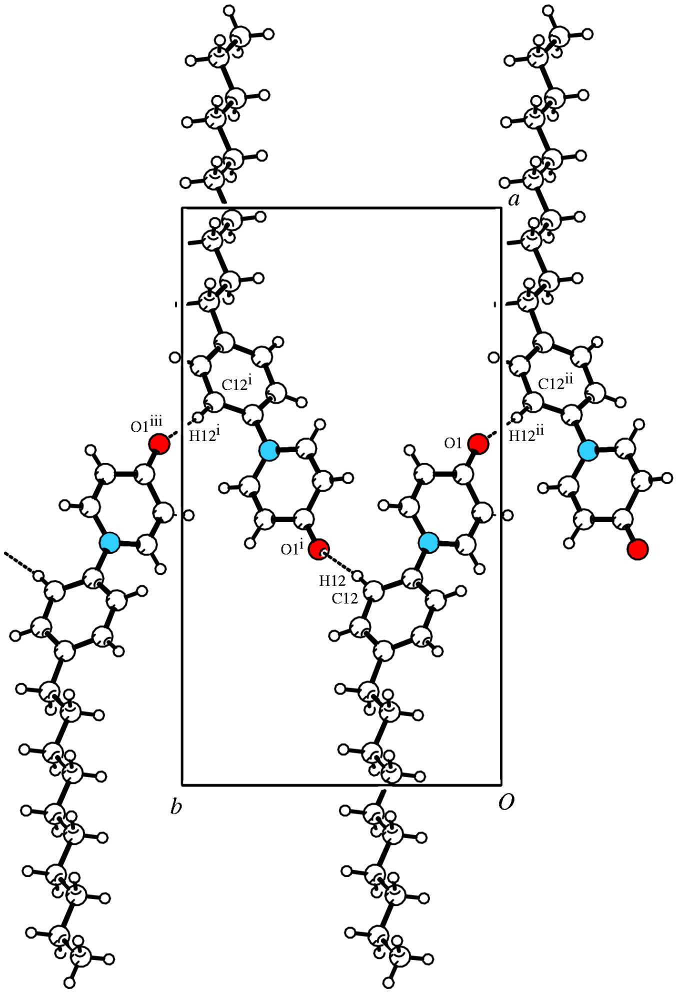


Figure 2
Hydrogen bonding in (I). The weak C—H···O bonds produce infinite molecular chains propagating in the *b*-axis direction. O and N atoms are colored red and blue, respectively. [Symmetry codes: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ii) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (iii) $x, 1 + y, z$.]

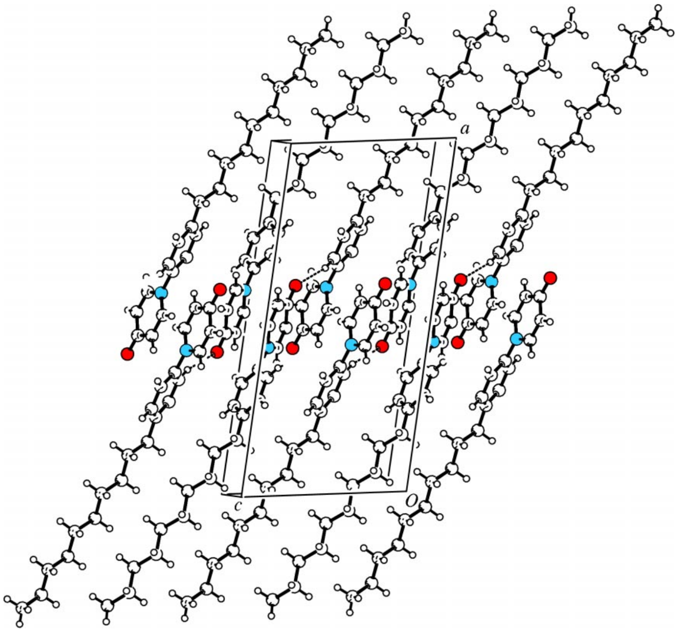


Figure 3
The molecular packing in (I). O and N atoms are colored red and blue, respectively; dashed lines represent hydrogen bonds.

aromatic core deviates rather more from planarity, the maximum deviation from its least-squares plane being 0.020 (2) Å (C7); the angle between the two least-squares planes is 50.39 (9)°. The long alkyl tail, with an 'all-*trans*' conformation, is twisted away from the benzene ring [C8—C9—C10—C13 = 175.2 (2)°] with a dihedral angle of 17.8 (3)° (C9—C10—C13—C14). In the crystal structure of the classic liquid crystal molecule 4-cyano-4′-octylbiphenyl (8CB) (Kuribayashi & Hori, 1998), the dihedral angle between the biphenyl rings is 39.12 (5)°, and the dihedral angle between the alkyl tail and the attached benzene ring is 34.92 (8)°. The similarities between the aromatic core structure of C10A-pyridone and 8CB suggests that the 1*H*-pyridin-4-one heterocycle should be an excellent rigid core for incorporation into rod-shaped liquid crystals.

Analysis of the molecular packing demonstrates weak C—H···O hydrogen-bonding interactions which form infinite polymeric chains along the *b*-axis direction as shown in Fig. 2. The C═O acts as the HB acceptor, and the C12 of the benzene ring as the HB donor. Such an asymmetric HB interaction, combined with the torsion between the pyridone and benzene rings, yields an asymmetric molecular geometry in the solid state even though the molecule itself is symmetrical. Details of the HB geometry are given in Table 2. The molecular packing, shown in Fig. 3, shows pairs of what appear to be potential π–π interactions involving the pyridone rings arranged about the center of the unit cell. *PLATON* (Spek, 2003) calculations show that these parallel ring pairs are quite close together (3.461 Å) when measured in a direction perpendicular to the planes. However, the slippage angle is 35.3°, which results in *ca* 2.45 Å of slippage and a centroid-to-centroid distance of 4.2382 (13) Å, values which appear to be out of the range of accepted π–π interactions. These data suggest that the C═O group of the pyridone ring could serve as an excellent HB acceptor, thus enabling robust interactions with HB donors such as benzoic acids and phenols.

Experimental

Chelidonic acid (2.02 g, 10 mmol) and 4-decylaniline (2.33 g, 10 mmol) were dissolved in dimethyl sulfoxide (10 ml), the solution was heated to 423 K under argon for 1 h, then the reaction mixture was heated to 453 K for an additional 30 min until gas evolution

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ceased. The mixture was cooled to room temperature, then distilled water (50 ml) was added and the mixture stirred overnight. The aqueous solution was extracted with chloroform. The combined organic layers were dried over anhydrous $MgSO_4$. The crude product was purified *via* column chromatography over silica gel (95/5 CH_2Cl_2–MeOH). The solid obtained after solvent evaporation was dissolved in MeOH and decolorized three times using activated charcoal. Pure crystals of compound (I) were obtained through recrystallization from toluene/hexane (1.51 g, 4.85 mmol, 48.5% yield). Single crystals of (I) were obtained by slow room-temperature evaporation of a dilute hexane/CH_2Cl_2 solution: R_F = 0.42 (95/5 CH_2Cl_2–MeOH); m.p. 335 K; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.57 (*d, J* = 7.8 Hz, 2H), 7.30 (*d, J* = 8.7 Hz, 2H), 7.23 (*d, J* = 8.7 Hz, 2H), 6.48 (*d, J* = 7.5 Hz, 2H), 2.65 (*t, J* = 7.8 Hz, 2H), 1.63 (*p, J* = 8.1 Hz, 2H), 1.26 (*m*, 14H), 0.88 (*t, J* = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 178.9, 143.7, 140.9, 139.2, 130.0, 122.6, 118.8, 35.3, 31.8, 31.3, 29.6, 29.5, 29.4, 29.3, 29.2, 22.6, 14.1. Anal calculated for $C_{21}H_{29}NO$: C 80.98, H 9.38, N 4.50%; found: C 80.53, H 9.47, N 4.51%. EI MS m/z = 311.3 (M^+). Quantum calculations were performed with *Gaussian03W* (Revision C.01) software (Frisch *et al.* 2004), at the DFT/UB3LYP level of theory with 6-31*G* basis set; energies were calculated on the *MP*2 level. DSC examination was performed on a DSC821^e from METTLER TOLEDO with a heating and cooling rate of 10 K min^{-1}.

Crystal data

$C_{21}H_{29}NO$
M_r = 311.45
Monoclinic, $P2_1/c$
a = 19.4607 (10) Å
b = 10.5889 (15) Å
c = 9.0394 (12) Å
β = 99.948 (8)°
V = 1834.7 (4) Å^3
Z = 4

D_x = 1.128 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 16.4–19.1°
μ = 0.07 mm^{-1}
T = 296 K
Prism, colorless
0.43 × 0.33 × 0.19 mm

Data collection

Rigaku AFC-5*S* diffractometer
ω scans
Absorption correction: none
3484 measured reflections
3254 independent reflections
1521 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.031

$\theta_{\rm max}$ = 25.0°
$h = -23 \rightarrow 22$
$k = -12 \rightarrow 0$
$l = 0 \rightarrow 10$
3 standard reflections every 100 reflections intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.129
S = 0.99
3254 reflections
210 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.14 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0107 (15)

Table 1
Selected bond lengths (Å).

O1—C4	1.247 (2)	N1—C7	1.441 (2)
N1—C2	1.363 (2)	C7—C12	1.380 (3)
N1—C6	1.365 (4)	C7—C8	1.379 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1$^{\rm i}$	0.93	2.37	3.279 (3)	166

Symmetry code: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$.

The rotational orientation of the methyl group was refined by the circular Fourier method available in *SHELXL*97 (Sheldrick, 1997). All H atoms were treated as riding with C—H distances ranging from 0.93 to 0.97 Å and $U_{\rm iso}$(H) values equal to 1.5 (methyl H atoms) or 1.2 (all other H atoms) times $U_{\rm eq}$ of the parent atom.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1996); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *PROCESS* in *TEXSAN* (Molecular Structure Corporation, 1997); program(s) used to solve structure: *SIR*92 (Burla *et al.*, 1989); program(s) used to refine structure: LS in *TEXSAN* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *TEXSAN, SHELXL*97 and *PLATON*.

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