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Crystal structure of 4-*n*-nonylbenzoic acid

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The title compound, 4-*n*-nonylbenzoic acid, $CH_3(CH_2)_8C_6H_4COOH$ (NBA), has been characterized thus: triclinic, $P1$, $a = 13.514(4)$ Å, $b = 23.4672(5)$ Å, $c = 7.658(3)$ Å, $\alpha = 90.914(3)°$, $\beta = 100.403(3)°$, $\gamma = 77.781(2)°$, $V = 2334(2)$ Å^3, $Z = 2$, and $F.W = 745.06$, $D_m = 1.161$ g cm^{-3}, $D_c = 1.061$ g cm^{-3}, $F_{000} = 816.00$, $\lambda = 0.71069$ Å, $\mu = 0.6$ cm^{-1}, goodness-of-fit is 1.029, final $R1 = 0.063$ and $wR2 = 0.16$.

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1. Introduction

The crystal structure studies of mesogens provide insight into the understanding of physical properties and phase transitions. In view of this a crystal structure study of 4-*n*-nonylbenzoic acid was undertaken. The compound melts into the nematic state at 97.7°C and into the isotropic phase at 114.8°C. The material exhibits a very small positive dielectric anisotropy and it has a very small dipole moment [1], as compared with other mesogens. The dielectric constant along the preferred direction (along the nematic director) is slightly greater than that in the transverse direction. The small value of the dielectric constant is due to the absence of a strongly polar end group. The dipole moment contributed by the COOH group is 1.7 D whereas the dielectric anisotropy is in the range 0.15–0.38 D. The dipole moment of the molecule is 0.40 D. 4-*n*-Nonyl benzoic acid in pure form is not used for electro-optic devices because of low birefringence, but there is a continued interest in nematic liquid crystals with low optical birefringence, as is evident from the work of Dalmolen *et al.* [2].

2. Experimental

Clear needle-shaped crystals of the title compound (Merck Ltd., England) were obtained from a solution in acetone. A crystal of approximate size $0.1 \times 0.1 \times 0.1$ mm^3 was mounted on a Rigaku AFC7S diffractometer equipped with a graphite monochromated MoK_α X-ray source ($\lambda = 0.71069$ Å). The unit cell parameters were obtained by using the method of short vectors followed by least squares refinement of 18 reflections. All reflections could be indexed with respect to a triclinic cell. Lorentz and polarization corrections were applied. The structure was solved using SHELXS-97 [3]. The structure solution did not yield any meaningful *E*-map in the space group $P\bar{1}$, even though the *E*-statistics showed better agreements of zonal and all data with the centrosymmetric system. A structure solution in $P\bar{1}$ did not give a good combined figure of merit. The resulting *E*-map did not reveal the complete structure nor could it be further expanded by a difference Fourier map after a few cycles of refinement.

Subsequently the structure was solved in the non-centric space group $P1$. The peak list from SHELXS-97 revealed all the phenyl rings and the side chains were revealed partially. The difference Fourier map showed the positions of all missing non-hydrogen atoms. The structure was refined by full matrix least-squares using SHELXL-97 [4], using 6002 unique reflections. The hydrogen atoms were generated at chemically acceptable positions and refined with isotropic thermal parameters assigned to them. 997 parameters were refined using 5352 observed reflections with $I > 2\sigma(I)$ to $R1 = 0.063$ and $wR2 = 0.16$. In the final difference map $\Delta\rho_{max} = 0.191$, $\Delta\rho_{min} = -0.203$ e Å^{-3}, and goodness-of-fit = 1.029. After the completion of the structure, the coordinates were checked for missing symmetry using BUNYIP [5]. No missing symmetry could be detected.

3. Results and discussion

The positional parameters and equivalent temperature factors for non-hydrogen atoms are given in table 1. Anisotropic parameters (U_{ij}) are listed in table 2. Tables 3 and 4 give the bond distances and angles. Figure 1

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Table 1. Atomic coordinates and U_{eq} of non-hydrogen atoms.

Atom	*x*	*y*	*z*	U_{eq}
O1A	0.8813(11)	0.2689(6)	0.7697(16)	0.113(4)
O2A	0.9867(11)	0.2275(6)	0.5825(15)	0.098(4)
C1A	0.9064(15)	0.2637(8)	0.616(3)	0.089(6)
C2A	0.8444(15)	0.3046(9)	0.467(2)	0.085(5)
C3A	0.8620(14)	0.2962(8)	0.295(2)	0.098(6)
C4A	0.8067(13)	0.3347(10)	0.156(3)	0.127(7)
C5A	0.7293(14)	0.3786(8)	0.189(2)	0.089(6)
C6A	0.7110(16)	0.3868(10)	0.361(3)	0.109(6)
C7A	0.7677(18)	0.3478(9)	0.491(2)	0.095(6)
C8A	0.6710(15)	0.4146(8)	0.035(2)	0.098(6)
C9A	0.7206(15)	0.4500(8)	− 0.062(2)	0.103(6)
C10A	0.6541(18)	0.4885(11)	− 0.218(3)	0.152(9)
C11A	0.716(2)	0.5214(14)	− 0.314(4)	0.228(15)
C12A	0.636(3)	0.5622(16)	− 0.458(4)	0.34(3)
C13A	0.670(3)	0.5812(14)	− 0.587(4)	0.229(14)
C14A	0.584(3)	0.620(2)	− 0.733(5)	0.30(3)
C15A	0.639(6)	0.634(3)	− 0.851(9)	0.41(5)
C16A	0.558(5)	0.682(2)	− 0.965(7)	0.40(3)
O1B	0.5800(11)	0.1074(7)	− 0.181(2)	0.122(5)
O2B	0.4761(15)	0.1515(8)	− 0.004(2)	0.143(6)
C1B	0.551(2)	0.1135(13)	− 0.033(3)	0.120(9)
C2B	0.6136(17)	0.0746(10)	0.120(3)	0.110(7)
C3B	0.5918(15)	0.0817(9)	0.285(3)	0.126(8)
C4B	0.6471(19)	0.0468(9)	0.425(3)	0.104(7)
C5B	0.7263(16)	0.0019(12)	0.401(3)	0.122(8)
C6B	0.7480(17)	− 0.0091(9)	0.238(4)	0.124(7)
C7B	0.6973(18)	0.0243(11)	0.088(3)	0.137(8)
C8B	0.7897(18)	− 0.0437(11)	0.561(3)	0.162(9)
C9B	0.729(2)	− 0.0766(12)	0.626(4)	0.206(13)
C10B	0.791(2)	− 0.1115(14)	0.773(4)	0.179(12)
C11B	0.756(2)	− 0.1428(12)	0.887(4)	0.206(15)
C12B	0.822(2)	− 0.1790(11)	1.061(4)	0.188(13)
C13B	0.783(4)	− 0.215(3)	1.157(9)	0.43(4)
C14B	0.849(4)	− 0.2418(13)	1.349(6)	0.30(3)
C15B	0.839(7)	− 0.277(3)	1.455(13)	0.54(6)
C16B	0.910(7)	− 0.302(3)	1.595(7)	0.38(7)
O1C	0.6204(11)	0.2423(6)	0.248(2)	0.112(4)
O2C	0.7202(12)	0.1992(7)	0.0593(19)	0.118(5)
C1C	0.650(2)	0.2350(10)	0.096(2)	0.096(8)
C2C	0.5723(17)	0.2764(9)	− 0.051(2)	0.089(6)
C3C	0.6000(14)	0.2717(8)	− 0.217(3)	0.096(6)
C4C	0.5399(15)	0.3045(10)	− 0.350(3)	0.126(8)
C5C	0.4484(15)	0.3479(9)	− 0.327(3)	0.096(7)
C6C	0.4265(16)	0.3513(10)	− 0.161(4)	0.112(7)
C7C	0.4858(17)	0.3171(9)	− 0.026(3)	0.104(7)
C8C	0.3780(16)	0.3817(8)	− 0.477(3)	0.124(7)
C9C	0.4164(15)	0.4216(9)	− 0.584(3)	0.115(7)
C10C	0.3385(17)	0.4552(10)	− 0.727(3)	0.148(9)
C11C	0.380(2)	0.4873(11)	− 0.846(3)	0.151(9)
C12C	0.300(2)	0.5177(13)	− 0.999(4)	0.206(13)
C13C	0.347(2)	0.5530(10)	− 1.128(4)	0.185(11)
C14C	0.283(3)	0.5832(15)	− 1.280(4)	0.229(19)
C15C	0.319(5)	0.624(3)	− 1.394(6)	0.39(4)
C16C	0.251(6)	0.656(3)	− 1.515(8)	0.47(4)
O1D	0.1104(11)	0.1664(5)	− 0.1456(18)	0.114(5)
O2D	0.0003(11)	0.2012(6)	0.0328(15)	0.099(4)
C1D	0.0885(17)	0.1709(9)	0.003(3)	0.098(6)
C2D	0.1531(15)	0.1351(8)	0.159(3)	0.098(6)

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Table 1. (*continued.*)

Atom	*x*	*y*	*z*	U_{eq}
C3D	0.1298(17)	0.1362(9)	0.319(2)	0.123(7)
C4D	0.201(2)	0.1047(10)	0.454(2)	0.119(8)
C5D	0.2995(15)	0.0732(9)	0.432(3)	0.106(7)
C6D	0.3182(17)	0.0758(10)	0.263(4)	0.130(10)
C7D	0.2494(15)	0.1071(8)	0.124(3)	0.106(7)
C8D	0.3735(16)	0.0448(9)	0.592(3)	0.149(9)
C9D	0.3429(17)	− 0.0013(10)	0.685(3)	0.136(7)
C10D	0.4218(17)	− 0.0288(10)	0.849(3)	0.134(7)
C11D	0.3861(17)	− 0.0696(11)	0.951(4)	0.161(9)
C12D	0.4641(18)	− 0.1011(10)	1.108(3)	0.144(8)
C13D	0.427(2)	− 0.1271(19)	1.227(4)	0.27(2)
C14D	0.493(3)	− 0.1661(12)	1.375(4)	0.208(14)
C15D	0.451(2)	− 0.198(2)	1.479(6)	0.42(4)
C16D	0.502(3)	− 0.226(2)	1.624(5)	0.33(2)
O1E	0.3518(11)	0.2102(7)	− 0.269(2)	0.127(5)
O2E	0.4634(15)	0.1734(8)	− 0.451(2)	0.127(5)
C1E	0.3829(19)	0.2045(9)	− 0.424(3)	0.094(7)
C2E	0.3088(17)	0.2370(9)	− 0.565(4)	0.100(8)
C3E	0.3327(16)	0.2380(9)	− 0.735(3)	0.103(7)
C4E	0.2691(16)	0.2680(9)	− 0.887(3)	0.120(7)
C5E	0.177(2)	0.2955(12)	− 0.862(3)	0.132(9)
C6E	0.1441(17)	0.3015(10)	− 0.701(4)	0.130(8)
C7E	0.214(3)	0.2697(12)	− 0.556(3)	0.141(11)
C8E	0.096(2)	0.3364(11)	− 1.021(3)	0.182(13)
C9E	0.109(2)	0.3842(13)	− 1.081(5)	0.268(19)
C10E	0.031(3)	0.4121(17)	− 1.231(5)	0.27(2)
C11E	0.057(3)	0.436(2)	− 1.356(5)	0.219(18)
C12E	− 0.009(3)	0.4580(15)	− 1.525(6)	0.213(16)
C13E	0.026(2)	0.5059(17)	− 1.612(5)	0.31(3)
C14E	− 0.029(2)	0.5306(15)	− 1.780(4)	0.207(13)
C16E	− 0.036(5)	0.606(3)	− 2.032(7)	0.48(5)
C15E	0.009(4)	0.579(2)	− 1.890(7)	0.42(4)
O1F	− 0.1598(12)	0.1341(6)	− 0.6769(18)	0.117(5)
O2F	− 0.2593(13)	0.1765(7)	− 0.4907(18)	0.117(4)
C1F	− 0.1789(16)	0.1405(10)	− 0.526(3)	0.109(7)
C2F	− 0.1230(18)	0.1030(9)	− 0.380(3)	0.104(7)
C3F	− 0.1412(16)	0.1061(10)	− 0.208(3)	0.114(7)
C4F	− 0.077(2)	0.0700(9)	− 0.068(2)	0.108(7)
C5F	0.010(2)	0.0362(12)	− 0.094(3)	0.124(9)
C6F	0.0327(16)	0.0297(9)	− 0.262(3)	0.109(7)
C7F	− 0.0288(16)	0.0633(9)	− 0.409(3)	0.105(6)
C8F	0.0861(18)	− 0.0073(12)	0.057(3)	0.157(10)
C9F	0.0425(19)	− 0.0449(12)	0.137(3)	0.156(9)
C10F	0.117(2)	− 0.0759(13)	0.303(4)	0.159(11)
C11F	0.075(2)	− 0.1099(14)	0.398(5)	0.201(16)
C12F	0.147(2)	− 0.1435(11)	0.564(4)	0.161(11)
C13F	0.112(3)	− 0.163(3)	0.686(6)	0.37(4)
C14F	0.189(3)	− 0.2031(13)	0.854(5)	0.231(17)
C15F	0.141(3)	− 0.244(2)	0.964(7)	0.34(2)
C16F	0.200(3)	− 0.2639(19)	1.115(6)	0.32(2)

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represents the ORTEP [6] diagram of one molecule of the asymmetric unit which comprises six molecules of NBA with thermal ellipsoids at 50% probability. Figures 2, 3 and 4 show the packing of molecules in the unit cell looking down the *a*, *b* and *c* axes respectively. Two molecules are bound into dimers through well defined hydrogen bonds, as is observed in the case of crystalline aggregates of fatty acids [7]. There is a possibility of cyclic dimer formation as well as an open dimer [8–10] see figure 5. A list of intermolecular and intramolecular

Table 2. Anisotropic displacement parameters for non-hydrogen atoms.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1A	0.106(11)	0.164(12)	0.071(8)	− 0.016(9)	0.039(8)	− 0.008(8)
O2A	0.093(9)	0.118(9)	0.073(8)	− 0.001(8)	0.014(8)	− 0.017(7)
C1A	0.070(14)	0.104(14)	0.101(16)	− 0.026(12)	0.026(13)	− 0.062(12)
C2A	0.072(12)	0.127(16)	0.061(11)	− 0.040(12)	0.003(11)	0.004(11)
C3A	0.093(13)	0.153(16)	0.054(9)	− 0.031(12)	0.032(10)	− 0.063(10)
C4A	0.057(12)	0.21(2)	0.102(15)	− 0.013(14)	− 0.010(12)	0.027(14)
C5A	0.065(12)	0.100(13)	0.093(14)	− 0.011(11)	0.003(11)	− 0.043(11)
C6A	0.110(16)	0.112(17)	0.104(15)	− 0.006(13)	0.037(13)	0.000(13)
C7A	0.114(17)	0.107(16)	0.078(12)	− 0.027(14)	0.052(13)	− 0.035(11)
C8A	0.085(14)	0.107(15)	0.098(13)	− 0.012(12)	0.015(12)	0.011(11)
C9A	0.112(15)	0.114(14)	0.095(12)	− 0.033(12)	0.039(12)	− 0.008(10)
C10A	0.124(17)	0.16(2)	0.17(2)	− 0.051(16)	− 0.016(16)	0.031(16)
C11A	0.21(3)	0.29(3)	0.22(3)	− 0.09(3)	0.07(2)	0.10(2)
C12A	0.36(4)	0.40(5)	0.22(3)	0.07(4)	0.11(3)	0.27(3)
C13A	0.28(4)	0.20(3)	0.17(2)	− 0.02(2)	− 0.01(2)	0.01(2)
C14A	0.27(3)	0.39(6)	0.25(4)	− 0.08(4)	0.01(3)	0.22(4)
C15A	0.52(11)	0.30(8)	0.32(10)	− 0.06(7)	− 0.10(8)	0.00(8)
C16A	0.53(7)	0.29(5)	0.34(6)	− 0.19(5)	− 0.15(5)	0.15(5)
O1B	0.103(11)	0.129(11)	0.128(12)	− 0.020(9)	0.014(9)	− 0.029(9)
O2B	0.124(14)	0.142(14)	0.160(15)	− 0.015(10)	0.038(12)	− 0.006(11)
C1B	0.12(2)	0.16(3)	0.091(16)	− 0.08(2)	− 0.004(17)	0.041(17)
C2B	0.086(17)	0.124(19)	0.14(2)	− 0.051(16)	0.037(16)	− 0.034(16)
C3B	0.087(14)	0.152(19)	0.144(17)	− 0.037(13)	0.014(13)	0.073(16)
C4B	0.140(19)	0.084(14)	0.112(15)	− 0.039(14)	0.067(15)	− 0.039(13)
C5B	0.086(16)	0.18(2)	0.129(18)	− 0.071(16)	0.060(15)	− 0.010(16)
C6B	0.095(17)	0.113(16)	0.16(2)	− 0.012(13)	0.020(18)	− 0.023(16)
C7B	0.107(18)	0.132(19)	0.16(2)	− 0.003(15)	0.007(16)	− 0.003(15)
C8B	0.14(2)	0.16(2)	0.17(2)	− 0.032(17)	− 0.013(19)	0.011(18)
C9B	0.16(2)	0.17(2)	0.26(3)	− 0.05(2)	− 0.06(2)	0.12(2)
C10B	0.23(3)	0.15(2)	0.17(3)	− 0.01(2)	0.09(2)	0.016(18)
C11B	0.23(3)	0.13(2)	0.19(3)	0.05(2)	− 0.03(3)	0.014(18)
C12B	0.15(2)	0.12(2)	0.30(4)	− 0.050(18)	0.04(3)	− 0.06(2)
C13B	0.26(5)	0.62(10)	0.49(12)	− 0.23(6)	0.09(6)	0.10(8)
C14B	0.38(7)	0.109(19)	0.37(5)	− 0.09(3)	− 0.11(5)	0.02(2)
C15B	0.48(12)	0.21(5)	0.90(18)	− 0.12(7)	0.01(11)	0.18(8)
C16B	0.55(18)	0.26(8)	0.29(6)	− 0.13(9)	− 0.09(7)	0.02(5)
O1C	0.085(9)	0.144(11)	0.110(10)	− 0.026(8)	0.021(8)	0.016(9)
O2C	0.105(11)	0.141(12)	0.106(10)	− 0.006(9)	0.036(8)	− 0.11(8)
C1C	0.14(2)	0.133(19)	0.056(11)	− 0.081(17)	0.056(14)	− 0.031(12)
C2C	0.098(17)	0.121(15)	0.057(11)	− 0.046(14)	0.010(11)	0.011(10)
C3C	0.053(12)	0.126(15)	0.103(16)	− 0.017(12)	− 0.003(12)	0.010(12)
C4C	0.044(12)	0.166(19)	0.15(2)	− 0.008(13)	− 0.008(13)	− 0.036(16)
C5C	0.075(15)	0.104(15)	0.104(16)	− 0.039(13)	− 0.023(13)	0.016(13)
C6C	0.079(14)	0.117(17)	0.137(19)	− 0.038(12)	− 0.010(15)	0.020(15)
C7C	0.094(16)	0.099(15)	0.14(2)	− 0.026(13)	0.061(15)	− 0.026(14)
C8C	0.123(16)	0.081(13)	0.155(19)	− 0.031(13)	− 0.017(16)	0.001(12)
C9C	0.094(14)	0.089(13)	0.152(17)	− 0.026(12)	− 0.013(14)	− 0.003(13)
C10C	0.099(16)	0.142(19)	0.17(2)	− 0.009(14)	− 0.037(17)	0.022(16)
C11C	0.14(2)	0.18(2)	0.118(14)	0.014(17)	0.023(15)	0.054(14)
C12C	0.16(2)	0.20(3)	0.22(3)	0.053(19)	0.02(2)	0.05(2)
C13C	0.22(3)	0.141(17)	0.21(3)	− 0.060(18)	0.03(2)	0.055(18)
C14C	0.27(4)	0.19(3)	0.17(3)	0.00(3)	− 0.07(3)	0.06(2)
C15C	0.42(8)	0.51(9)	0.22(4)	− 0.08(7)	− 0.03(4)	0.22(5)
C16C	0.75(13)	0.38(7)	0.32(7)	− 0.23(7)	0.07(8)	0.04(5)
O1D	0.144(13)	0.128(10)	0.081(9)	− 0.034(9)	0.041(9)	− 0.004(8)
O2D	0.103(10)	0.119(10)	0.074(8)	− 0.023(9)	0.015(8)	− 0.020(7)
C1D	0.099(16)	0.107(14)	0.091(16)	− 0.016(12)	0.028(14)	− 0.005(12)
C2D	0.069(13)	0.114(15)	0.086(15)	− 0.007(11)	− 0.033(11)	− 0.007(12)

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Table 2. (*continued.*)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3D	0.145(19)	0.146(16)	0.057(11)	0.005(14)	0.001(13)	0.031(11)
C4D	0.20(2)	0.139(18)	0.056(10)	− 0.088(18)	0.054(14)	− 0.010(11)
C5D	0.055(12)	0.115(16)	0.146(19)	− 0.004(11)	0.033(13)	0.002(14)
C6D	0.082(17)	0.13(2)	0.21(3)	− 0.054(15)	0.08(2)	− 0.066(19)
C7D	0.055(13)	0.111(14)	0.126(15)	0.015(11)	− 0.015(11)	0.031(11)
C8D	0.113(16)	0.155(18)	0.20(2)	− 0.084(14)	− 0.005(15)	0.084(16)
C9D	0.137(18)	0.130(16)	0.143(17)	− 0.038(14)	0.014(15)	0.043(13)
C10D	0.117(17)	0.131(16)	0.162(17)	− 0.030(13)	0.041(14)	0.035(13)
C11D	0.113(15)	0.144(17)	0.22(3)	− 0.039(15)	0.005(18)	0.016(18)
C12D	0.142(18)	0.128(17)	0.17(2)	− 0.047(14)	0.015(17)	0.046(14)
C13D	0.17(3)	0.47(6)	0.19(3)	− 0.09(3)	0.06(2)	0.12(3)
C14D	0.27(4)	0.17(2)	0.22(3)	− 0.09(2)	0.08(3)	0.01(2)
C15D	0.15(3)	0.74(9)	0.30(5)	0.10(4)	0.07(3)	0.32(6)
C16D	0.31(5)	0.48(6)	0.24(4)	− 0.21(4)	0.04(4)	0.07(4)
O1E	0.078(10)	0.173(15)	0.114(11)	− 0.009(9)	− 0.003(10)	− 0.005(11)
O2E	0.101(12)	0.133(13)	0.147(14)	− 0.014(11)	0.033(11)	− 0.013(10)
C1E	0.080(17)	0.075(13)	0.13(2)	− 0.037(12)	0.015(17)	− 0.034(14)
C2E	0.062(14)	0.097(15)	0.17(3)	− 0.030(12)	0.074(17)	− 0.027(15)
C3E	0.073(16)	0.110(16)	0.150(19)	− 0.047(13)	0.054(16)	− 0.054(14)
C4E	0.045(12)	0.139(17)	0.16(2)	0.004(11)	0.017(13)	0.001(14)
C5E	0.14(3)	0.17(2)	0.099(17)	− 0.10(2)	− 0.001(19)	− 0.026(16)
C6E	0.085(15)	0.17(2)	0.114(19)	− 0.005(14)	− 0.019(15)	0.001(16)
C7E	0.19(3)	0.17(2)	0.120(18)	− 0.12(2)	0.08(2)	− 0.080(17)
C8E	0.14(2)	0.18(2)	0.16(2)	0.04(2)	− 0.059(19)	− 0.077(19)
C9E	0.14(2)	0.15(2)	0.44(5)	− 0.03(2)	− 0.11(3)	0.08(3)
C10E	0.18(3)	0.27(4)	0.30(5)	− 0.08(3)	− 0.11(3)	0.16(3)
C11E	0.15(3)	0.26(5)	0.21(4)	0.02(3)	− 0.02(3)	− 0.01(3)
C12E	0.20(3)	0.15(3)	0.28(4)	− 0.02(2)	0.03(3)	0.02(3)
C13E	0.17(3)	0.28(4)	0.33(5)	0.10(3)	− 0.17(3)	− 0.11(3)
C14E	0.12(2)	0.28(3)	0.20(3)	− 0.02(2)	0.02(2)	− 0.02(2)
C16E	0.57(8)	0.42(8)	0.35(7)	0.20(7)	0.14(6)	0.19(6)
C15E	0.48(8)	0.53(8)	0.37(6)	− 0.36(7)	0.11(6)	0.07(5)
O1F	0.126(12)	0.145(12)	0.079(9)	− 0.019(9)	0.027(9)	− 0.026(8)
O2F	0.101(11)	0.129(11)	0.117(11)	− 0.014(9)	0.021(9)	− 0.031(8)
C1F	0.060(14)	0.114(17)	0.15(2)	− 0.017(13)	0.004(15)	0.044(16)
C2F	0.092(18)	0.089(15)	0.15(2)	− 0.041(14)	0.055(16)	− 0.052(15)
C3F	0.106(16)	0.143(19)	0.090(16)	− 0.015(14)	0.022(14)	− 0.003(15)
C4F	0.18(2)	0.102(15)	0.065(12)	− 0.044(15)	0.065(15)	− 0.024(11)
C5F	0.17(2)	0.15(2)	0.085(16)	− 0.08(2)	0.054(17)	− 0.029(15)
C6F	0.094(16)	0.098(14)	0.128(18)	0.002(12)	0.031(15)	− 0.007(13)
C7F	0.084(15)	0.120(16)	0.110(15)	− 0.029(14)	0.006(13)	− 0.002(13)
C8F	0.086(17)	0.22(3)	0.16(2)	− 0.008(17)	0.022(17)	0.042(18)
C9F	0.138(19)	0.19(2)	0.150(19)	− 0.046(18)	0.027(17)	0.058(17)
C10F	0.14(2)	0.16(2)	0.19(3)	− 0.052(19)	0.05(2)	0.02(2)
C11F	0.15(3)	0.14(3)	0.28(4)	− 0.02(2)	− 0.02(3)	− 0.01(3)
C12F	0.18(3)	0.14(2)	0.19(3)	− 0.08(2)	0.08(2)	− 0.035(19)
C13F	0.14(3)	0.70(12)	0.23(5)	− 0.04(4)	0.01(3)	− 0.06(5)
C14F	0.28(4)	0.19(2)	0.28(4)	− 0.13(3)	0.12(4)	− 0.03(2)
C15F	0.23(4)	0.39(7)	0.41(5)	− 0.13(4)	− 0.02(4)	0.06(5)
C16F	0.25(5)	0.37(5)	0.29(4)	− 0.07(4)	− 0.06(4)	0.02(3)

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hydrogen bonds [11] is given in table 5. These dimers are stacked in layers down two directions as can be seen from the packing diagrams. We should have expected the material to be smectic from the layering, but it exhibits the nematic phase only. This may be explained by the formation of open instead of cyclic dimers, by the breaking of one of the two hydrogen bonds that help in the formation of a cyclic dimer. In this compound there is only one hydrogen bond between molecules A and D, and C and F. In the case of a lower homologous

Table 3. Bond lengths (Å).

Atoms	Length	Atoms	Length
O1A–C1A	1.28(2)	C2C–C7C	1.38(2)
O2A–C1A	1.29(2)	C3C–C4C	1.33(3)
C1A–C2A	1.51(2)	C4C–C5C	1.46(3)
C2A–C7A	1.32(2)	C5C–C6C	1.35(3)
C2A–C3A	1.38(2)	C5C–C8C	1.48(2)
C3A–C4A	1.40(2)	C6C–C7C	1.34(3)
C4A–C5A	1.36(2)	C8C–C9C	1.48(2)
C5A–C6A	1.38(2)	C9C–C10C	1.48(3)
C5A–C8A	1.47(2)	C10C–C11C	1.45(3)
C6A–C7A	1.37(3)	C11C–C12C	1.52(3)
C8A–C9A	1.46(2)	C12C–C13C	1.59(3)
C9A–C10A	1.53(3)	C13C–C14C	1.42(3)
C10A–C11A	1.53(3)	C14C–C15C	1.51(5)
C11A–C12A	1.57(4)	C15C–C16C	1.31(8)
C12A–C13A	1.29(3)	O1D–C1D	1.23(2)
C13A–C14A	1.59(5)	O2D–C1D	1.31(2)
C14A–C15A	1.36(9)	C1D–C2D	1.50(3)
C15A–C16A	1.55(6)	C2D–C3D	1.32(3)
01B–C1B	1.27(3)	C2D–C7D	1.40(3)
O2B–C1B	1.24(3)	C3D–C4D	1.38(3)
C1B–C2B	1.51(3)	C4D–C5D	1.41(3)
C2B–C3B	1.35(3)	C5D–C6D	1.37(3)
C2B–C7B	1.50(3)	C5D–C8D	1.50(3)
C3B–C4B	1.36(3)	C6D–C7D	1.39(3)
C4B–C5B	1.37(3)	C8D–C9D	1.47(2)
C5B–C6B	1.34(3)	C9D–C10D	1.54(3)
C5B–C8B	1.63(3)	C10D–C11D	1.46(3)
C6B–C7B	1.39(3)	C11D–C12D	1.53(3)
C8B–C9B	1.40(3)	C12D–C13D	1.33(3)
C9B–C10B	1.43(4)	C13D–C14D	1.50(4)
C10B–C11B	1.36(3)	C14D–C15D	1.37(4)
C11B–C12B	1.60(4)	C15D–C16D	1.30(4)
C12B–C13B	1.37(5)	O1E–C1E	1.33(3)
C13B–C14B	1.63(6)	O2E–C1E	1.22(2)
C14B–C15B	1.21(8)	C1E–C2E	1.44(3)
C15B–C16B	1.34(9)	C2E–C7E	1.37(3)
O1C–C1C	1.291(19)	C2E–C3E	1.39(3)
O2C–C1C	1.20(2)	C3E–C4E	1.41(3)
C1C–C2C	1.58(3)	C4E–C5E	1.32(3)
C2C–C3C	1.38(2)	C5E–C6E	1.38(3)
C5E–C8E	1.65(3)	C2F–C7F	1.46(3)
C6E–C7E	1.43(3)	C3F–C4F	1.41(3)
C8E–C9E	1.28(4)	C4F–C5F	1.31(3)
C9E–C10E	1.47(4)	C5F–C6F	1.38(2)
C10E–C11E	1.25(4)	C5F–C8F	1.61(3)
C11E–C12E	1.46(4)	C6F–C7F	1.42(3)
C12E–C13E	1.51(5)	C8F–C9F	1.37(3)
C13E–C14E	1.42(4)	C9F–C10F	1.55(3)
C14E–C15E	1.63(4)	C10F–C11F	1.36(4)
C16E–C15E	1.26(6)	C11F–C12F	1.56(4)
O1F–C1F	1.23(2)	C12F–C13F	1.26(5)
O2F–C1F	1.30(2)	C13F–C14F	1.66(5)
C1F–C2F	1.43(3)	C14F–C15F	1.59(5)
C2F–C3F	1.38(3)	C15F–C16F	1.31(5)

member, viz. octylbenzoic acid [12] there is one hydrogen bond for one pair of molecules. This compound also exhibits the nematic phase instead of smectic as per the packing. The melting points and mesophase ranges of

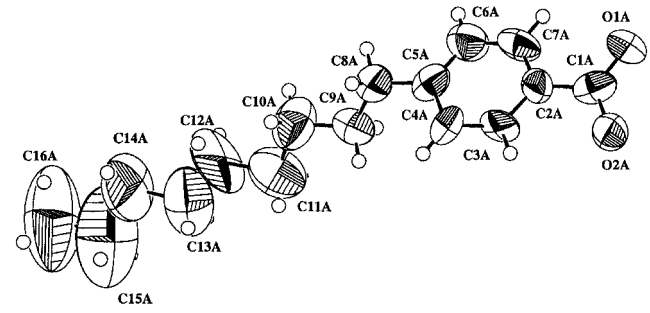

Figure 1. ORTEP of one 4-*n*-nonylbenzoic acid molecule at 50% probability.

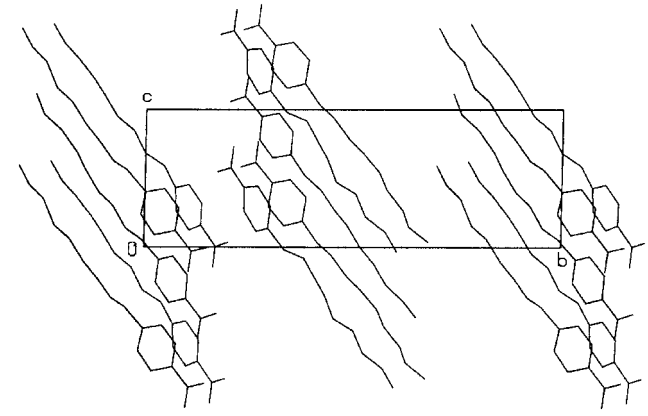

Figure 2. Packing of molecules down the *a*-axis.

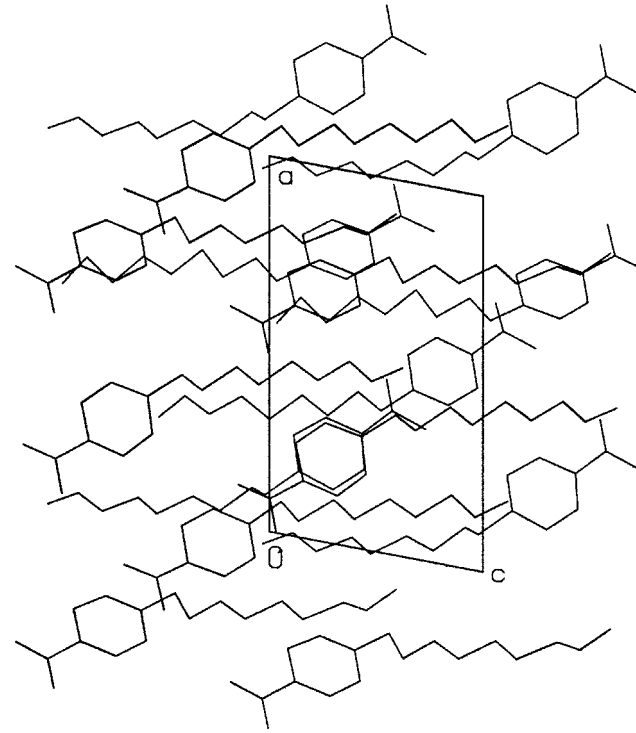

Figure 3. Packing of molecules down the *b*-axis.

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Table 4. Bond angles (°).

Atoms	Angle	Atoms	Angle
O1A–C1A–O2A	124(2)	C15B–C14B–C13B	135(6)
O1A–C1A–C2A	119.3(17)	C14B–C15B–C16B	127(9)
O2A–C1A–c2A	116.9(18)	O2C–C1C–O1C	128(2)
C7A–C2A–C3A	116.9(18)	O2C–C1C–C2C	121.2(16)
C7A–C2A–C1A	122.2(17)	O1C–C1C–C2C	111(2)
C3A–C2A–C1A	120.8(19)	C3C–C2C–C7C	119.6(18)
C2A–C3A–C4A	121.2(18)	C3C–C2C–C1C	113.9(19)
C5A–C4A–C3A	119(2)	C7C–C2C–C1C	126.4(19)
C4A–C5A–C6A	120(2)	C4C–C3C–C2C	119(2)
C4A–C5A–C8A	115.5(18)	C3C–C4C–C5C	122(2)
C6A–C5A–C8A	124.8(19)	C6C–C5C–C4C	116(2)
C5A–C6A–C7A	118.5(19)	C6C–C5C–C8C	121(2)
C2A–C7A–C6A	124.4(17)	C4C–C5C–C8C	122(2)
C9A–C8A–C5A	120.8(17)	C7C–C6C–C5C	122(2)
C8A–C9A–C10A	118.1(17)	C6C–C7C–C2C	121(2)
C9A–C10A–C11A	113.0(19)	C9C–C8C–C5C	119.8(18)
C10A–C11A–C12A	106(2)	C8C–C9C–C10C	115.3(18)
C13A–C12A–C11A	117(3)	C9C–C10C–C11C	114(2)
C12A–C13A–C14A	115(3)	C10C–C11C–C12C	114(2)
C15A–C14A–C13A	103(5)	C11C–C12C–C13C	113(2)
C14A–C15A–C16A	101(6)	C14C–C13C–C12C	120(3)
O2B–C1B–O1B	124(2)	C13C–C14C–C15C	123(3)
O2B–C1B–C2B	119(2)	C16C–C15C–C14C	118(6)
O1B–C1B–C2B	118(3)	O1D–C1D–O2D	122(2)
C3B–C2B–C1B	121(2)	O1D–C1D–C2D	122(2)
C3B–C2B–C7B	119(2)	O2D–C1D–C2D	114.6(19)
C1B–C2B–C7B	120(2)	C3D–C2D–C7D	122.8(18)
C2B–C3B–C4B	122(2)	C3D–C2D–C1D	125(2)
C3B–C4B–C5B	120(2)	C7D–C2D–C1D	112(2)
C6B–C5B–C4B	120(2)	C2D–C3D–C4D	118(2)
C6B–C5B–C8B	117(2)	C3D–C4D–C5D	123.9(18)
C4B–C5B–C8B	122(2)	C6D–C5D–C4D	114(2)
C5B–C6B–C7B	124(2)	C6D–C5D–C8D	127(2)
C6B–C7B–C2B	115(2)	C4D–C5D–C8D	119(2)
C9B–C8B–C5B	113.4(19)	C7D–C6D–C5D	124(2)
C8B–C9B–C10B	108(3)	C6D–C7D–C2D	116.8(19)
C11B–C10B–C9B	125(3)	C9D–C8D–C5D	116.9(17)
C10B–C11B–C12B	127(3)	C8D–C9D–C10D	114.6(18)
C13B–C12B–C11B	123(3)	C11D–C10D–C9D	114.2(19)
C12B–C13B–C14B	120(4)	C10D–C11D–C12D	116.2(18)
C13D–C12D–C11D	117(2)	C13E–C14E–C15E	123(3)
C12D–C13D–C14D	124(3)	C16E–C15E–C14E	129(5)
C15D–C14D–C13D	121(3)	O1F–C1F–O2F	123(2)
C16D–C15D–C14D	124(4)	O1F–C1F–C2F	123(2)
O2E–C1E–O1E	125(2)	O2F–C1F–C2F	114(2)
O2E–C1E–C2E	122(3)	C3F–C2F–C1F	126(2)
O1E–C1E–C2E	113(2)	C3F–C2F–C7F	117(2)
C7E–C2E–C3E	113(2)	C1F–C2F–C7F	116(2)
C7E–C2E–C1E	127(3)	C2F–C3F–C4F	122(2)
C3E–C2E–C1E	120(2)	C5F–C4F–C3F	121(2)
C2E–C3E–C4E	127(2)	C4F–C5F–C6F	120(2)
C5E–C4E–C3E	115(2)	C4F–C5F–C8F	124(2)
C4E–C5E–C6E	126(2)	C6F–C5F–C8F	115(3)
C4E–C5E–C8E	121(2)	C5F–C6F–C7F	122(2)
C6E–C5E–C8E	113(3)	C6F–C7F–C2F	117(2)
C5E–C6E–C7E	115(2)	C9F–C8F–C5F	116(2)
C2E–C7E–C6E	125(2)	C8F–C9F–C10F	112(2)
C9E–C8E–C5E	125(3)	C11F–C10F–C9F	115(3)
C8E–C9E–C10E	116(3)	C10F–C11F–C12F	117(3)
C11E–C10E–C9E	120(4)	C13F–C12F–C11F	122(3)
C10E–C11E–C12E	127(4)	C12F–C13F–C14F	121(3)
C11E–C12E–C13E	114(4)	C15F–C14F–C13F	118(3)
C14E–C13E–C12E	120(4)	C16F–C15F–C14F	114(4)

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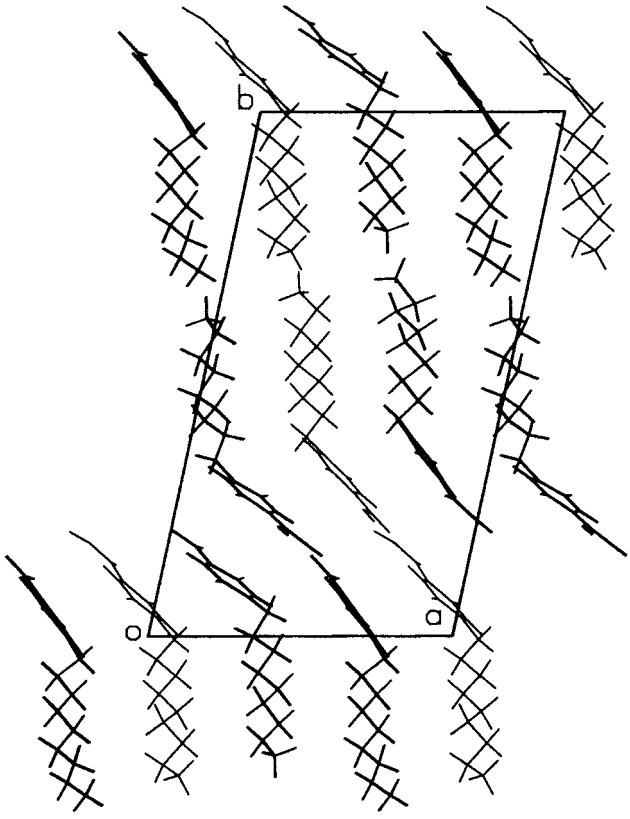

Figure 4. Packing of molecules down the *c*-axis.

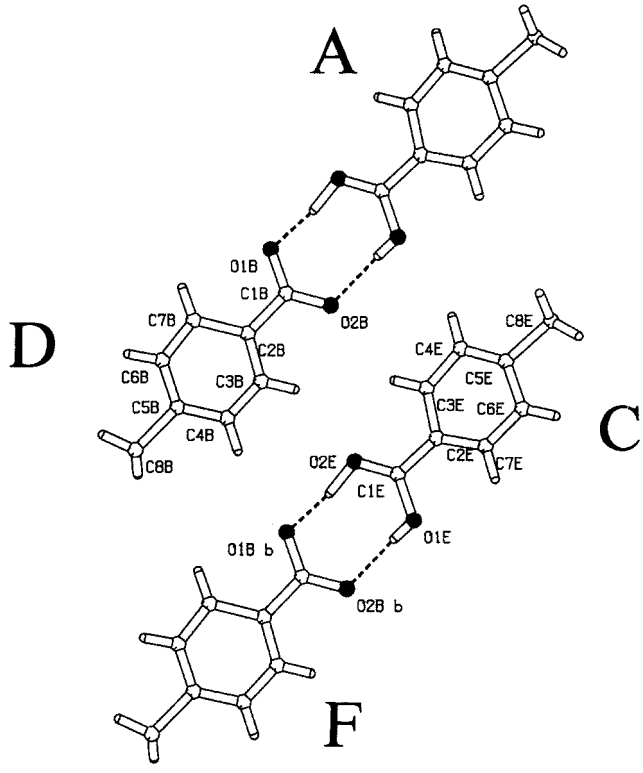

Figure 5. Cyclic dimer formation in 4-*n*-nonylbenzoic acid: hydrogen bonds are shown as dashed lines.

Table 5. Hydrogen bond distances and angles.

Atoms	Length/Å	Angle/°
O(2A)--H(1A)--O(2D)	3.478(16)	153.24
O(2E)--H(1B)--O(1B)	2.66(2)	161(16)
O(1C)--H(1C)--O(2F)	2.63(2)	172(11)
O(1E)--H(1E)--O(2B)	2.59(2)	175(16)
O(3B)--H(3B)--O(2E)	3.36(3)	142.71
C(3C)--H(3C)--O(2C)	2.78(3)	101.46
C(3E)--H(3E)--O(2E)	2.78(3)	100.78
C(7A)--H(7A)--O(1A)	2.84(2)	101.16
C(7D)--H(7D)--O(1D)	2.70(3)	100.67

the octyl and nonyl members may be understood in terms of the formation of cyclic and open dimers. The two benzene rings of the dimer are coplanar; alkyl chains are in an extended conformation. The dimer formation clearly explains the small dipole moment of this mesogen.

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