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Crystal structure of a cholesterol-based dimesogen

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The title compound, cholesteryl 6[4-(4-pentyloxyphenylethynyl)phenoxy]hexanoate (DMT5), a cholesterol-based dimesogen, crystallizes in the monoclinic space group $P2_1$ with the parameters $a = 9.812(3)$ Å, $b = 9.713(2)$ Å, $c = 24.179(2)$ Å, $\beta = 92.48(1)°$ $V = 2302.2(9)$ Å^3, $Z = 2$, $F_{000} = 836$, $\lambda(\mathrm{MoK}_\alpha) = 0.71069$ Å, $\mu = 0.067$ cm^{-1}, final $R = 0.0772$. The structure has intermolecular hydrogen bonds; it is stabilized by the presence of intermolecular contacts whose spacings are less than van der Waals' radii.

1. Introduction

Liquid crystalline dimers consisting of two identical mesogenic units connected linearly via a flexible spacer, such as polymethylene or oligosiloxyl group, are well known [1]. Compounds in which the chemical structures of the two mesogenic units are different have also been studied [2]. Such compounds, also called dimesogens, have been reported to exhibit an interesting polymorphic sequence including incommensurate smectic phases [3]. We previously synthesized a dimesogen referred to as DMT4, which has a cholesteryl ester unit and tolane moiety connected by a polymethylene (C_5) spacer. It shows just a single mesophase—a cholesteric phase having a wide temperature range of about 130° [4]. To get a better understanding of the effect of the length of the side chain on the mesophase, we have synthesized a number

Figure 1. ORTEP of the DMT5 molecule at 50% probability.

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of higher and lower homologues of DMT4. Owing to their exotic nature and properties, it will be interesting to look at the crystal structure of these dimesogens. In this paper we report the crystal structure of one of the homologues of DMT4, namely cholesteryl 6[4-(4-pentyl-oxyphenylethyn yl)phenoxy]hexanoate, DMT5 (figure 1). This compound melts to the cholesteric phase at 124.8°C and goes to the isotropic phase at 199.3°C. It is evident that this homologue has a greatly reduced mesophase range as compared with DMT4.

2. Experimental

The crystals were colourless. A sample of size $0.3 \times 0.3 \times 0.5\,mm^3$ was selected for data collection. The crystal was mounted on a glass fibre and the data collection was carried out on an Enraf-Nonius CAD4 single crystal X-ray diffractometer with graphite monochromated MoK_α radiation. Data were collected upto $2\theta = 50°$. The index ranges are as follows: $-11 \leqslant h \leqslant 11$, $0 \leqslant k \leqslant 11$, $0 \leqslant l \leqslant 28$. A total of 4308 reflections were collected of which 1597 has $I \geqslant 2\sigma(I)$. Lorentz and polarization corrections were applied. The structure was solved by direct methods (SHELXS-97 [5]). Structure was revealed in the first map; it was refined (SHELXL-97

Table 1. Crystal data and structure refinement details.

Empirical formula	$C_{52}H_{74}O_4$
Formula weight	763.11
Temperature	293(2) K
Wavelength	0.71060 Å
Crystal system	Monoclinic
Space group	$P2_1$
Cell dimensions	$a = 9.812(3)$ Å, $\alpha = 90°$ $b = 9.713(2)$ Å, $\beta = 92.485(15)°$ $c = 24.179(2)$ Å, $\gamma = 90°$
Volume	2302.2(9) Å^3
Z	2
Density (calculated)	1.101 Mg/m^3
Absorption coefficient	0.067 cm^{-1}
F_{000}	836
Crystal size	$0.3 \times 0.3 \times 0.5\,mm^3$
Theta range for data collection	1.69–48.97°
Index ranges	$-11 \leqslant h \leqslant 11$, $0 \leqslant k \leqslant 11$, $0 \leqslant l \leqslant 28$
Independent reflections	4308 [$R_{(int)} = 0.0000$]
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4308/1/566
Goodness-of-fit on F^2	0.879
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0772$, $wR2 = 0.1838$
R indices (all data)	$R1 = 0.1781$, $wR2 = 0.2236$
Absolute structure parameter	1(4)
Extinction coefficient	0.0034(15)
Largest diff. peak and hole	0.154 and −0.141 e Å^{-3}

Table 2. Atomic coordinates and equivalent isotropic temperature factors of non-hydrogen atoms.

Atom	X	Y	Z	U_{eq}
C1	−0.7742(16)	1.062(2)	−0.2202(8)	0.237(8)
C2	−0.7192(13)	0.9386(19)	−0.2078(6)	0.179(6)
C3	−0.6081(12)	0.9328(15)	−0.1618(6)	0.157(4)
C4	−0.5484(13)	0.8088(13)	−0.1535(6)	0.170(5)
C5	−0.4370(10)	0.8027(13)	−0.1077(4)	0.125(4)
C6	−0.3401(7)	0.9054(8)	−0.1184(2)	0.134(2)
C7	−0.2164(11)	0.8949(12)	−0.0882(4)	0.101(3)
C8	−0.1220(14)	0.9914(13)	−0.1012(4)	0.125(4)
C9	0.0052(11)	0.9946(12)	−0.0778(4)	0.111(3)
C10	0.0423(11)	0.8946(11)	−0.0377(3)	0.102(3)
C11	−0.0524(13)	0.7989(10)	−0.0239(4)	0.109(3)
C12	−0.1851(10)	0.7993(11)	−0.0510(4)	0.102(3)
C13	0.1774(10)	0.9001(10)	−0.0136(3)	0.105(3)
C14	0.2896(10)	0.9018(10)	0.0086(4)	0.102(3)
C15	0.4212(10)	0.9046(12)	0.0338(4)	0.099(3)
C16	0.5069(11)	1.0087(13)	0.0201(4)	0.105(3)
C17	0.6379(11)	1.0231(10)	0.0458(4)	0.104(3)
C18	0.6757(11)	0.9312(14)	0.0862(5)	0.120(4)
C19	0.5936(12)	0.8319(15)	0.1011(4)	0.122(4)
C20	0.4678(13)	0.8154(11)	0.0765(5)	0.118(3)
C21	0.7971(7)	0.9333(8)	0.1172(3)	0.130(2)
C22	0.8902(10)	1.0349(14)	0.1078(4)	0.135(4)
C23	1.0097(12)	1.0285(15)	0.1504(5)	0.153(4)
C24	1.0868(11)	0.9030(16)	0.1429(5)	0.157(4)
C25	1.1944(11)	0.8669(15)	0.1903(5)	0.159(5)
C26	1.3072(10)	0.9672(13)	0.1974(4)	0.139(4)
C27	1.4130(14)	0.928(2)	0.2394(5)	0.159(5)
C28	1.4211(14)	0.8202(16)	0.2568(6)	0.339(11)
C29	1.4211(8)	1.0148(8)	0.2540(3)	0.132(2)
C30	1.5973(9)	0.9881(10)	0.2972(4)	0.100(3)
C31	1.5886(8)	1.0988(10)	0.3381(4)	0.109(3)
C32	1.6971(8)	1.0783(9)	0.3850(3)	0.100(3)
C33	1.8432(7)	1.0749(8)	0.3652(3)	0.075(2)
C34	1.8476(9)	0.9747(10)	0.3173(3)	0.090(2)
C35	1.7363(9)	0.9890(11)	0.2721(3)	0.114(3)
C36	1.8806(9)	1.2183(9)	0.3448(3)	0.106(3)
C37	1.9398(7)	1.0284(7)	0.4133(3)	0.074(2)
C38	2.0817(7)	0.9828(9)	0.3931(3)	0.087(2)
C39	2.0602(8)	0.8616(10)	0.3535(3)	0.104(3)
C40	1.9434(10)	0.8808(11)	0.3133(4)	0.108(3)
C41	1.9548(8)	1.1289(9)	0.4602(3)	0.102(3)
C42	2.0565(8)	1.0879(8)	0.5075(3)	0.093(2)
C43	2.1945(7)	1.0555(7)	0.4859(3)	0.078(2)
C44	2.1708(7)	0.9437(8)	0.4426(3)	0.079(2)
C45	2.2577(9)	1.1872(9)	0.4651(4)	0.125(3)
C46	2.2972(7)	0.9790(8)	0.5259(3)	0.083(2)
C47	2.3880(8)	0.9013(11)	0.4869(3)	0.117(3)
C48	2.3143(8)	0.8920(13)	0.4310(4)	0.133(4)
C49	2.3790(9)	1.0554(10)	0.5707(4)	0.105(3)
C50	2.2883(11)	1.1408(10)	0.6080(4)	0.145(4)
C51	2.4669(9)	0.9595(11)	0.6052(4)	0.119(3)
C52	2.5775(10)	1.0217(11)	0.6429(5)	0.161(5)
C53	2.6534(10)	0.9159(13)	0.6783(4)	0.144(4)
C54	2.7645(14)	0.961(2)	0.7167(6)	0.201(7)
C55	2.858(2)	1.019(2)	0.6885(12)	0.42(2)
C56	2.8197(12)	0.837(2)	0.7478(5)	0.200(6)

Table 3. Anisotropic thermal parameters of the non-hydrogen atoms.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.186(15)	0.25(2)	0.270(18)	0.004(16)	− 0.038(13)	− 0.023(19)
C2	0.134(10)	0.202(16)	0.197(12)	− 0.001(11)	− 0.030(10)	− 0.026(13)
C3	0.139(9)	0.113(10)	0.215(12)	− 0.015(8)	− 0.033(9)	− 0.011(9)
C4	0.161(11)	0.102(9)	0.250(16)	− 0.043(10)	0.067(11)	− 0.043(10)
C5	0.102(7)	0.164(10)	0.106(7)	− 0.003(8)	− 0.026(6)	− 0.005(7)
C6	0.113(5)	0.169(7)	0.120(5)	− 0.036(5)	− 0.013(4)	0.026(5)
C7	0.114(8)	0.102(7)	0.086(6)	− 0.003(7)	0.004(6)	0.010(6)
C8	0.136(9)	0.121(10)	0.115(8)	0.011(9)	− 0.016(8)	0.035(7)
C9	0.107(7)	0.126(9)	0.100(7)	0.001(7)	− 0.007(6)	0.003(7)
C10	0.140(9)	0.099(7)	0.067(5)	0.031(8)	− 0.004(6)	− 0.007(6)
C11	0.152(10)	0.080(6)	0.097(7)	− 0.001(7)	0.035(7)	0.018(6)
C12	0.097(7)	0.108(8)	0.100(7)	− 0.002(6)	− 0.001(6)	0.019(7)
C13	0.104(7)	0.119(8)	0.090(6)	0.030(7)	− 0.018(6)	0.003(6)
C14	0.104(7)	0.105(7)	0.098(6)	0.019(6)	0.012(6)	− 0.011(5)
C15	0.092(7)	0.109(8)	0.096(7)	0.000(7)	− 0.005(6)	− 0.034(6)
C16	0.102(7)	0.123(9)	0.088(7)	0.021(7)	− 0.025(6)	− 0.011(6)
C17	0.129(9)	0.088(7)	0.095(7)	0.008(7)	0.006(6)	0.014(5)
C18	0.083(7)	0.152(11)	0.124(8)	− 0.044(8)	0.005(7)	− 0.015(8)
C19	0.083(7)	0.167(13)	0.113(8)	0.014(8)	− 0.034(7)	0.007(8)
C20	0.137(10)	0.107(8)	0.110(7)	0.000(7)	0.017(7)	0.010(7)
C21	0.084(4)	0.151(6)	0.153(6)	− 0.014(5)	0.007(4)	0.039(5)
C22	0.086(7)	0.194(12)	0.122(8)	0.020(8)	− 0.030(6)	0.002(8)
C23	0.151(10)	0.154(11)	0.157(10)	0.016(10)	0.049(8)	− 0.005(9)
C24	0.136(9)	0.165(12)	0.170(11)	− 0.009(10)	0.025(8)	− 0.013(10)
C25	0.115(7)	0.211(13)	0.148(9)	− 0.005(9)	− 0.041(7)	0.040(10)
C26	0.122(8)	0.152(10)	0.142(9)	− 0.015(8)	0.011(7)	0.010(8)
C27	0.142(10)	0.195(15)	0.134(8)	− 0.062(11)	− 0.049(8)	0.081(10)
C28	0.305(14)	0.273(15)	0.416(19)	− 0.173(13)	− 0.252(14)	0.190(14)
C29	0.116(5)	0.118(6)	0.160(6)	− 0.025(5)	− 0.034(5)	0.015(5)
C30	0.108(7)	0.087(6)	0.102(6)	− 0.003(6)	− 0.026(6)	0.006(6)
C31	0.082(6)	0.116(8)	0.130(7)	0.003(5)	0.006(5)	0.008(7)
C32	0.090(6)	0.096(6)	0.114(6)	0.001(5)	0.004(5)	0.018(6)
C33	0.068(5)	0.065(5)	0.092(6)	0.002(4)	0.016(4)	0.023(5)
C34	0.097(6)	0.100(7)	0.073(5)	− 0.009(6)	0.001(5)	− 0.003(6)
C35	0.118(7)	0.121(8)	0.101(6)	0.007(7)	− 0.007(6)	− 0.014(6)
C36	0.112(6)	0.092(6)	0.113(6)	0.002(5)	− 0.014(5)	0.031(5)
C37	0.080(5)	0.061(5)	0.083(5)	0.002(4)	0.024(4)	0.002(4)
C38	0.073(5)	0.086(6)	0.100(6)	− 0.006(5)	− 0.002(5)	0.012(5)
C39	0.093(6)	0.128(8)	0.093(6)	0.008(6)	0.013(5)	− 0.023(6)
C40	0.104(7)	0.125(8)	0.094(6)	0.014(7)	− 0.006(6)	− 0.011(6)
C41	0.095(6)	0.097(6)	0.116(7)	0.022(5)	0.013(5)	− 0.023(6)
C42	0.099(6)	0.078(6)	0.102(6)	0.006(5)	− 0.001(5)	− 0.019(5)
C43	0.079(5)	0.056(5)	0.099(5)	− 0.006(4)	0.013(5)	− 0.002(5)
C44	0.073(5)	0.079(6)	0.085(5)	0.018(4)	0.023(4)	− 0.003(5)
C45	0.130(7)	0.089(7)	0.152(7)	− 0.050(6)	− 0.026(6)	0.037(6)
C46	0.087(5)	0.067(5)	0.096(5)	0.002(5)	0.025(5)	− 0.015(5)
C47	0.103(6)	0.123(8)	0.127(7)	0.027(6)	0.012(6)	0.011(7)
C48	0.106(7)	0.180(11)	0.111(7)	0.042(7)	0.001(6)	− 0.025(7)
C49	0.116(7)	0.079(6)	0.120(7)	− 0.022(6)	− 0.009(6)	− 0.016(6)
C50	0.172(9)	0.100(7)	0.157(9)	0.023(7)	− 0.073(8)	− 0.039(7)
C51	0.106(6)	0.118(8)	0.131(7)	0.003(7)	− 0.009(6)	− 0.012(7)
C52	0.150(9)	0.121(9)	0.204(10)	− 0.049(8)	− 0.091(9)	0.017(8)
C53	0.112(7)	0.158(10)	0.160(9)	− 0.032(8)	− 0.021(7)	− 0.004(9)
C54	0.143(11)	0.247(19)	0.209(13)	0.001(12)	− 0.051(11)	0.096(14)
C55	0.24(2)	0.30(3)	0.70(5)	− 0.11(2)	− 0.14(3)	0.32(3)
C56	0.140(9)	0.31(2)	0.150(10)	0.009(12)	− 0.034(8)	− 0.006(13)

Table 4. BondLengths for non-hydrogen atoms.

Atoms	Length	Atoms	Length
C1–C2	1.344(19)	C30–C31	1.465(11)
C2–C3	1.524(15)	C30–C35	1.516(11)
C3–C4	1.351(15)	C31–C32	1.535(10)
C4–C5	1.525(15)	C32–C33	1.531(10)
C5–O6	1.410(11)	C33–C34	1.514(10)
O6–C7	1.393(10)	C33–C36	1.528(10)
C7–C12	1.319(12)	C33–C37	1.538(9)
C7–C8	1.364(13)	C34–C40	1.317(11)
C8–C9	1.349(13)	C34–C35	1.518(10)
C9–C10	1.407(12)	C37–C41	1.498(9)
C10–C11	1.367(12)	C37–C38	1.560(9)
C10–C13	1.426(12)	C38–C44	1.500(8)
C11–C12	1.433(12)	C38–C39	1.525(10)
C12–C14	1.204(11)	C39–C40	1.483(10)
C14–C15	1.404(12)	C41–C42	1.538(9)
C15–C16	1.366(13)	C42–C43	1.505(10)
C15–C20	1.408(13)	C43–C45	1.517(10)
C16–C17	1.410(12)	C43–C44	1.521(9)
C17–C18	1.364(13)	C43–C46	1.555(9)
C18–C19	1.317(14)	C44–C48	1.532(10)
C18–O21	1.378(10)	C46–C49	1.513(9)
C19–C20	1.357(15)	C46–C47	1.526(10)
O21–C22	1.370(12)	C47–C48	1.508(10)
C22–C23	1.528(12)	C49–C51	1.499(11)
C23–C24	1.451(15)	C49–C50	1.538(12)
C24–C25	1.564(12)	C51–C52	1.512(10)
C25–C26	1.478(14)	C52–C53	1.513(13)
C26–C27	1.471(14)	C53–C54	1.467(15)
C27–O28	1.130(15)	C54–C55	1.29(2)
C27–O29	1.205(14)	C54–C56	1.50(2)
O29–C30	1.443(9)		

Table 5. BondAngles for non-hydrogen atoms.

Atoms	Angle	Atoms	Angle
C1–C2–C3	117.6(15)	C30–C31–C32	110.1(8)
C4–C3–C2	115.7(13)	C31–C32–C33	113.6(7)
C3–C4–C5	115.8(11)	C34–C33–C36	108.9(6)
O6–C5–C4	107.9(9)	C34–C33–C32	108.1(7)
C7–O6–C5	115.6(8)	C36–C33–C32	108.9(7)
C12–C7–C8	120.1(9)	C34–C33–C37	110.6(6)
C12–C7–O6	125.5(10)	C36–C33–C37	111.3(6)
C8–C7–O6	114.4(9)	C32–C33–C37	108.9(6)
C9–C8–C7	122.9(10)	C40–C34–C33	123.1(8)
C8–C9–C10	118.7(11)	C40–C34–C35	120.3(8)
C11–C10–C9	118.7(9)	C33–C34–C35	116.6(8)
C11–C10–C13	123.7(10)	C30–C35–C34	110.1(7)
C9–C10–C13	117.6(11)	C41–C37–C33	114.7(6)
C10–C11–C12	119.9(9)	C41–C37–C38	111.3(6)
C7–C12–C11	119.7(9)	C33–C37–C38	112.0(6)
C14–C13–C10	177.4(10)	C44–C38–C39	111.4(7)
C13–C14–C15	179.3(11)	C44–C38–C37	108.6(6)
C16–C15–C14	118.2(11)	C39–C38–C37	108.4(6)
C16–C15–C20	116.7(9)	C40–C39–C38	113.3(8)
C14–C15–C20	124.8(12)	C34–C40–C39	124.9(9)
C15–C16–C17	121.7(10)	C37–C41–C42	115.7(6)
C18–C17–C16	117.8(10)	C43–C42–C41	111.1(7)
C19–C18–C17	121.6(10)	C42–C43–C45	109.0(7)
C19–C18–O21	112.8(11)	C42–C43–C44	106.0(6)
C17–C18–O21	125.5(11)	C45–C43–C44	115.2(7)
C18–C19–C20	121.5(11)	C42–C43–C46	116.9(6)
C19–C20–C15	120.7(11)	C45–C43–C46	110.2(6)
C22–O21–C18	119.2(8)	C44–C43–C46	99.4(6)
O21–C22–C23	110.9(10)	C38–C44–C43	115.9(6)
C24–C23–C22	109.8(11)	C38–C44–C48	116.5(6)
C23–C24–C25	115.8(11)	C43–C44–C48	104.2(6)
C26–C25–C24	114.5(10)	C49–C46–C47	112.3(7)
C25–C26–C27	114.3(10)	C49–C46–C43	121.3(7)
O28–C27–O29	120.3(13)	C47–C46–C43	103.4(6)
O28–C27–C26	122.2(16)	C48–C47–C46	108.3(6)
O29–C27–C26	117.5(14)	C47–C48–C44	103.0(6)
C27–O29–C30	121.4(10)	C51–C49–C46	111.6(7)
O29–C30–C31	107.3(8)	C51–C49–C50	110.0(7)
O29–C30–C35	108.7(7)	C46–C49–C50	112.4(7)
C31–C30–C35	110.2(7)	C49–C51–C52	117.9(8)
C51–C52–C53	113.1(9)	C55–C54–C56	111.2(15)
C54–C53–C52	119.4(11)	C53–C54–C56	108.8(15)
C55–C54–C53	108.6(16)		

[6]) by the method of full-matrix least-squares on F^2. Initial refinement was done with isotropic temperature factors for the non-hydrogen atoms which saturated at $R = 0.1548$. At this stage the hydrogens were placed at calculated positions and refinement was carried out with anisotropic temperature factors for the non-hydrogens. The hydrogens were treated as riding on the parent atom. The final cycle of the refinement was carried out with 4308 reflections with 566 parameters which saturated at $R = 0.0772$. The largest peak and the deepest hole in the final difference Fourier map were 0.154 and -0.141 e Å^{-3} respectively. Crystal data and refinement details are given in table 1.

3. Results and discussion

The final atomic coordinates with equivalent isotropic temperature factors are given in table 2 for non-hydrogen atoms. The anisotropic thermal parameters are listed in table 3. Tables 4 and 5 give bond lengths and bond angles, respectively, for non-hydrogen atoms. The ORTEP diagram of the molecule with 50% probability [7] is shown in figure 1. Figures 2–4 show the packing of the molecules down the *a*, *b* and *c* axes, respectively [8]. The bond distances and angles are in good agreement with the values for compounds containing phenyl and cholesterol moieties [9–11]. DMT5 crystallizes in the $P2_1$ space group, as in the case of a similar dimesogen, DM, 4-(cholesteroxycarbonyl)pentyloxy-4′-heptyloxycarbonylbiphenyl [12]. This indicates that the dimesogens should conform to either $P2_1$ or $P2_12_12_1$ space groups for them to exhibit a chiral mesophase. Intermolecular hydrogen bonds of the type CH … O are present, viz. C3-H3A … O6, with length 2.802(2) Å and C24-H24B … O21 with length 2.898(7) Å. The two phenyl rings are independently planar and are almost parallel as the dihedral angle between them is 4°. The

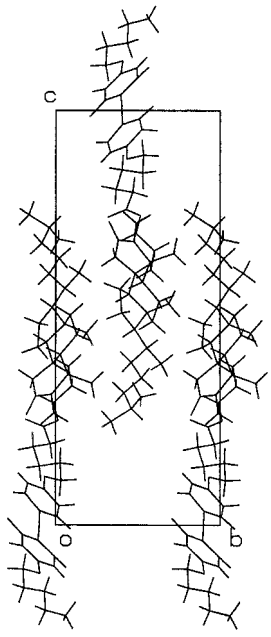

Figure 2. Packing of DMT5 molecules down the *a*-axis.

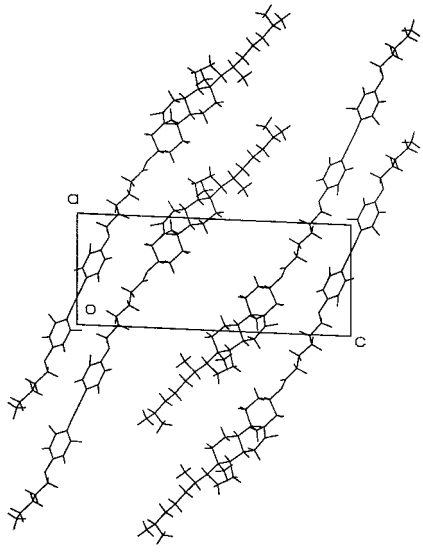

Figure 3. Packing of DMT5 molecules down the *b*-axis.

fused rings of the cholesterol moiety are almost perpendicular to the phenyl rings. The dihedral angles between the planes of the fused rings of the cholesterol moiety and the phenyl rings are 87.7° and 88.3°. This is in contrast to the structure of DM in reference [12] where the angles are 18.9° and 19.75°. Further the molecule is extended, unlike the molecule of DM. The deviations can be attributed to the presence of a triple bond between the phenyl groups which reduces the flexibility. The structure also has many intermolecular contacts closer than van der Waals' radii which stabilize the structure. The greater flexibility of DM results in the occurrence of multiple mesophases, unlike in this structure where only a single mesophase is exhibited.

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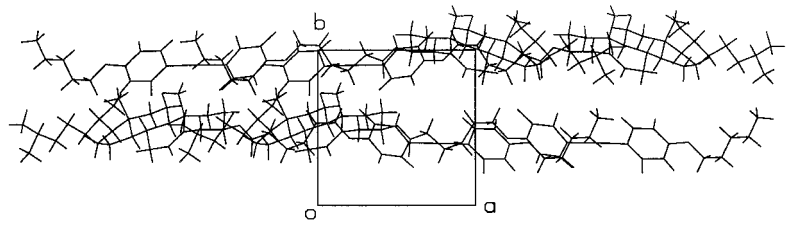

Figure 4. Packing of DMT5 molecules down the *c*-axis.