Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

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Online publication date: 06 August 2010

To cite this Article Surendranath, V. , Lokanath, N. K. , Sridhar, M. A. and Prasad, J. Shashidhara(1998) 'Crystal structure of di-(2,7-disubstituted-9 fluorenyl)glutamate', Liquid Crystals, 24: 3, 361 — 368
To link to this Article: DOI: 10.1080/026782998207163
URL: http://dx.doi.org/10.1080/026782998207163

LIQUID CRYSTALS, 1998, VOL. 24, NO. 3, 361–368

Crystal structure of di-(2,7-disubstituted-9 fluorenyl)glutamate

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(*Received 23 July 1997; accepted 6 August 1997*)

The title compound, di-(2,7-disubstituted-9 fluorenyl)glutamate, $C_{82}H_{86}O_{12}$, has been characterized thus: triclinic, $P\bar{1}$, $a=16{\cdot}173(5)$ Å, $b=16{\cdot}233(5)$ Å, $c=14{\cdot}320(5)$ Å, $\alpha=91{\cdot}124(5)°$, $\beta=105{\cdot}098(5)°$, $\gamma=92{\cdot}270(5)°$, $V=3625(1)$ Å^3, $Z=2$ and F.W.$=1248{\cdot}54$, $D_m=1{\cdot}125$ g cm^{-3}, $D_c=1{\cdot}169$ g cm^{-3}. $F_{000}=1356{\cdot}00$, λ(Mo-K_α)$=0{\cdot}71069$ Å, $\mu=0{\cdot}77$ cm^{-1}, final $R1$ and $\omega R2$ are 0·094 and 0·28 respectively.

1. Introduction

New exotic liquid crystals are being continuously synthesized for the generation of properties that are of great academic and technological interest. Here we report the structure of a nematogen, di-(2,7-disubstituted-9 fluorenyl)glutamate which is obtained by bridging two identical mesogens at their centres, a method for generating polymeric liquid crystals. This structural work will assist in the understanding of underlying molecular forces.

2. Experimental

A pale green prismatic crystal having the approximate dimensions $0{\cdot}20\times0{\cdot}10\times0{\cdot}15$ mm^3 was mounted on a glass fibre. All measurements were made on a Rigaku AFC7S diffractometer with graphite monochromated Mo-$K\alpha$ radiation.

Cell constants and an orientation matrix for data collection obtained from a least-squares refinement, using the setting angles of 17 carefully centred reflections in the range $13{\cdot}89<2\theta<15{\cdot}97°$, corresponded to a primitive triclinic cell. Based on statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be $P\bar{1}$.

The data were collected at a temperature of 20 ± 1°C using the ω–2θ scan technique to a maximum 2θ value of 50·0°. Of the 10179 reflections which were measured, 9682 were unique ($R_{int}=0{\cdot}101$). Over the course of data collection, the intensity of the standards decreased by 1·6%, and a linear correction factor was applied to the data to account for this phenomenon. Data were reduced by the teXsan data reduction program [1]; a semi-empirical absorption correction based on ψ-scans [1] was applied. The transmission factors range from 0·64 to 1·00. The data were corrected for Lorentz and polarization effects. The structure was solved by direct methods SHELXS86 [2].

All the non-hydrogen atoms were revealed in the first map. Full-matrix least-squares refinement based on 3205 observed reflections ($I>2\sigma(I)$) with isotropic

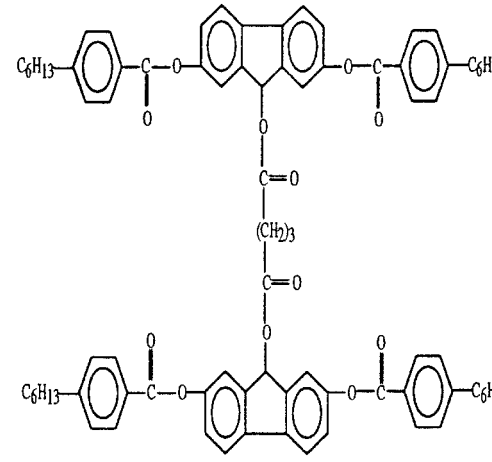

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Table 1. Atomic coordinates and U_{eq} of non-hydrogen atoms.

Atom	*x*	*y*	*z*	U_{eq}
C1A	−0·2980(13)	−0·7339(16)	0·3360(14)	0·292(11)
C2A	−0·2265(10)	−0·7405(18)	0·3669(20)	0·328(14)
C3A	−0·2000(13)	−0·6513(12)	0·3160(13)	0·317(12)
C4A	−0·1595(11)	−0·5924(9)	0·3562(11)	0·229(7)
C5A	−0·1182(9)	−0·5284(9)	0·3008(10)	0·232(7)
C6A	−0·0649(8)	−0·4725(7)	0·3545(8)	0·167(4)
C7A	−0·0160(8)	−0·4106(6)	0·3101(8)	0·113(3)
C8A	−0·0568(6)	−0·3625(6)	0·2363(7)	0·113(3)
C9A	−0·0121(5)	−0·3034(5)	0·1993(6)	0·099(2)
C10A	0·0753(5)	−0·2924(6)	0·2351(7)	0·092(2)
C11A	0·1152(6)	−0·3412(6)	0·3083(8)	0·112(3)
C12A	0·0697(8)	−0·4010(6)	0·3437(7)	0·122(3)
C13A	0·1262(6)	−0·2282(6)	0·2007(7)	0·105(3)
O14A	0·2039(4)	−0·2216(4)	0·2272(6)	0·184(3)
O15A	0·0820(3)	−0·1804(4)	0·1365(4)	0·104(2)
C16A	0·1143(4)	−0·1177(5)	0·0888(6)	0·087(2)
C17A	0·0613(5)	−0·0978(5)	0·0014(7)	0·099(2)
C18A	0·0805(5)	−0·0331(6)	−0·0528(6)	0·101(2)
C19A	0·1593(4)	0·0093(5)	−0·0149(6)	0·076(2)
C20A	0·2114(5)	−0·0085(5)	0·0698(6)	0·085(2)
C21A	0·1934(4)	−0·0729(5)	0·1264(6)	0·095(2)
C22A	0·1963(5)	0·0811(5)	−0·0543(6)	0·085(2)
C23A	0·2748(5)	0·1044(5)	0·0116(6)	0·090(2)
C24A	0·2891(4)	0·0511(4)	0·0993(5)	0·086(2)
C25A	0·1684(5)	0·1258(5)	−0·1366(6)	0·097(2)
C26A	0·2196(7)	0·1893(6)	−0·1557(6)	0·109(3)
C27A	0·2970(6)	0·2109(6)	−0·0920(7)	0·108(3)
C28A	0·3260(5)	0·1701(5)	−0·0076(6)	0·096(2)
O29A	0·3599(5)	0·2724(5)	−0·1138(5)	0·139(3)
C30A	0·3400(7)	0·3467(12)	−0·1151(7)	0·157(6)
O31A	0·2691(5)	0·3694(4)	−0·1032(5)	0·151(2)
C32A	0·4029(6)	0·4097(9)	−0·1308(6)	0·114(3)
C33A	0·3918(8)	0·4917(10)	−0·1207(8)	0·150(4)
C34A	0·4516(10)	0·5475(8)	−0·1304(7)	0·146(4)
C35A	0·5250(7)	0·5249(9)	−0·1503(6)	0·119(3)
C36A	0·5371(6)	0·4449(8)	−0·1594(7)	0·122(3)
C37A	0·4766(7)	0·3842(6)	−0·1499(6)	0·124(3)
C38A	0·5892(6)	0·5955(6)	−0·1589(7)	0·151(4)
C39A	0·5669(5)	0·6325(5)	−0·2578(7)	0·119(3)
C40A	0·6310(5)	0·6995(5)	−0·2702(7)	0·126(3)
C41A	0·6078(5)	0·7343(5)	−0·3672(6)	0·109(3)
C42A	0·6703(5)	0·8002(5)	−0·3831(8)	0·129(3)
C43A	0·6479(6)	0·8360(6)	−0·4812(8)	0·156(4)
O44A	0·3653(3)	0·0030(3)	0·1064(3)	0·098(2)
C45A	0·4398(6)	0·0377(7)	0·1614(7)	0·116(3)
O46A	0·4422(4)	0·1061(5)	0·2014(5)	0·163(3)
C47A	0·5110(6)	−0·0109(8)	0·1600(7)	0·162(4)
C1B	0·6155(8)	−0·9641(8)	0·6076(11)	0·222(7)
C2B	0·5907(7)	−0·8850(9)	0·6443(8)	0·180(5)
C3B	0·6112(6)	−0·8151(8)	0·5879(9)	0·169(4)
C4B	0·5922(7)	−0·7276(8)	0·6236(8)	0·166(4)
C5B	0·6257(5)	−0·6589(7)	0·5692(8)	0·145(4)
C6B	0·6145(7)	−0·5761(6)	0·5996(8)	0·151(4)
C7B	0·6592(6)	−0·5101(5)	0·5541(9)	0·111(3)
C8B	0·7324(6)	−0·4666(6)	0·6088(6)	0·114(3)
C9B	0·7731(5)	−0·4056(5)	0·5692(7)	0·096(2)
C10B	0·7436(4)	−0·3859(5)	0·4731(6)	0·082(2)
C11B	0·6707(5)	−0·4296(5)	0·4168(6)	0·099(2)
C12B	0·6307(5)	−0·4908(6)	0·4576(9)	0·121(3)
C13B	0·7843(5)	−0·3204(5)	0·4284(7)	0·094(2)
O14B	0·7641(4)	−0·3049(4)	0·3458(5)	0·129(2)

Table 1. (*continued*).

Atom	x	y	z	U_{eq}
O15B	0·8524(3)	−0·2818(3)	0·4942(3)	0·101(2)
C16B	0·9004(6)	−0·2182(6)	0·4602(5)	0·091(2)
C17B	0·9831(5)	−0·2338(5)	0·4588(5)	0·100(2)
C18B	1·0300(5)	−0·1706(6)	0·4278(5)	0·093(2)
C19B	0·9949(4)	−0·0974(6)	0·4002(5)	0·080(2)
C20B	0·9118(5)	−0·0829(5)	0·4072(5)	0·083(2)
C21B	0·8621(5)	−0·1441(6)	0·4375(5)	0·088(2)
C22B	1·0294(5)	−0·0232(5)	0·3621(5)	0·079(2)
C23B	0·9695(4)	0·0363(6)	0·3459(5)	0·079(2)
C24B	0·8891(4)	0·0059(5)	0·3786(5)	0·083(2)
C25B	1·095(5)	−0·0083(6)	0·3460(6)	0·097(2)
C26B	1·1258(5)	0·0648(6)	0·3080(7)	0·109(3)
C27B	1·0631(6)	0·1190(6)	0·2911(6)	0·104(3)
C28B	0·9824(4)	0·1090(5)	0·3076(5)	0·089(2)
O29B	1·0715(5)	0·2055(7)	0·2563(6)	0·185(5)
C30B	1·0965(8)	0·2054(7)	0·2002(10)	0·167(7)
O31B	1·1376(5)	0·1571(5)	0·1498(5)	0·178(3)
C32B	1·1125(7)	0·3007(6)	0·1446(11)	0·118(3)
C33B	1·1499(7)	0·3184(11)	0·0785(10)	0·151(5)
C34B	1·1513(7)	0·3931(12)	0·0470(8)	0·139(5)
C35B	1·1171(7)	0·4591(8)	0·0811(10)	0·124(3)
C36B	1·0773(7)	0·4424(10)	0·1562(12)	0·152(4)
C37B	1·0746(6)	0·3578(14)	0·1866(6)	0·137(4)
C38B	1·1232(8)	0·5392(8)	0·0312(11)	0·227(7)
C39B	1·1970(7)	0·5845(8)	0·0474(9)	0·179(5)
C40B	1·2016(9)	0·6634(8)	−0·0068(9)	0·201(5)
C41B	1·2854(9)	0·7022(8)	0·0128(10)	0·212(6)
C42B	1·2960(10)	0·7811(8)	−0·0344(10)	0·214(6)
C43B	1·3848(11)	0·8083(9)	−0·0220(12)	0·269(9)
O44B	0·8150(3)	0·0056(3)	0·2968(3)	0·0851(13)
C45B	0·7380(5)	0·0119(5)	0·3176(7)	0·098(2)
O46B	0·7353(3)	0·0188(4)	0·4016(5)	0·124(2)
C47B	0·6666(5)	0·0018(5)	0·2323(6)	0·120(3)
C48	0·5877(5)	0·0110(8)	0·2449(7)	0·199(6)

temperature factors for all the atoms converged the residuals to $R1=0{\cdot}124$ and $\omega R2=0{\cdot}5478$. At this stage, the hydrogen atoms were generated and placed at a distance of 0·98 Å from the parent atom. The isotropic temperature factors of the hydrogen atoms were set to 1·2 times the equivalent isotropic temperature factor of the parent atom; they were not refined. The non-hydrogen atoms were refined anisotropically. The final cycle of full-matrix least-squares refinement (SHELXL93[3]) was based on 3205 observed reflections ($I>2\sigma(I)$) and 939 variable parameters. The final residuals were $R1=0{\cdot}097$ and $\omega R2=0{\cdot}28$. In the final difference map, the maximum and minimum electron densities were 0·73 and $-0{\cdot}26\,e-\text{Å}^{-3}$ respectively.

3. Results and discussion

The final coordinates with equivalent isotropic temperature factors for all atoms are given in table 1. Anisotropic thermal parameters (U_{ij}) for non-hydrogen atoms are listed in table 2. Tables 3 and 4 give bond distances and angles of the non-hydrogen atoms, respectively. Table 5 lists the hydrogen bonds in the structure.

Figure 1 represents the ORTEP [4] diagram of the molecule. Figures 2, 3 and 4 show the packing of the molecules in the unit cell, which are projected down the *a*, *b* and *c* axes, respectively.

The bond distances and angles are in good agreement with those of other mesogenic materials containing either phenyl or cyclohexane rings [5]. Some disorder is observed in atoms O14A, C30A, C29B, C30B, C37B and C48. However, this trend is found in many of the structures of mesogenic materials reported in the literature [5]; this is attributed to geometrical anisotropy of the molecule. The crystalline cohesion is due to van der Waals interaction. The torsion angles indicate

Table 2. Anisotropic displacement parameters (Å^2) for non-hydrogen atoms.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1A	0·304(27)	0·370(26)	0·253(23)	0·021(19)	0·155(22)	0·051(28)
C2A	0·174(16)	0·415(31)	0·385(29)	0·129(23)	0·054(19)	−0·027(21)
C3A	0·450(30)	0·263(21)	0·272(22)	0·007(16)	0·187(20)	−0·196(20)
C4A	0·311(20)	0·149(12)	0·253(17)	0·001(11)	0·133(15)	−0·074(12)
C5A	0·304(16)	0·197(13)	0·190(13)	−0·015(10)	0·077(12)	−0·131(12)
C6A	0·216(12)	0·130(9)	0·179(11)	0·005(8)	0·100(10)	−0·015(8)
C7A	0·123(9)	0·118(8)	0·103(8)	−0·007(6)	0·040(7)	−0·006(7)
C8A	0·095(6)	0·132(8)	0·108(7)	−0·010(6)	0·027(6)	−0·025(6)
C9A	0·083(6)	0·101(6)	0·108(6)	−0·006(5)	0·015(5)	0·005(5)
C10A	0·067(6)	0·103(7)	0·099(6)	−0·021(5)	0·009(5)	0·002(5)
C11A	0·097(6)	0·110(7)	0·124(8)	−0·009(6)	0·021(6)	0·008(6)
C12A	0·144(10)	0·104(8)	0·116(7)	−0·007(6)	0·028(7)	0·018(7)
C13A	0·070(6)	0·106(7)	0·118(7)	−0·010(6)	−0·009(5)	−0·007(6)
O14A	0·090(4)	0·174(6)	0·256(8)	0·076(6)	−0·011(5)	−0·031(4)
O15A	0·067(3)	0·118(5)	0·119(5)	0·003(4)	0·015(3)	−0·018(3)
C16A	0·057(5)	0·102(6)	0·095(6)	−0·014(5)	0·009(5)	−0·002(4)
C17A	0·067(5)	0·119(7)	0·099(6)	−0·023(5)	0·003(5)	−0·008(5)
C18A	0·082(6)	0·124(7)	0·089(6)	−0·021(5)	0·011(5)	−0·004(5)
C19A	0·055(4)	0·097(6)	0·068(5)	−0·015(4)	0·000(4)	0·015(4)
C20A	0·076(5)	0·092(6)	0·088(6)	−0·007(5)	0·028(5)	−0·011(4)
C21A	0·063(5)	0·118(7)	0·094(6)	−0·025(5)	0·003(4)	−0·003(5)
C22A	0·080(5)	0·106(6)	0·065(5)	−0·011(5)	0·012(4)	0·002(5)
C23A	0·095(6)	0·096(6)	0·076(6)	−0·006(5)	0·020(5)	−0·002(5)
C24A	0·049(4)	0·099(6)	0·100(6)	−0·003(5)	0·004(4)	−0·009(4)
C25A	0·102(6)	0·101(6)	0·085(7)	−0·022(5)	0·022(5)	−0·012(5)
C26A	0·136(8)	0·110(7)	0·075(6)	−0·003(5)	0·016(6)	0·019(6)
C27A	0·128(8)	0·116(7)	0·082(7)	−0·012(6)	0·038(6)	−0·020(6)
C28A	0·110(6)	0·095(6)	0·080(6)	−0·011(5)	0·021(5)	−0·006(5)
O29A	0·157(6)	0·111(5)	0·131(5)	0·016(4)	0·007(4)	−0·017(5)
C30A	0·113(9)	0·281(19)	0·084(7)	−0·016(9)	0·033(6)	0·049(13)
O31A	0·148(6)	0·159(6)	0·157(6)	−0·029(4)	0·067(5)	−0·010(5)
C32A	0·080(7)	0·176(11)	0·087(6)	0·008(6)	0·032(5)	−0·061(7)
C33A	0·147(11)	0·166(12)	0·142(9)	−0·013(9)	0·051(7)	−0·021(9)
C34A	0·157(11)	0·153(11)	0·118(8)	−0·009(7)	0·018(8)	−0·001(10)
C35A	0·094(7)	0·179(13)	0·083(6)	0·011(7)	0·021(5)	−0·004(8)
C36A	0·114(8)	0·112(8)	0·143(8)	0·002(7)	0·034(6)	0·010(7)
C37A	0·117(8)	0·130(8)	0·122(7)	0·013(6)	0·031(6)	−0·034(7)
C38A	0·162(9)	0·136(8)	0·130(9)	0·014(7)	0·005(7)	−0·055(7)
C39A	0·119(7)	0·121(7)	0·112(7)	−0·018(6)	0·032(5)	−0·030(6)
C40A	0·131(8)	0·110(7)	0·125(8)	−0·027(6)	0·021(6)	−0·046(6)
C41A	0·091(6)	0·116(7)	0·121(7)	−0·005(6)	0·034(5)	−0·021(5)
C42A	0·107(6)	0·101(7)	0·173(10)	−0·007(6)	0·033(6)	−0·035(5)
C43A	0·120(8)	0·163(10)	0·199(11)	0·028(8)	0·073(8)	−0·028(7)
O44A	0·060(3)	0·114(4)	0·108(4)	−0·005(3)	0·007(3)	−0·027(3)
C45A	0·081(7)	0·156(10)	0·110(7)	−0·005(7)	0·025(6)	−0·018(7)
O46A	0·119(5)	0·178(7)	0·165(6)	−0·043(5)	0·001(4)	−0·043(5)
C47A	0·078(6)	0·261(13)	0·139(9)	0·007(8)	0·021(6)	−0·041(8)
C1B	0·237(15)	0·130(10)	0·307(19)	−0·042(11)	0·083(13)	0·035(10)
C2B	0·134(9)	0·219(14)	0·179(11)	0·072(11)	0·029(8)	−0·045(9)
C3B	0·130(8)	0·163(11)	0·202(12)	0·033(10)	0·027(8)	−0·042(8)
C4B	0·168(10)	0·150(10)	0·161(10)	0·028(8)	0·017(7)	−0·042(8)
C5B	0·098(6)	0·129(9)	0·207(11)	0·025(8)	0·038(7)	−0·015(6)
C6B	0·181(10)	0·106(8)	0·193(11)	0·012(7)	0·096(8)	−0·011(7)
C7B	0·104(7)	0·096(7)	0·143(9)	0·001(7)	0·050(7)	−0·004(6)
C8B	0·134(8)	0·115(7)	0·098(6)	0·000(6)	0·038(6)	0·011(6)
C9B	0·105(6)	0·086(6)	0·099(7)	0·000(5)	0·030(5)	−0·005(5)
C10B	0·083(5)	0·089(6)	0·072(6)	−0·012(5)	0·018(4)	0·001(4)
C11B	0·094(6)	0·096(6)	0·099(6)	0·004(5)	0·014(5)	−0·014(5)
C12B	0·095(6)	0·126(8)	0·138(9)	−0·013(7)	0·029(6)	−0·034(5)
C13B	0·092(6)	0·110(7)	0·084(6)	−0·015(6)	0·032(5)	−0·019(5)
O14B	0·159(5)	0·138(5)	0·081(4)	−0·008(4)	0·027(4)	−0·054(4)
O15B	0·097(4)	0·122(4)	0·076(3)	−0·010(3)	0·011(3)	−0·023(3)
C16B	0·096(7)	0·097(7)	0·072(5)	−0·009(5)	0·016(4)	−0·027(6)

Table 2. (*continued*).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C17B	0·079(6)	0·102(7)	0·112(6)	−0·040(5)	0·015(5)	0·002(5)
C18B	0·075(5)	0·100(7)	0·103(6)	−0·037(5)	0·026(4)	−0·017(6)
C19B	0·054(5)	0·096(7)	0·087(5)	−0·017(5)	0·013(4)	0·005(5)
C20B	0·072(5)	0·097(6)	0·076(5)	−0·031(4)	0·022(4)	−0·023(5)
C21B	0·078(5)	0·104(6)	0·082(5)	−0·015(5)	0·023(4)	−0·023(5)
C22B	0·063(5)	0·089(6)	0·079(5)	−0·026(4)	0·014(4)	−0·018(5)
C23B	0·050(4)	0·103(6)	0·084(5)	−0·031(4)	0·025(4)	−0·022(5)
C24B	0·051(4)	0·102(6)	0·089(5)	−0·008(4)	0·009(4)	−0·030(4)
C25B	0·067(6)	0·108(7)	0·121(7)	−0·025(5)	0·040(4)	−0·016(5)
C26B	0·054(5)	0·110(8)	0·168(8)	−0·032(6)	0·042(5)	−0·005(5)
C27B	0·096(7)	0·110(7)	0·110(6)	−0·015(5)	0·046(5)	−0·062(6)
C28B	0·069(5)	0·106(7)	0·099(6)	−0·025(5)	0·040(4)	−0·033(4)
O29B	0·107(5)	0·318(13)	0·144(7)	−0·059(7)	0·077(5)	−0·086(6)
C30B	0·151(11)	0·093(9)	0·198(13)	−0·110(10)	−0·061(9)	0·084(9)
O31B	0·176(7)	0·156(6)	0·202(7)	−0·024(5)	0·058(5)	−0·031(5)
C32B	0·073(6)	0·124(9)	0·142(10)	−0·034(8)	0·007(6)	−0·015(6)
C33B	0·107(8)	0·227(18)	0·125(10)	−0·040(9)	0·051(8)	−0·016(9)
C34B	0·131(8)	0·183(13)	0·119(8)	0·024(10)	0·064(6)	−0·020(10)
C35B	0·091(7)	0·123(9)	0·150(10)	−0·011(8)	0·016(6)	0·002(6)
C36B	0·105(8)	0·170(13)	0·180(12)	−0·074(9)	0·042(8)	0·018(8)
C37B	0·072(6)	0·256(15)	0·084(6)	−0·014(10)	0·031(5)	−0·036(9)
C38B	0·188(13)	0·142(10)	0·306(18)	0·067(11)	−0·015(11)	−0·044(9)
C39B	0·186(11)	0·177(12)	0·183(11)	−0·048(10)	0·076(9)	−0·063(10)
C40B	0·276(17)	0·153(11)	0·183(12)	0·018(9)	0·084(11)	−0·053(11)
C41B	0·274(17)	0·137(10)	0·240(15)	0·014(9)	0·108(13)	−0·076(10)
C42B	0·289(19)	0·172(13)	0·197(13)	0·007(10)	0·101(13)	−0·053(12)
C43B	0·329(22)	0·184(14)	0·286(19)	0·024(12)	0·076(17)	−0·082(15)
O44B	0·060(3)	0·106(4)	0·089(3)	−0·015(3)	0·024(3)	−0·013(2)
C45B	0·069(6)	0·123(6)	0·103(7)	−0·024(5)	0·031(6)	−0·019(4)
O46B	0·071(3)	0·187(6)	0·123(5)	−0·006(4)	0·041(3)	0·004(3)
C47B	0·066(5)	0·166(8)	0·120(7)	−0·013(6)	0·016(5)	−0·038(5)
C48	0·046(6)	0·395(18)	0·136(8)	−0·020(9)	−0·004(6)	−0·013(7)

Table 3. Bond lengths (Å).

Atoms	Length	Atoms	Length	Atoms	Length	Atoms	Length
C1A–C2A	1·14(2)	C23A–C28A	1·400(9)	C1B–C2B	1·487(14)	C23B–C28B	1·343(9)
C2A–C3A	1·72(3)	C23A–C24A	1·513(9)	C2B–C3B	1·482(12)	C23B–C24B	1·559(8)
C3A–C4A	1·19(2)	C24A–O44A	1·468(8)	C3B–C4B	1·569(14)	C24B–O44B	1·442(7)
C4A–C5A	1·55(2)	C25A–C26A	1·373(10)	C4B–C5B	1·534(11)	C25B–C26B	1·360(10)
C5A–C6A	1·312(13)	C26A–C27A	1·370(10)	C5B–C6B	1·437(11)	C26B–C27B	1·346(10)
C6A–C7A	1·505(12)	C27A–C28A	1·372(10)	C6B–C7B	1·518(11)	C27B–C28B	1·390(10)
C7A–C12A	1·345(11)	C27A–O29A	1·491(10)	C7B–C12B	1·385(11)	C27B–O29B	1·512(14)
C7A–C8A	1·367(11)	O29A–C30A	1·261(14)	C7B–C8B	1·394(11)	O29B–C30B	0·99(2)
C8A–C9A	1·375(10)	C30A–O31A	1·269(10)	C8B–C9B	1·378(10)	C30B–O31B	1·358(12)
C9A–C10A	1·375(9)	C30A–C32A	1·48(2)	C9B–C10B	1·382(9)	C30B–C32B	1·79(2)
C10A–C11A	1·365(10)	C32A–C37A	1·367(12)	C10B–C11B	1·400(9)	C32B–C33B	1·281(13)
C10A–C13A	1·472(11)	C32A–C33A	1·360(13)	C10B–C13B	1·471(10)	C32B–C37B	1·346(13)
C11A–C12A	1·379(11)	C33A–C34A	1·335(13)	C11B–C12B	1·384(10)	C33B–C34B	1·303(14)
C13A–O14A	1·215(9)	C34A–C35A	1·354(12)	C13B–O14B	1·178(8)	C34B–C35B	1·365(13)
C13A–O15A	1·299(9)	C35A–C36A	1·329(12)	C13B–O15B	1·369(8)	C35B–C36B	1·416(14)
O15A–C16A	1·396(8)	C35A–C38A	1·544(12)	O15B–C16B	1·435(8)	C35B–C38B	1·507(14)
C16A–C17A	1·372(9)	C36A–C37A	1·394(11)	C16B–C21B	1·380(10)	C36B–C37B	1·452(14)
C16A–C21A	1·417(9)	C38A–C39A	1·511(10)	C16B–C17B	1·376(10)	C38B–C39B	1·342(12)
C17A–C18A	1·390(9)	C39A–C40A	1·518(9)	C17B–C18B	1·400(9)	C39B–C40B	1·520(14)
C18A–C19A	1·396(9)	C40A–C41A	1·472(10)	C18B–C19B	1·357(9)	C40B–C41B	1·428(14)
C19A–C20A	1·329(8)	C41A–C42A	1·504(9)	C19B–C20B	1·403(9)	C41B–C42B	1·484(14)
C19A–C22A	1·476(10)	C42A–C43A	1·493(11)	C19B–C22B	1·481(9)	C42B–C43B	1·45(2)
C20A–C21A	1·402(9)	O44A–C45A	1·352(10)	C20B–C21B	1·397(9)	O44B–C45B	1·361(8)
C20A–C24A	1·518(9)	C45A–O46A	1·234(10)	C20B–C24B	1·539(9)	C45B–O46B	1·218(8)
C22A–C25A	1·379(9)	C45A–C47A	1·425(12)	C22B–C23B	1·375(9)	C45B–C47B	1·447(10)
C22A–C23A	1·403(9)	C47A–C48	1·518(11)	C22B–C25B	1·386(9)	C47B–C48	1·347(10)

Table 4. Bond angles (°).

Atoms	Angle	Atoms	Angle
C1A–C2A–C3A	93·2(25)	C22A–C23A–C24A	110·0(7)
C4A–C3A–C2A	127·7(19)	C28A–C23A–C24A	129·4(7)
C3A–C4A–C5A	121·4(16)	O44A–C24A–C23A	109·7(6)
C6A–C5A–C4A	116·0(12)	O44A–C24A–C20A	107·3(6)
C5A–C6A–C7A	121·2(11)	C23A–C24A–C20A	100·9(6)
C12A–C7A–C8A	118·6(10)	C26A–C25A–C22A	119·8(8)
C12A–C7A–C6A	119·9(12)	C25A–C26A–C27A	120·8(8)
C8A–C7A–C6A	121·5(11)	C28A–C27A–C26A	121·5(8)
C7A–C8A–C9A	121·0(8)	C28A–C27A–O29A	114·9(9)
C8A–C9A–C10A	120·3(8)	C26A–C27A–O29A	123·2(9)
C11A–C10A–C9A	118·0(9)	C27A–C28A–C23A	118·1(8)
C11A–C10A–C13A	119·3(8)	C30A–O29A–C27A	116·3(10)
C9A–C10A–C13A	122·7(9)	O31A–C30A–O29A	123·1(15)
C10A–C11A–C12A	121·0(9)	O31A–C30A–C32A	119·1(15)
C7A–C12A–C11A	120·9(10)	O29A–C30A–C32A	117·7(11)
O14A–C13A–O15A	121·8(9)	C37A–C32A–C33A	119·6(9)
O14A–C13A–C10A	123·1(9)	C37A–C32A–C30A	118·6(13)
O15A–C13A–C10A	115·0(8)	C33A–C32A–C30A	121·6(13)
C13A–O15A–C16A	126·7(6)	C34A–C33A–C32A	120·6(12)
C17A–C16A–O15A	115·1(7)	C33A–C34A–C35A	121·5(12)
C17A–C16A–C21A	120·0(8)	C36A–C35A–C34A	118·4(11)
O15A–C16A–C21A	124·7(8)	C36A–C35A–C38A	125·2(11)
C16A–C17A–C18A	122·9(7)	C34A–C35A–C38A	116·3(14)
C17A–C18A–C19A	116·0(7)	C35A–C36A–C37A	122·2(9)
C20A–C19A–C18A	122·2(8)	C32A–C37A–C36A	117·5(9)
C20A–C19A–C22A	109·2(7)	C39A–C38A–C35A	112·3(7)
C18A–C19A–C22A	128·5(8)	C40A–C39A–C38A	113·7(7)
C19A–C20A–C21A	123·1(7)	C41A–C40A–C39A	112·5(7)
C19A–C20A–C24A	112·2(7)	C40A–C41A–C42A	114·2(7)
C21A–C20A–C24A	124·7(7)	C43A–C42A–C41A	114·9(8)
C20A–C21A–C16A	115·8(7)	C45A–O44A–C24A	115·7(7)
C25A–C22A–C23A	119·2(8)	O46A–C45A–O44A	120·9(10)
C25A–C22A–C19A	133·3(7)	O46A–C45A–C47A	126·9(10)
C23A–C22A–C19A	107·5(7)	O44A–C45A–C47A	112·0(10)
C22A–C23A–C28A	120·6(8)	C45A–C47A–C48	111·9(10)
C3B–C2B–C1B	110·8(11)	C22B–C23B–C24B	110·0(7)
C2B–C3B–C4B	115·3(11)	O44B–C24B–C23B	108·9(5)
C5B–C4B–C3B	111·4(9)	O44B–C24B–C20B	110·5(5)
C6B–C5B–C4B	115·6(9)	C23B–C24B–C20B	101·3(6)
C5B–C6B–C7B	114·1(8)	C26B–C25B–C22B	118·4(8)
C12B–C7B–C8B	116·9(8)	C27B–C26B–C25B	117·2(8)
C12B–C7B–C6B	122·5(10)	C26B–C27B–C28B	127·5(8)
C8B–C7B–C6B	120·6(11)	C26B–C27B–O29B	124·8(8)
C9B–C8B–C7B	121·5(9)	C28B–C27B–O29B	107·6(9)
C8B–C9B–C10B	121·3(8)	C23B–C28B–C27B	113·2(8)
C9B–C10B–C11B	118·0(7)	C30B–O29B–C27B	110·9(13)
C9B–C10B–C13B	123·0(7)	O29B–C30B–O31B	142·4(17)
C11B–C10B–C13B	118·9(8)	O29B–C30B–C32B	119·7(12)
C12B–C11B–C10B	120·0(8)	O31B–C30B–C32B	97·1(13)
C7B–C12B–C11B	122·3(8)	C33B–C32B–C37B	122·3(12)
O14B–C13B–O15B	123·5(8)	C33B–C32B–C30B	132·1(15)
O14B–C13B–C10B	125·0(8)	C37B–C32B–C30B	105·7(16)
O15B–C13B–C10B	111·4(8)	C34B–C33B–C32B	121·1(13)
C13B–O15B–C16B	117·7(6)	C33B–C34B–C35B	125·1(12)
C21B–C16B–C17B	124·9(8)	C34B–C35B–C36B	115·3(10)
C21B–C16B–O15B	117·5(8)	C34B–C35B–C38B	116·0(16)
C17B–C16B–O15B	117·5(9)	C36B–C35B–C38B	128·6(17)
C18B–C17B–C16B	117·0(8)	C35B–C36B–C37B	117·6(10)
C19B–C18B–C17B	121·1(7)	C32B–C37B–C36B	118·4(10)
C18B–C19B–C20B	119·9(8)	C39B–C38B–C35B	121·7(11)
C18B–C19B–C22B	131·4(7)	C38B–C39B–C40B	120·3(12)

Table 4. (*continued*).

Atoms	Angle	Atoms	Angle
C20B–C19B–C22B	108·7(7)	C41B–C40B–C39B	114·2(12)
C21B–C20B–C19B	121·2(8)	C40B–C41B–C42B	118·3(13)
C21B–C20B–C24B	128·8(7)	C43B–C42B–C41B	113·6(14)
C19B–C20B–C24B	110·0(7)	C45B–O44B–C24B	116·1(5)
C16B–C21B–C20B	115·8(7)	O46B–C45B–O44B	119·7(7)
C23B–C22B–C25B	121·0(7)	O46B–C45B–C47B	127·7(7)
C23B–C22B–C19B	109·7(7)	O44B–C45B–C47B	112·4(7)
C25B–C22B–C19B	129·2(8)	C48–C47B–C45B	116·8(8)
C28B–C23B–C22B	122·5(7)	C47B–C48–C47A	118·0(9)
C28B–C23B–C24B	127·4(8)		

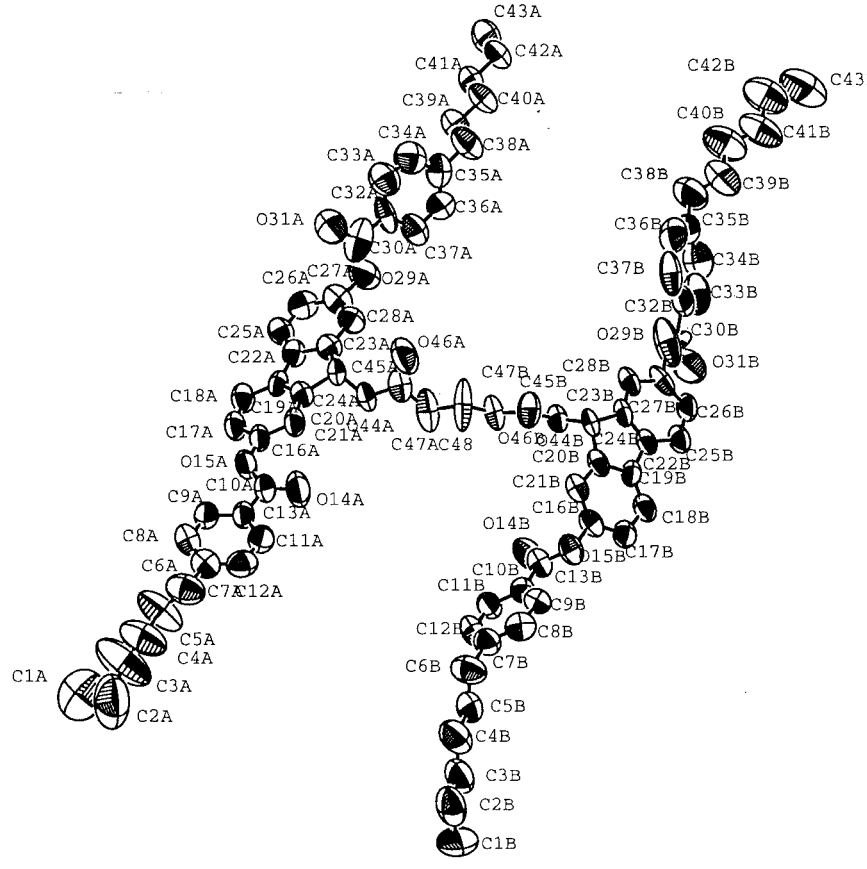

Figure 1. ORTEP of the molecule with 50% probability.

that the end chains assume extended conformation. The packing of molecules indicates strong imbrication about all axes. The results are consistent with the necessary requirement to form a nematic liquid crystal. Packing of molecules down the *a*-axis shows the stacking of molecules one above the other. The limbs of the bridged molecule penetrate into the limbs of the neighbouring molecules. All the phenyl rings are independently planar.

The authors would like to thank DST, Government of India for financial assistance under project No. SP/12/FOO/93.

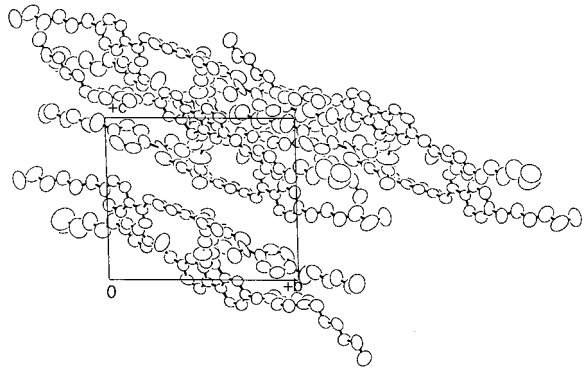

Figure 2. Packing of molecules down the *a*-axis.

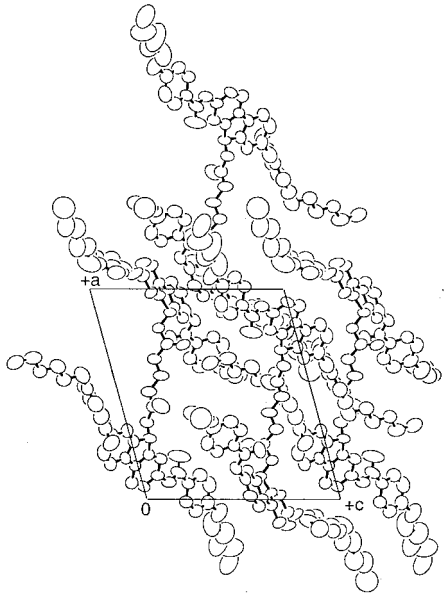

Figure 3. Packing of molecules down the *b*-axis.

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Table 5. Hydrogen bond lengths (Å) and angles (°).

Atoms	Length	Angle
C9A–H9A…O15A	2·767	98·41
C11A–H11A…O14A	2·813	98·43
C21A–H21A…O14A	2·825	110·78
C26A–H26A…O31A	3·028	88·62
C28A–H28A…O46A	3·304	122·88
C33A–H33A…O31A	2·812	98·45
C37A–H37A…O29A	2·720	98·33
C9B–H9B…O15B	2·727	100·39
C11B–H11B…O14B	2·838	96·65
C21B–H21B…O46B	3·376	120·63
C26B–H26B…O31B	2·784	102·99
C33B–H33B…O31B	2·847	97·60
C37B–H37B…O29B	2·688	104·47
C48–H48A…O46A	2·805	108·17
C48–H48B…O46B	2·815	93·58
C8A–H8A…O31A	3·462	164·64
C26A–H26A…O14B	3·396	150·45
C25A–H25A…O44B	3·172	93·35
C17A–H17A…O31B	3·465	151·45
C40A–H40A…O46A	3·621	139·37
C4B–H4B…O14A	3·568	119·45
C1B–H1B…O46A	3·882	156·83
C3B–H3B…O14A	3·461	118·01
C34B–H34B…O31A	3·250	154·99

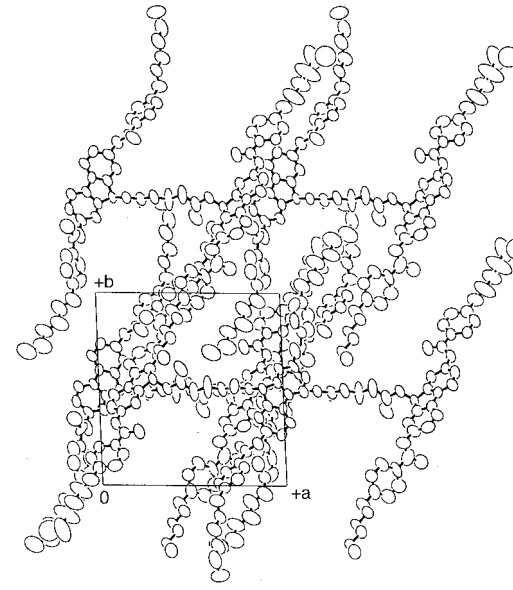

Figure 4. Packing of molecules down the *c*-axis.