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Unit cell dimensions and space groups of some liquid crystals

M M M Abdoh [a] , Srinivasa [a] , N C Shivaprakash [a] & J Shashidhara Prasad [a]
[a] Department of Physics, Univeristy of Mysore, Mysore, 570 006, India
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UNIT CELL DIMENSIONS AND SPACE GROUPS OF SOME LIQUID CRYSTALS

M M M ABDOH, SRINIVASA, N C SHIVAPRAKASH and J SHASHIDHARA PRASAD
Department of Physics, University of Mysore, Mysore 570 006, India.

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It is now very well established that for a proper understanding and interpretation of several physical properties of liquid crystalline phases, a knowledge of the molecular structure in the crystalline state is very useful, as the molecular conformation in the crystalline state predetermines the molecular organisation in the mesomorphic state. Also, it is believed that the stabilisation of liquid crystalline phase and hence the micro variations in the physical properties depend strongly on the long side chains and are essentially independent of the central rigid core. In view of this, we communicate the preliminary crystallographic data for some liquid crystalline materials, the detailed structure of which has been taken up.

The compounds for which the crystal data are presented, are listed below.

(1) Trans-4-propyl cyclohexyl-4-(trans-4-pentyl cyclohexyl)benzoate (TPPEB)
(2) Trans-4-butyl-(trans-4-cyanophenyl) cyclohexane (TBCC)
(3) Cholesteryl cinnamate (CC)

The first two compounds manufactured by E.Merck, West Germany were gifted by Prof A.Bauer. Cholesteryl cinnamate was purchased from Varilight Corporation, USA. Crystals of the samples were grown by successive recrystallization.

Oscillation and Weissenberg photographs were taken using CuK_α radiation(λ= 1.5418Å). The density was measured by flotation technique in a solution of potassium iodide. The data are presented in Table I.

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Table I: Crystal data

		TPPEB	TBCC	CC
Chemical formula		$C_{27}H_{42}O_2$	$C_{17}H_{23}N$	$C_{36}H_{52}O_2$
Molecular weight		398.61	241.36	516.80
Solvent		Acetone	Benzene	Acetone+ Toluene
Unit cell dimensions	a	14.52(1)Å	8.923Å	28.38(1)Å
	b	10.94(1)Å	9.246Å	10.14(1)Å
	c	7.00(1)Å	9.470Å	9.95(1)Å
		90.00(2)°	82.75(2)°	90.00(2)°
		97.00(2)°	88.89(2)°	81.00(2)°
		85.0(2)°	76.37(2)°	90.00(2)°
Volume of unit cell	v	1099.32Å^3	753.23Å^3	2828.09Å^3
No.of molecules in the unit cell	z	2	2	4
Density	d_m	1.199	1.195	1.239
($Mg\ m^{-3}$)	d_c	1.204	1.199	1.243
Space group		P1 or $P\bar{1}$	P1 or $P\bar{1}$	$P2_1$
Crystal class		Triclinic	Triclinic	Monoclinic