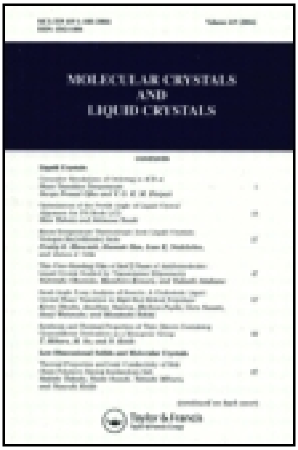

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Crystal and Molecular Structure of the Discogen bis[1,3-di(p-n-octyloxy-phenyl)propane-1,3-dionato]copper(II)

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Crystal and Molecular Structure of the Discogen bis[1,3-di(*p*-*n*-octyloxyphenyl)propane-1,3-dionato]copper(II)

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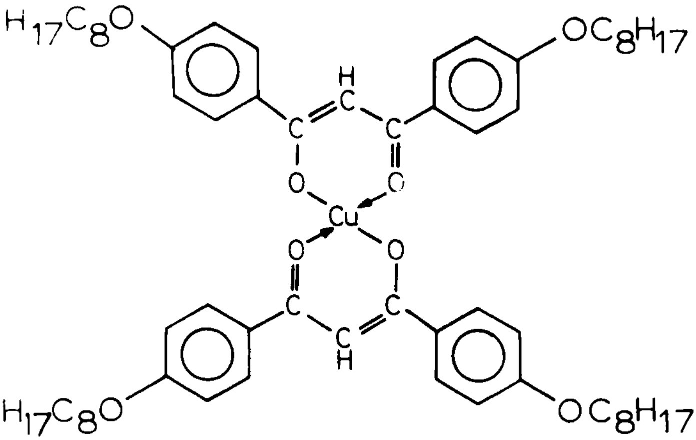
The transition metal containing discogenic bis[1,3-di(*p*-*n*-octyloxy phenyl)propane-1,3-dionato]copper(II) crystallizes in the triclinic space group $P\bar{1}$ with two molecules in a unit cell of dimensions $a = 11.300(9)$, $b = 16.101(1)$, $c = 17.089(2)$Å, $\alpha = 82.23(1)$, $\beta = 74.88(4)$, $\gamma = 77.43(3)°$. The crystal structure was solved by direct methods and refined to $R = 0.097$ by the structure factor least squares procedure. The copper atom is surrounded by four oxygen atoms in a square planar arrangement. The octyloxy chains are fully extended. The crystal structure has both layer-like and columnar characteristics. The repeating unit along the column is a molecular pair. The copper atoms are distributed about the column axis in a zig-zag fashion.

Keywords: discotic, copper complex, crystal structure

INTRODUCTION

Since the first discovery of the discotic phase,[1] there have been a number of x-ray investigations on the mesophases of disc-like molecules, which have led to a systematic classification of their structural characteristics.[2] However, the solid phase of discogens appears to have received little attention so far. It is known from x-ray studies of rod-like systems that knowledge of the molecular arrangement in the crystalline state is very useful in understanding the properties of the mesophase (see for example, Bernal and Crowfoot,[3] Krigbaum and Barber,[4] Astheimer *et al.*,[5] Walz *et al.*,[6] Vani,[7] Vani and Vijayan[8]). However, as yet, the crystal structure of no discogen seems to have been accurately determined by conventional crystallographic procedures. Cotrait *et al.*[9] have reported the molecular arrangement in the crystalline state of triphenylene hexaester. However, on account of the limited intensity data, the atomic coordinates and the molecular dimensions have not been reported for this discogen. In this paper, we report the results of the first detailed x-ray analysis of the crystal and the molecular structure of a discogen.

A number of copper complexes are known to exhibit mesomorphism[10-13] and x-ray studies on their mesophases have been reported.[14-16] The complex chosen for the present study was bis[1,3-di(*p*-*n*-octyloxyphenyl)propane-1,3-dionato]copper(II), hereafter referred to as (A). A preliminary report discussing the broad structural features of (A) has already been published.[17] In this paper, we present a more detailed description of the analysis, the final atomic coordinates and the molecular dimensions.



(A)

EXPERIMENTAL

Greenish prismatic single crystals of (A) were obtained by slow evaporation from a solution in acetone. The unit cell dimensions and space group were determined from oscillation, Weissenberg and precession photographs. The unit cell parameters were later refined on the diffractometer by least squares method, using 25 reflections. The crystal data are given in the abstract and in reference 17. The estimated standard deviation, e.s.d. of the *a*-axial length is 0.009Å and is considerably larger than the corresponding values of 0.001 and 0.002Å for the *b* and the *c*-axial lengths respectively. As mentioned later in this paper, the crystallographic *a*-axis corresponds to the column axis of the structure and whether the comparatively high e.s.d. of the *a*-length is indicative of the fact that this is a preferential direction for slip between adjacent columns of the structure is a matter for further study.

Three dimensional intensity data were collected on a CAD-4 single crystal diffractometer in the ω-2θ scan mode. Intensities of the reflections (132) and (033) were checked once after every 100 reflections. For $\theta \leq 47°$, the intensities of 5217 independent reflections were measured of which 4043 have $I \geq 3\sigma(I)$. The intensities were corrected for Lorentz and polarization factors.

STRUCTURE DETERMINATION

Based on the statistical distribution of the normalized structure factors which was unambiguously centric, the space group $P\bar{1}$ was chosen for the analysis. The crystal structure was solved by direct methods using the program MULTAN 80[18] and refined to $R = 0.097$ by block diagonal structure factor least squares procedure, using anisotropic thermal parameters for all the nonhydrogen atoms. The hydrogen atoms were placed at their calculated positions, assuming a C-H distance of 1.08Å[19] and were assigned temperature factors which were the same as the equivalent isotropic temperature factors,[20] B_{eq}, of the respective carbon atoms to which they are attached. The parameters of the hydrogen atoms were not refined but their contributions to the structure factors were included in the least squares refinement. The weighting function was of the form[21]

$$\omega = 1/(a_o + b_oF_o + c_oF_o^2)$$

with $a_o = 0.632$, $b_o = 0.172$ and $c_o = -0.0002$. The computer program used for the refinement of the crystal structure was the modified version of a block diagonal structure factor least squares program, SFLS, written originally by R. Shiono. The atomic scattering factors used in the calculations were those of Cromer and Waber.[22]

In the course of the least squares refinement, the thermal parameters of the atoms C(22) to C(25) and C(51) to C(55) which correspond to the terminal regions of two of the octyloxy chains (Figure 1) were found to be rather high. Also, the molecular dimensions involving these atoms were found to deviate significantly from the expected values. These features suggested the possibility of disorder in the octyloxy chains and hence, a difference electron density map was computed after removing the contributions from these nine atoms. The difference electron density map did not provide any evidence for the presence of positionally resolvable disorder. It was therefore concluded that the high thermal parameters and the unusual molecular dimensions were due to the existence of alternative positions separated by distances too small to be resolved by x-ray analysis.

In the course of the least squares refinement, the observed intensity of the reflection (224) was corrected for secondary extinction effect.

RESULTS AND DISCUSSION

Figure 1 shows the atomic numbering scheme. Although the two halves of the molecule are chemically identical, they are not related crystallographically by symmetry elements. Table I lists the positional and the B_{eq} values of all the nonhydrogen

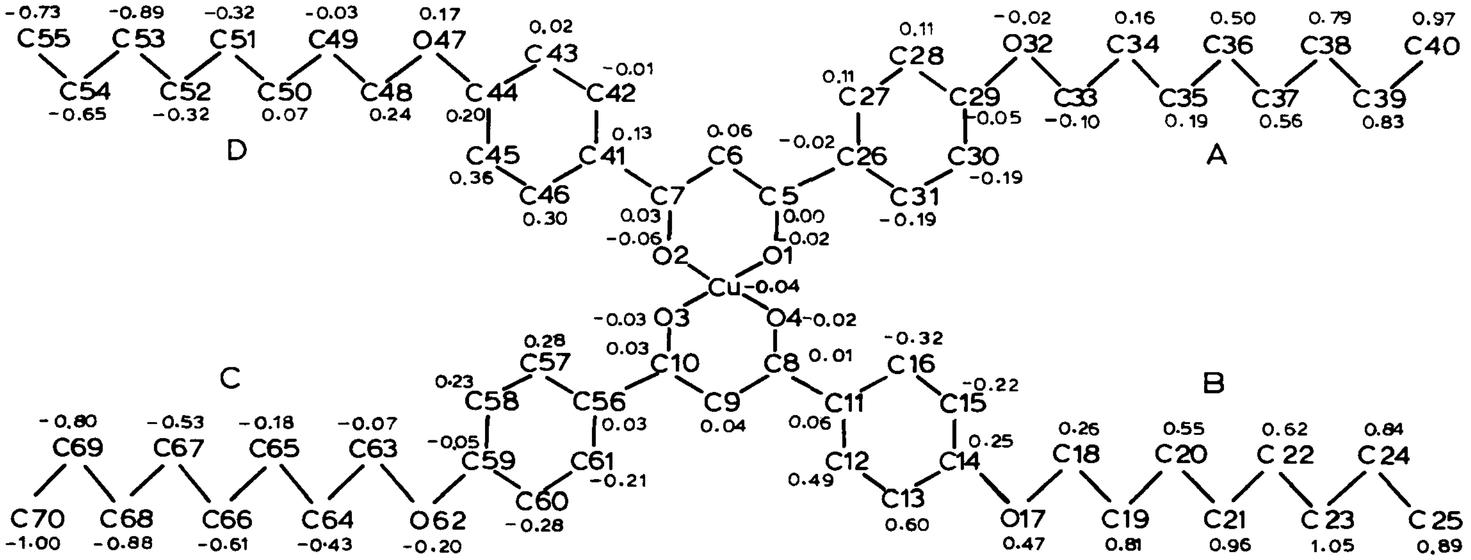


FIGURE 1 Displacements in Å of the non-hydrogen atoms from the least squares plane of the molecular core. A, B, C and D refer to the four octyloxy chains.

TABLE I

Final fractional atomic coordinates

	X	Y	Z	B_{eq}(Å)^2
Cu	0.7692(2)	0.4120(1)	0.0424(2)	6.0
O(1)	0.880(1)	0.4683(7)	−0.0408(7)	5.7
O(2)	0.639(1)	0.5099(7)	0.0512(7)	5.7
O(3)	0.658(1)	0.3554(7)	0.1241(7)	5.2
O(4)	0.897(1)	0.3147(6)	0.0343(7)	5.5
C(5)	0.856(2)	0.544(1)	−0.072(1)	4.8
C(6)	0.741(2)	0.599(1)	−0.052(1)	4.9
C(7)	0.638(1)	0.579(1)	0.008(1)	4.4
C(8)	0.896(1)	0.244(1)	0.071(1)	4.4
C(9)	0.792(2)	0.220(1)	0.130(1)	5.1
C(10)	0.679(2)	0.278(1)	0.152(1)	5.0
C(11)	0.013(2)	0.177(1)	0.050(1)	4.5
C(12)	0.024(2)	0.089(1)	0.063(1)	4.9
C(13)	0.136(2)	0.035(1)	0.032(1)	5.1
C(14)	0.240(2)	0.069(1)	−0.011(1)	5.1
C(15)	0.231(2)	0.156(1)	−0.022(1)	5.2
C(16)	0.120(2)	0.209(1)	0.008(1)	5.4
O(17)	0.343(1)	0.0078(7)	−0.0404(7)	6.2
C(18)	0.445(2)	0.042(1)	−0.093(1)	6.2
C(19)	0.539(2)	0.961(1)	0.870(1)	6.6
C(20)	0.655(2)	0.996(2)	0.815(1)	9.1
C(21)	0.754(2)	0.924(2)	0.780(2)	11.7
C(22)	0.877(4)	0.971(3)	0.720(2)	15.5
C(23)	0.957(7)	0.915(3)	0.685(3)	27.2
C(24)	0.050(6)	0.972(5)	0.624(4)	29.3
C(25)	0.125(6)	0.929(6)	0.610(6)	35.5
C(26)	0.964(2)	0.571(1)	−0.136(1)	4.6
C(27)	0.955(2)	0.650(1)	−0.183(1)	5.4
C(28)	0.056(2)	0.669(1)	−0.241(1)	5.6
C(29)	0.171(2)	0.613(1)	−0.252(1)	5.1
C(30)	0.180(2)	0.536(1)	−0.206(1)	5.3
C(31)	0.078(2)	0.517(1)	−0.148(1)	5.0
O(32)	0.265(1)	0.6386(8)	−0.3122(8)	6.6
C(33)	0.382(2)	0.581(1)	−0.330(1)	5.8
C(34)	0.462(2)	0.620(1)	−0.406(1)	6.6
C(35)	0.588(2)	0.561(1)	−0.435(1)	6.8
C(36)	0.668(2)	0.596(1)	−0.512(1)	6.5
C(37)	0.790(2)	0.538(1)	−0.542(1)	6.9
C(38)	0.876(2)	0.574(1)	−0.617(1)	7.2
C(39)	0.999(2)	0.515(1)	−0.645(1)	7.4
C(40)	0.086(2)	0.554(2)	−0.715(2)	9.2
C(41)	0.516(2)	0.641(1)	0.025(1)	4.4
C(42)	0.500(1)	0.728(1)	−0.005(1)	4.5
C(43)	0.386(2)	0.781(1)	0.017(1)	4.9
C(44)	0.285(2)	0.750(1)	0.068(1)	4.6
C(45)	0.298(2)	0.665(1)	0.098(1)	5.4
C(46)	0.415(2)	0.613(1)	0.076(1)	4.7
O(47)	0.178(1)	0.8094(7)	0.0882(7)	6.0
C(48)	0.076(2)	0.781(1)	0.147(1)	6.2
C(49)	−0.022(2)	0.862(1)	0.167(1)	7.1
C(50)	0.859(2)	0.831(2)	0.232(2)	11.8
C(51)	0.766(3)	0.911(3)	0.259(2)	14.3
C(52)	0.656(4)	0.872(4)	0.331(3)	25.4
C(53)	0.603(7)	0.909(4)	0.374(3)	26.1
C(54)	0.486(6)	0.844(4)	0.448(3)	22.8
C(55)	0.431(6)	0.912(4)	0.441(3)	24.5

TABLE I

(continued)

C(56)	0.570(2)	0.254(1)	0.216(1)	4.7
C(57)	0.454(2)	0.308(1)	0.224(1)	5.5
C(58)	0.351(2)	0.294(1)	0.283(1)	5.5
C(59)	0.360(2)	0.222(1)	0.337(1)	5.8
C(60)	0.474(2)	0.164(1)	0.330(1)	6.2
C(61)	0.575(2)	0.179(1)	0.270(1)	5.9
O(62)	0.267(1)	0.2018(8)	0.4008(8)	7.2
C(63)	0.151(2)	0.260(1)	0.415(1)	7.1
C(64)	0.071(2)	0.225(1)	0.495(1)	7.0
C(65)	0.938(2)	0.281(1)	0.510(1)	7.9
C(66)	0.857(2)	0.251(1)	0.593(1)	7.4
C(67)	0.730(2)	0.307(1)	0.616(1)	7.4
C(68)	0.649(2)	0.274(1)	0.696(1)	7.2
C(69)	0.519(2)	0.331(2)	0.719(1)	9.1
C(70)	0.435(2)	0.294(2)	0.793(1)	9.1

atoms.† The average value of B_{eq} for the core of the molecule (comprising of the copper-oxygen polyhedron and the six nonbenzenoid carbon atoms, viz., C(5) to C(7) and C(8) to C(10)) is 5.2 Å^2. In the phenyl rings, to which the chains A to D (Figure 1) are attached, the B_{eq} values average to 4.9, 5.2, 5.6 and 5.1 Å^2 respectively and are comparable to that of the core. In the octyloxy chains, the thermal parameters are higher. The average values of B_{eq} in the chains A, B, C and D are 7.0, 17.6, 7.8 and 17.6 Å^2 respectively. It is very striking that the thermal parameters of only the diametrically opposite chains are comparable. Also, the B_{eq} values of chains B and D are conspicuously higher than those of A and C. Examination of the molecular arrangement in the unit cell shows that the octyloxy chains A and C point towards the aromatic, central regions of molecules in the neighboring unit cells. The chains B and D, on the other hand, point towards the octyloxy chains. The difference in the type of packing of the octyloxy chains seems to have a significant bearing on their respective B_{eq} values. Further, it is also well known that in the discotic mesophase, the chains which form the fringe of disclike molecules are likely to be flexible and disordered.[1,23] It is therefore likely, that the characteristics of the chains B and D observed in the crystalline state are only indicative of the possible disorder in these chains in the mesophase of (A). Similar high thermal vibrations and consequent abnormal molecular dimensions have been observed in the crystal structures of several other mesogens also.[24-26]

In Table II, final bond lengths and bond angles with their respective estimated standard deviations are listed. For the phenyl rings and the octyloxy chains only the average values are given. Within the limits of experimental error, the molecular dimensions are normal in all parts other than in chains B and D. The core of the molecule is only nearly planar. The least squares planes through the atoms Cu, O(1), O(2), C(5) to C(7) makes an angle of ~3° with that through the group of

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†A listing of the structure factors can be obtained from the authors, on request.

TABLE II

Bond Lengths (Å) and Bond Angles (°). The quantities in parentheses represent the respective e.s.d's.

Bond lengths			
Cu - O(1)	1.90(1)	Bond angles	
Cu - O(2)	1.90(1)	O(1) - Cu - O(2)	92.7(5)
Cu - O(3)	1.90(1)	O(3) - Cu - O(4)	92.4(5)
Cu - O(4)	1.88(1)	O(1) - Cu - O(4)	87.7(5)
O(1) - C(5)	1.26(2)	O(2) - Cu - O(3)	87.2(5)
O(2) - C(7)	1.25(2)	O(1) - Cu - O(3)	179.1(5)
O(3) - C(10)	1.27(2)	O(2) - Cu - O(4)	179.6(5)
O(4) - C(8)	1.23(2)	Cu - O(1) - C(5)	127(1)
C(5) - C(6)	1.40(2)	Cu - O(2) - C(7)	128(1)
C(6) - C(7)	1.40(2)	Cu - O(3) - C(10)	127(1)
C(7) - C(41)	1.50(2)	Cu - O(4) - C(8)	129(1)
C(8) - C(9)	1.41(2)	C(44) - O(47) - C(48)	116(1)
C(9) - C(10)	1.41(2)	O(47) - C(48) - C(49)	105(2)
C(10) - C(56)	1.51(2)	C(59) - O(62) - C(63)	118(2)
C(8) - C(11)	1.51(2)	O(1) - C(5) - C(6)	124(2)
C(5) - C(26)	1.50(2)	C(5) - C(6) - C(7)	124(2)
C(14) - O(17)	1.37(2)	O(2) - C(7) - C(6)	124(2)
O(17) - C(18)	1.43(2)	O(4) - C(8) - C(9)	124(2)
C(29) - O(32)	1.36(2)	O(3) - C(10) - C(9)	125(2)
O(32) - C(33)	1.43(2)	C(8) - C(9) - C(10)	122(2)
C(44) - O(47)	1.36(2)	C(14) - O(17) - C(18)	114(1)
O(47) - C(48)	1.43(2)	O(17) - C(18) - C(19)	104(1)
C(59) - O(62)	1.36(2)	C(29) - O(32) - C(33)	118(1)
O(62) - C(63)	1.42(2)	O(32) - C(33) - C(34)	107(2)
$(\overline{\text{C - C}})_{\text{PhA}}$	1.38(2)	O(62) - C(63) - C(64)	106(2)
$(\overline{\text{C - C}})_{\text{PhB}}$	1.39(2)	$(\overline{\text{C - C - C}})_{\text{PhA,B,C \& D}}$	120(2)
$(\overline{\text{C - C}})_{\text{PhC}}$	1.39(2)	$(\overline{\text{C - C - C}})_{\text{OctA}}$	114(2)
$(\overline{\text{C - C}})_{\text{PhD}}$	1.39(2)	$(\overline{\text{C - C - C}})_{\text{OctB}}$	105(4)
$(\overline{\text{C - C}})_{\text{OctA}}$	1.51(3)	$(\overline{\text{C - C - C}})_{\text{OctC}}$	112(2)
$(\overline{\text{C - C}})_{\text{OctB}}$	1.46(6)	$(\overline{\text{C - C - C}})_{\text{OctD}}$	103(4)
$(\overline{\text{C - C}})_{\text{OctC}}$	1.53(3)		
$(\overline{\text{C - C}})_{\text{OctD}}$	1.49(5)		
Intermolecular contact distances			
C(10) - C(43)′	3.46(3)		
C(8) - C(44)′	3.50(3)		

(—) indicates the average value for the group.
PhA . . . PhD denote the phenyl groups.
OctA . . . OctD denote the octyloxy chains.
′ represents the centrosymmetrically related molecules.

atoms Cu, O(3), O(4), C(8) to C(10). The planar phenyl rings are tilted with respect to the core. The angles between the normals to the least squares planes of the four phenyl rings and the core vary from 7 to 20°. In Figure 1 the displacements of all the non-hydrogen atoms from the least squares plane of the core are shown. Atoms of the phenyl rings and the octyloxy chains are significantly displaced from the core.

The copper atom is surrounded by four oxygen atoms in a square planar arrangement, with the copper-oxygen distance averaging to 1.90(1)Å. The conformation of (A) observed in the crystal strongly resembles the model B proposed by

Ohta et al.[14] for its mesophase. The linear dimensions 31 and 11 Å of the molecule (estimated as the respective average of the distances

(i) C(25) . . . C(70) and C(40) . . . C(55) and

(ii) C(25) . . . C(40) and C(55) . . . C(70))

are, however, slightly lower than the theoretical values obtained by Ohta et al., from CPK models. If the dimensions 31 and 11 Å are retained in the mesophase also, the tilt of the molecule within the layers characterising the mesophase should decrease to ~42° from the value of ~52° proposed by Ohta et al.[14]

Details of the molecular arrangement in the crystal of (A) have already been presented in Ref. 17. The crystal structure of (A) has both layer-like and columnar

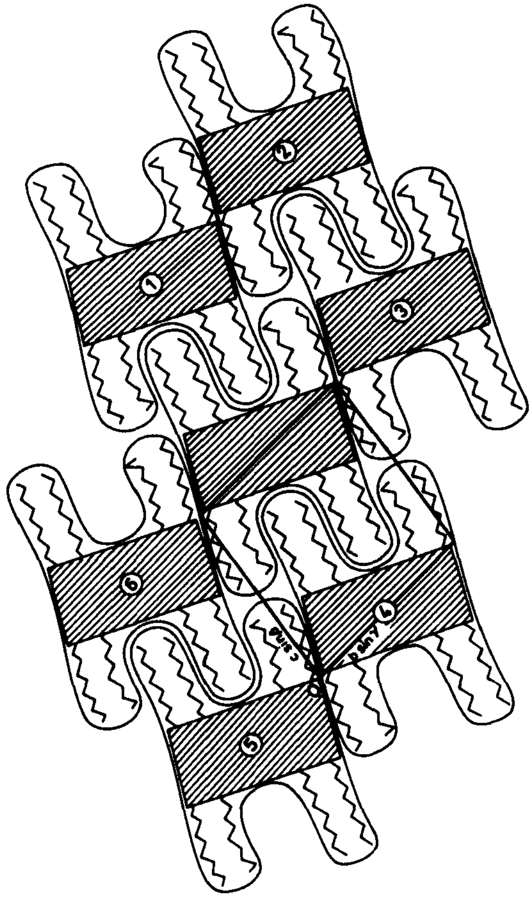

FIGURE 2 Schematic representation of a section of the columnar structure. The repeating unit of the column has been enclosed within solid lines. The shaded portions represent the cores of the repeating unit. The sixfold coordination of a column has been indicated by the numerals 1 to 6.

characteristics. The columnar characteristics arise from the periodic repetition of the unit cell contents along the crystallographic a-axis. Therefore, unlike in conventional columnar structures which characterise many discotic mesophases,[1,23,27,28] in the crystal structure of (A), the repeating unit of the column consists of the centrosymmetrically related molecular pair. The concept of molecular pair is further supported by the presence of short, intermolecular contact distances. In Table II, the contact distances which are less than the sum of the van der Waal's radius (for carbon, 1.8Å)[29] have been included. The preferential occurrence of short contacts only between adjacent, centrosymmetrically related pairs of molecules suggests that they tend to associate in pairs. Similar pairing of molecules has been suggested[9] for the discogen triphenylene hexaester which also has a columnar structure in the crystalline phase. The cores of the molecular pair of (A) are tilted with respect to the column axis, viz., the crystallographic *a*-axis. Each column in the crystal is surrounded by six others situated at ± **b**, ± **c** and ± (**b** + **c**). This arrangement deviates from the ideally hexagonal arrangement. In Figure 2, a section of the columnar arrangement of molecular pairs has been schematically shown. The rigid central cores of columns (marked shaded in Figure 2), are separated by distinct pockets consisting of octyloxy chains.

The copper atoms are distributed about the column axis in a zig-zag fashion, the zig-zag distances being 6.3 and 6.6 Å respectively. The angle at the zig-zag is 124°.

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