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Structures of 1,3-Di(9-carbazolyl)propane and 1,5-Di(9-carbazolyl)pentane. Polyvinylcarbazole Model Compounds

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Abstract. 9,9′-Propylenedicarbazole, $C_{27}H_{22}N_2$, M_r = 374·49, monoclinic, $P2_1/c$, a = 9·303 (3), b = 17·697 (3), c = 12·477 (3) Å, β = 98·30 (3)°, V = 2033 (2) Å^3, Z = 4, D_m = 1·221, D_x = 1·224 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 0·7 cm^{-1}, F(000) = 792, T = 302 K, R = 0·075, wR = 0·095 for 1650 independent reflections with $I \geq 3\sigma(I)$ and 262 variables. 9,9′-Pentylenedicarbazole, $C_{29}H_{26}N_2$, M_r = 402·54, monoclinic, $P2_1/c$, a = 9·158 (3), b = 28·204 (8), c = 8·717 (3) Å, β = 100·97 (3)°, V = 2210 (2) Å^3, Z = 4, D_m = 1·21, D_x = 1·210 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 0·7 cm^{-1}, F(000) = 856, T = 302 K, R = 0·054, wR = 0·052 for 2115 independent reflections with $I \geq 2\sigma(I)$ and 280 variables. The stereochemistry of the carbazole substituents is *gauche*, *anti* for 1,3-di(9-carbazolyl)propane and *gauche*, *gauche* for 1,5-di(9-carbazolyl)pentane, two polyvinylcarbazole model compounds. Although no intramolecular interactions between carbazole rings are evident, one carbazole of each molecule associates in a shifted parallel planar orientation with that of another molecule.

Introduction. Poly(9-vinylcarbazole) (PVC) is one of the most useful conducting organic polymers (Masuhara, Ohwada, Mataga, Itaya, Okamoto & Kusabayashi, 1978). Overlap between the carbazole groups is believed to be responsible for the electronic transport properties (Turner & Pai, 1979). Structural studies of PVC have been conducted in order to establish the role of polymer structure in photoconductivity (Tsuchihashi, Hatano & Sohna, 1976; Limburg & Williams, 1973).

1,3-Di(9-carbazolyl)propane (I) and related compounds which contain two neighboring carbazole substituents have been employed to model the interactions of the pendant carbazole groups in PVC (Masuhara *et al.*, 1978; Itaya, Okamoto & Kusabayashi, 1979; Masuhara, Tamai, Mataga, De Schryver & Vandendriessche, 1983; Klöpffer, 1969). We found that spatial relationships in such model systems affect the electronic interactions between the carbazole groups (Masnovi, Krafcik, Baker & Towns, 1990). Therefore, we have undertaken single-crystal X-ray structure determinations of (I) and of a higher analog, 1,5-di(9-carbazolyl)pentane (II), in order to establish the preferred relative orientation of the carbazole groups in these compounds. The structures and properties of molecular complexes of PVC model compounds with electron-accepting dopants are also of interest (Masnovi, Baker, Towns & Chen, 1991) and will be reported subsequently.

Experimental. The title compounds were prepared by reaction of the potassium salt of carbazole and 1,3-dibromopropane and 1,5-dibromopentane in dimethyl sulfoxide (Johnson, 1974). The reaction mixtures were poured into water and the crude products collected by filtration. Purification was accomplished by chromatography on silica gel, eluting fractionally using petroleum ether and dichloromethane.

Colorless crystals of (I) and (II) were attached to the end of glass capillaries using quick-drying epoxy cement at room temperature. An Enraf–Nonius CAD-4 X-ray diffractometer equipped with a graphite monochromator (Mo $K\alpha$ radiation) was used for data collection. Cell parameters were determined

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from accurately measured goniometer settings for 25 reflections, $3\cdot6 < \theta < 12\cdot6^\circ$. Systematically absent reflections ($0k0$ for k odd and $h0l$ for l odd) uniquely determined the space group to be $P2_1/c$ for both compounds. Three intensity controls were measured at 1 h intervals and showed no decay over 43 h exposure for each crystal. Both structures were solved by direct methods. The H atoms were located or generated in chemically reasonable positions. $F_{\rm obs}$ were corrected for Lorentz and polarization effects. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). All calculations were performed with Enraf–Nonius (1983) *SDP-Plus* on a PDP-11 minicomputer.

1,3-*Dicarbazolylpropane*. Crystals of (I) suitable for X-ray diffraction were grown by slow evaporation from a concentrated solution in chloroform/cyclohexane (crystal dimensions $0\cdot39 \times 0\cdot24 \times 0\cdot48$ mm); $1 \le \theta \le 27^\circ$. Of 4580 unique reflections collected with $\omega - 2\theta$ scans over the index ranges $0 \le h \le 11$, $0 \le k \le 22$, $-15 \le l \le 15$, 1650 reflections were considered observed [$I > 3\sigma(I)$]. An empirical transmission correction ranging from 0·908 to 1·000 was applied on the basis of ψ scans for eight reflections with χ near 90°. The final refinement parameters for 262 variables are $R = 0\cdot075$, $wR = 0\cdot095$; $w = 1/\sigma^2(F_o)$, $S = 2\cdot67$; $(\Delta/\sigma)_{\rm max} < 0\cdot01$. The largest peak in the resulting difference Fourier map was 0·18 and the deepest hole $-0\cdot31$ e Å^{-3}.

Final positional parameters and equivalent displacement parameters are listed in Table 1.* Important bond lengths and angles are given in Table 3. The conformation of the molecule is illustrated by the *ORTEP* (Johnson, 1976) drawing shown in Fig. 1(*a*), which also defines the atom-labeling scheme.

1,5-*Dicarbazolylpentane*. Crystals of (II) were grown by slow evaporation from a concentrated solution in ethyl acetate (crystal dimensions $0\cdot19 \times 0\cdot32 \times 0\cdot36$ mm); $1 \le \theta \le 25^\circ$. Of 3997 unique reflections collected with ω–2θ scans over the index ranges $-10 \le h \le 10$, $0 \le k \le 33$, $0 \le l \le 10$, 2115 reflections were considered observed [$I > 2\sigma(I)$]. The final refinement parameters for 280 variables are $R = 0\cdot054$, $wR = 0\cdot054$; $w = 1/\sigma^2(F_o)$, $S = 1\cdot79$; $(\Delta/\sigma)_{\rm max} < 0\cdot01$. The largest peak in the difference Fourier map was 0·16 and the deepest hole $-0\cdot22$ e Å^{-3}.

Final positional parameters and equivalent displacement parameters are listed in Table 2, and bond lengths and angles are given in Table 3. The conformation of the molecule is illustrated by the *ORTEP* (Johnson, 1976) drawing shown in Fig. 1(*b*), which also defines the atom-labeling scheme.

Table 1. *Positional parameters and their e.s.d.'s for the non*-H *atoms of* (I)

	x	y	z	$B_{\rm eq}$(Å^2)
C1	0·4790 (5)	0·1576 (3)	0·3360 (4)	6·8 (1)
C2	0·5042 (7)	0·2303 (3)	0·3696 (5)	9·0 (2)
C3	0·5977 (7)	0·2761 (3)	0·3222 (5)	9·0 (2)
C4	0·6694 (6)	0·2503 (3)	0·2416 (5)	7·9 (2)
C4a	0·6453 (5)	0·1758 (3)	0·2060 (4)	5·6 (1)
C4b	0·7020 (5)	0·1297 (3)	0·1269 (4)	5·6 (1)
C5	0·8030 (5)	0·1414 (3)	0·0565 (4)	7·4 (1)
C6	0·8370 (6)	0·0815 (3)	−0·0060 (4)	8·4 (2)
C7	0·7745 (5)	0·0125 (3)	−0·0006 (4)	7·5 (1)
C8	0·6731 (5)	−0·0024 (3)	0·0683 (4)	6·3 (1)
C8a	0·6380 (5)	0·0580 (3)	0·1307 (3)	5·1 (1)
N9	0·5426 (4)	0·0602 (2)	0·2073 (3)	4·93 (8)
C9a	0·5501 (4)	0·1304 (3)	0·2535 (3)	5·1 (1)
C1′	0·7526 (6)	−0·2249 (3)	0·4178 (5)	8·6 (2)
C2′	0·7862 (8)	−0·2929 (4)	0·4657 (7)	12·4 (2)
C3′	0·8612 (8)	−0·2947 (4)	0·5685 (7)	14·3 (2)
C4′	0·8994 (7)	−0·2348 (4)	0·6298 (5)	11·7 (2)
C4a′	0·8650 (5)	−0·1624 (4)	0·5802 (4)	8·0 (1)
C4b′	0·8880 (5)	−0·0868 (4)	0·6171 (4)	8·1 (2)
C5′	0·9517 (6)	−0·0505 (5)	0·7114 (4)	11·9 (2)
C6′	0·9535 (6)	0·0271 (5)	0·7162 (5)	15·4 (2)
C7′	0·8929 (6)	0·0697 (4)	0·6293 (6)	12·8 (2)
C8′	0·8260 (5)	0·0374 (3)	0·5358 (4)	8·1 (2)
C8a′	0·8258 (4)	−0·0394 (3)	0·5319 (4)	6·3 (1)
N9′	0·7680 (4)	−0·0855 (2)	0·4471 (3)	5·9 (1)
C9a′	0·7925 (5)	−0·1595 (3)	0·4770 (4)	6·4 (1)
C10	0·4647 (4)	−0·0038 (3)	0·2421 (4)	5·5 (1)
C11	0·5382 (4)	−0·0374 (3)	0·3483 (3)	5·5 (1)
C12	0·6935 (5)	−0·0595 (3)	0·3440 (3)	5·9 (1)

Discussion. The structure of the carbazole rings of (I) and (II) agrees with that reported for carbazole (Kurahashi, Fukuyo & Shimada, 1969). The only notable discrepancy between the carbazole rings of (I) and (II) and that of carbazole is found in the C4a—C4b distance, which is 1·43 Å for (I) and (II) (Table 3) but 1·48 Å for carbazole. This distance is 1·43 Å in the structure of dicarbazolylmethane (Masnovi *et al.*, 1990) and 1·40 Å in the disordered carbazoletetracyanoethylene (1/2) complex (Masnovi *et al.*, 1991).

The conformations of (I) and (II) are shown in Fig. 1. The 13 atoms defining each carbazole ring are essentially coplanar, and the methylene carbons attached to nitrogen also lie close to these planes. The carbazole substituents of (I) define a *gauche*, *anti* relationship with respect to the methylene carbons, whereas both carbazole rings of (II) are *gauche*. The conformation of the methylene chain of (II) is *anti*, *anti*; hence, all five methylene carbons of (II) also are coplanar.

The structure of (II) reveals no apparent disorder. However, the atoms in the carbazole ring with *anti* stereochemistry (bearing the prime designations) of (I) exhibit anomalous temperature factors. Data collected independently on a second crystal of (I) led to a solution essentially the same as reported, with large temperature factors observed in the plane of the carbazole ring for the same set of atoms. Evidently,

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, and bond lengths and angles involving H-atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54135 (30 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

this is a result of dynamic or static disorder in the crystal. A similar situation has been described for other planar systems, such as acridine (Toupet, Miniewicz & Ecolivet, 1989).

Comparison of packing diagrams of (I) and (II) (Fig. 2) indicates the spatial demands made by two larger planar groups attached to a flexible spacer moiety. Experimental and theoretical models suggest that aromatic rings prefer to associate in shifted

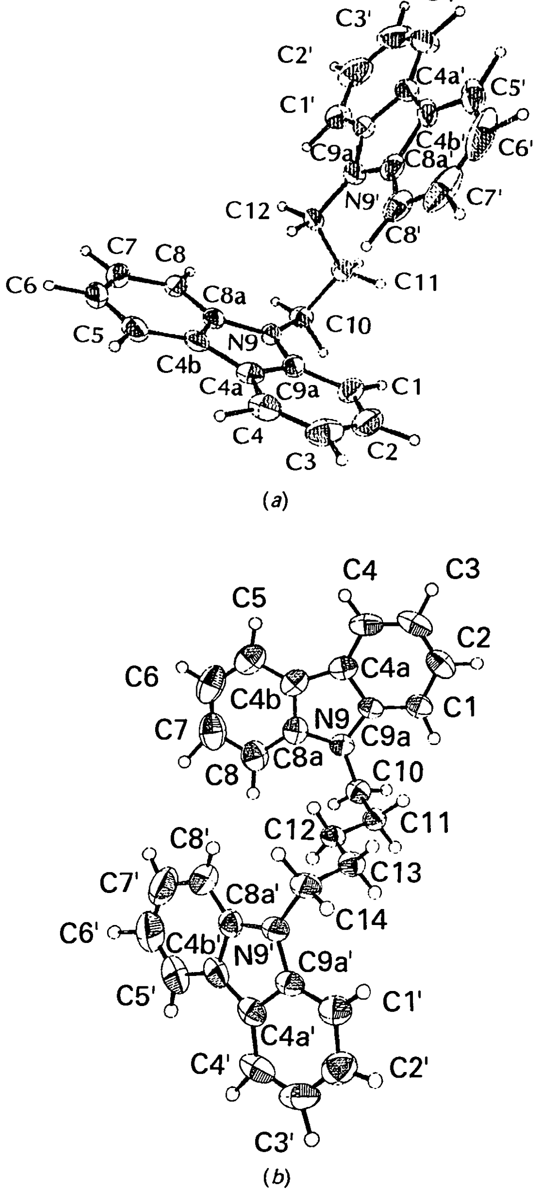

Fig. 1. (*a*) *ORTEP* drawing of 1,3-dicarbazolylpropane (I) (thermal ellipsoids are drawn at 20% probability level), and (*b*) *ORTEP* drawing of 1,5-dicarbazolylpropane (II) (thermal ellipsoids are drawn at 50% probability level).

Table 2. *Positional parameters and their e.s.d.'s for the non*-H *atoms of* (II)

	x	y	z	B_{eq}(Å^2)
C1	0·2678 (4)	0·4843 (1)	0·1459 (4)	4·40 (9)
C2	0·3086 (4)	0·5225 (1)	0·2412 (4)	5·6 (1)
C3	0·2135 (5)	0·5422 (1)	0·3297 (4)	6·1 (1)
C4	0·0732 (4)	0·5241 (1)	0·3245 (4)	5·20 (9)
C4a	0·0271 (4)	0·4851 (1)	0·2285 (4)	4·03 (8)
C4b	−0·1056 (4)	0·4567 (1)	0·1940 (4)	4·21 (8)
C5	−0·2424 (4)	0·4582 (1)	0·2431 (4)	5·9 (1)
C6	−0·3472 (4)	0·4254 (2)	0·1871 (5)	7·0 (1)
C7	−0·3219 (4)	0·3903 (2)	0·0854 (5)	6·8 (1)
C8	−0·1881 (4)	0·3873 (1)	0·0331 (5)	5·5 (1)
C8a	−0·0805 (4)	0·4213 (1)	0·0897 (4)	4·14 (8)
N9	0·0601 (3)	0·42733 (9)	0·0567 (3)	3·80 (6)
C9a	0·1265 (4)	0·4654 (1)	0·1412 (4)	3·61 (8)
C1′	0·3979 (4)	0·1708 (1)	0·1982 (4)	4·37 (9)
C2′	0·4472 (4)	0·1301 (1)	0·1337 (4)	5·7 (1)
C3′	0·3515 (5)	0·1004 (1)	0·0383 (4)	6·1 (1)
C4′	0·2020 (4)	0·1100 (1)	0·0010 (4)	5·1 (1)
C4a′	0·1470 (4)	0·1503 (1)	0·0640 (4)	3·83 (8)
C4b′	0·0029 (4)	0·1709 (1)	0·0541 (4)	4·22 (8)
C5′	−0·1383 (4)	0·1589 (1)	−0·0297 (5)	6·0 (1)
C6′	−0·2550 (4)	0·1873 (2)	−0·0140 (5)	7·8 (1)
C7′	−0·2393 (4)	0·2259 (2)	0·0832 (6)	7·8 (1)
C8′	−0·1019 (4)	0·2392 (1)	0·1656 (5)	5·9 (1)
C8a′	0·0189 (4)	0·2113 (1)	0·1489 (4)	3·94 (8)
N9′	0·1679 (3)	0·21675 (9)	0·2154 (3)	3·75 (6)
C9a′	0·2471 (4)	0·1799 (1)	0·1631 (4)	3·48 (8)
C10	0·1346 (4)	0·3976 (1)	−0·0417 (4)	4·24 (8)
C11	0·2472 (4)	0·3642 (1)	0·0535 (4)	3·72 (8)
C12	0·1798 (3)	0·3248 (1)	0·1358 (4)	3·68 (8)
C13	0·2967 (4)	0·2952 (1)	0·2416 (4)	3·82 (8)
C14	0·2337 (4)	0·2547 (1)	0·3217 (4)	4·10 (8)

Table 3. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s for* (I) *and* (II)

	(I)	(II)
C1—C2	1·362 (8)	1·367 (5)
C1—9a	1·389 (7)	1·393 (5)
C2—C3	1·382 (9)	1·386 (6)
C3—C4	1·363 (9)	1·375 (6)
C4—C4a	1·398 (7)	1·399 (5)
C4a—C4b	1·439 (7)	1·438 (5)
C4b—C5	1·391 (7)	1·400 (5)
C4b—C8a	1·404 (6)	1·398 (5)
C4a—C9a	1·390 (6)	1·407 (5)
C5—C6	1·379 (8)	1·356 (6)
C6—C7	1·359 (8)	1·377 (6)
C7—C8	1·390 (7)	1·389 (6)
C8—C8a	1·390 (7)	1·397 (5)
C8a—N9	1·396 (6)	1·382 (4)
N9—C10	1·445 (6)	1·459 (4)
C9a—N9	1·366 (6)	1·377 (4)
C1′—C2′	1·360 (9)	1·390 (5)
C1′—C9a′	1·395 (7)	1·380 (5)
C2′—C3′	1·37 (1)	1·373 (5)
C3′—C4′	1·33 (1)	1·372 (6)
C4′—C4a′	1·440 (9)	1·397 (5)
C4a′—C4b′	1·420 (9)	1·430 (5)
C4a′—C9a′	1·366 (6)	1·409 (4)
C4b′—C5′	1·396 (8)	1·400 (5)
C4b′—C8a′	1·410 (7)	1·398 (5)
C5′—C6′	1·37 (1)	1·364 (6)
C6′—C7′	1·37 (1)	1·371 (7)
C7′—C8′	1·366 (8)	1·377 (5)
C8′—C8a′	1·360 (8)	1·389 (5)
C8a′—N9′	1·382 (6)	1·385 (4)
C9a′—N9′	1·373 (6)	1·392 (4)
N9′—C12(C14)*	1·445 (5)	1·469 (4)
C10—C11	1·521 (6)	1·520 (4)
C11—C12	1·505 (6)	1·517 (5)
C12—C13	—	1·523 (4)
C13—C14	—	1·508 (5)
C2—C1—C9a	118·5 (5)	117·7 (3)
C1—C2—C3	120·9 (6)	121·8 (4)
C2—C3—C4	121·6 (5)	121·0 (3)
C3—C4—C4a	118·5 (5)	119·1 (4)
C4—C4a—C4b	134·0 (5)	135·2 (3)
C4—C4a—C9a	119·5 (5)	118·8 (3)
C9a—C4a—C4b	106·5 (5)	106·0 (3)

Table 3 (*cont.*)

	(I)	(II)
C4a—C4b—C5	134·2 (5)	133·6 (3)
C4a—C4b—C8a	106·8 (4)	107·2 (3)
C8a—C4b—C5	118·9 (4)	119·2 (3)
C4b—C5—C6	118·2 (5)	118·9 (4)
C5—C6—C7	121·9 (5)	121·9 (4)
C6—C7—C8	122·3 (5)	121·4 (4)
C7—C8—C8a	115·8 (5)	116·7 (4)
C4b—C8a—C8	122·8 (4)	121·9 (3)
C4b—C8a—N9	108·2 (4)	108·8 (3)
C8—C8a—N9	129·0 (4)	129·3 (3)
C8a—N9—C9a	108·4 (4)	108·6 (3)
C8a—N9—C10	125·5 (4)	127·6 (3)
C9a—N9—C10	125·7 (4)	123·7 (3)
C1—C9a—N9	128·9 (4)	128·9 (3)
C4a—C9a—C1	121·1 (4)	121·7 (3)
C4a—C9a—N9	110·1 (4)	109·3 (3)
C2′—C1′—C9a′	118·3 (5)	116·9 (3)
C1′—C2′—C3′	119·1 (6)	122·0 (3)
C2′—C3′—C4′	125·4 (7)	121·1 (4)
C3′—C4′—C4a′	116·1 (6)	119·0 (3)
C4′—C4a′—C4b′	133·3 (5)	134·8 (3)
C4′—C4a′—C9a′	119·1 (5)	118·9 (3)
C9a′—C4a′—C4b′	107·5 (4)	106·3 (3)
C4a′—C4b′—C5′	137·1 (6)	133·0 (3)
C4a′—C4b′—C8a′	106·9 (4)	107·7 (3)
C8a′—C4b′—C5′	116·1 (6)	119·3 (3)
C4b′—C5′—C6′	119·8 (6)	117·9 (4)
C5′—C6′—C7′	120·8 (6)	122·5 (4)
C6′—C7′—C8′	122·0 (7)	121·1 (4)
C7′—C8′—C8a′	116·5 (5)	117·2 (4)
C4b′—C8a′—N9′	107·3 (4)	108·8 (3)
C4a′—C9a′—N9′	109·4 (4)	108·9 (3)
C4a′—C9a′—C1′	121·8 (5)	122·1 (3)
C4b′—C8a′—C8′	124·7 (5)	121·9 (3)
C8′—C8a′—N9′	127·9 (4)	129·3 (3)
C8a′—N9′—C9a′	108·9 (4)	108·3 (3)
C8a′—N9′—C12(C14)†	125·3 (4)	126·7 (3)
C9a′—N9′—C12(C14)†	125·8 (4)	125·0 (3)
C1′—C9a′—N9′	128·8 (4)	128·9 (3)
N9—C10—C11	112·7 (3)	112·3 (3)
N9′—C12(C14)—C11(C13)†	113·0 (4)	114·0 (3)
C10—C11—C12	112·6 (4)	114·7 (3)
C11—C12—C13	—	112·7 (3)
C12—C13—C14	—	114·1 (3)

* Distance N9′—C12 (I), N9′—C14 (II).
† Angles N9′—C12 (I), N9′—C14 (II).

stack structures, and this stacking becomes increasingly favorable with increasing arene size (Jorgensen & Severance, 1990). Although no intramolecular interaction between the carbazole rings is apparent for either (I) or (II), one carbazole ring of each molecule [designated the primed ring for (I) and the unprimed ring for (II)] associates in a parallel planar orientation with a centrosymmetrically related carbazole ring of another molecule. Interactions between the π systems of the two associated rings are considerably more extensive in (II) (3·85 Å between the centers of gravity) than in (I) (5·30 Å between the centers).

Such interactions reflect on the formation and structure of inclusion complexes, as will be reported subsequently.

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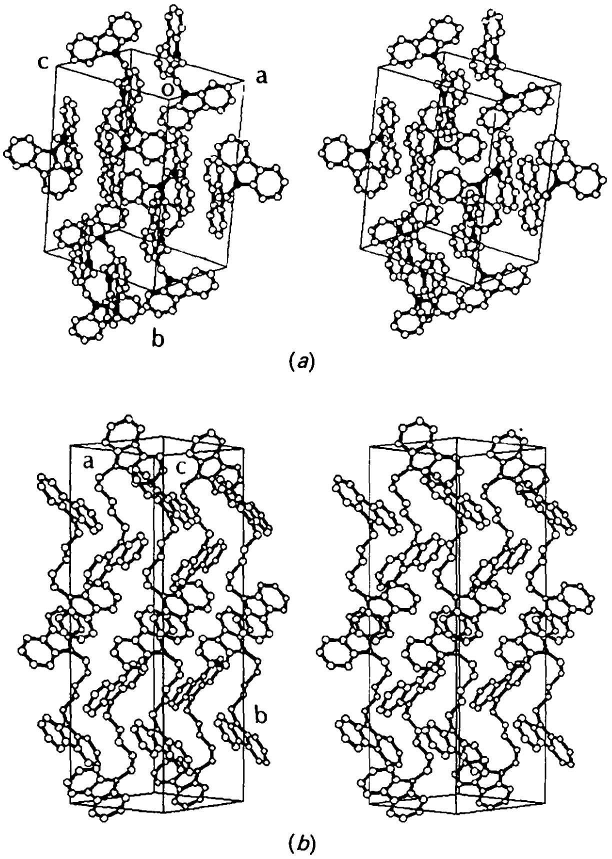

Fig. 2. Packing diagrams of (*a*) (I) and (*b*) (II).

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