with three pairs of atoms simultaneously eclipsed whereas rotational barriers about C(1)—N(2) and C(3)—O(3) will involve the eclipsing of one pair of atoms at a time and are therefore likely to be lower. The question of whether these two forms of DINA are polymorphs or rotational isomers depends upon whether the difference in conformation is brought about by packing or intramolecular effects. The coexistence of the two forms during crystallization from solution indicates a similar degree of thermodynamic stability. Solid–solid transitions between DINA (II) and DINA (I) have not been observed; the spatial requirements involved in the change of conformation imply a severe mechanistic barrier to transformation in the solid state. Crystals of DINA (II) become opaque and slightly discoloured over a period of one year or more but an oscillation photograph shows them to be structurally unchanged.

The shortest intermolecular contacts in DINA (II) are 3·12 Å between O(6) and N(3) of 2_1-related molecules; none of the other O···N intermolecular contacts are significantly less than the sum of the van der Waals radii across π-bonding electrons (Bondi, 1964). Closer interactions (2·9 Å) have been found in DINA (I) (Halfpenny & Small, 1978) and in other nitramines (Cobbledick & Small, 1973).

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6,9-Dimethoxy-2,13-diaza[4]paracyclo[4](3,5)pyridinophane-1,14-dione, $C_{19}H_{21}N_3O_4$, and 19-Benzyl-16,19-dihydro-2,13-diaza[4]paracyclo[4](3,5)pyridinophane-1,4-dione, $C_{24}H_{25}N_3O_2$

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Abstract

$C_{19}H_{21}N_3O_4$: $P2_1/n$, with a = 10·2801 (4), b = 9·4333 (4), c = 18·7174 (7) Å, β = 101·42 (1)°, Z = 4. Final R = 0·041 for 2519 observed reflexions. The pyridine ring is above and roughly perpendicular to the benzene ring with the H atom at the 4 position of the pyridine ring close to the benzene ring (shortest H—C distance 2·80 Å). The molecules are interconnected by means of N···O hydrogen bonds to form sheets parallel to (001). $C_{24}H_{25}N_3O_2$: $P2_1/c$, with a = 12·980 (2), b = 5·719 (2), c = 26·721 (2) Å, β = 99·26 (2)°, Z = 4. Final R = 0·048 for 2704 observed reflexions. The 1,4-dihydropyridine ring is in a boat conformation. One of the H atoms of its CH_2 group is roughly above the centre of the benzene ring with shortest H—C distance of 2·94 Å.

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Table 1. *Fractional coordinates* ($\times 10^4$, *for* H $\times 10^3$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$) *with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j.$$

	x	y	z	U_{eq} or U
(*a*) PP				
N(1)	4309 (2)	1272 (3)	704 (1)	64 (1)
C(2)	5310 (2)	449 (3)	1042 (1)	51 (1)
C(3)	5695 (2)	375 (2)	1791 (1)	34 (1)
C(4)	4969 (2)	1133 (2)	2211 (1)	33 (1)
C(5)	3908 (2)	1954 (2)	1875 (2)	33 (1)
C(6)	3640 (2)	2019 (3)	1125 (1)	51 (1)
C(7)	6838 (2)	−521 (2)	2167 (1)	38 (1)
N(8)	7647 (2)	129 (2)	2716 (1)	54 (1)
C(9)	8580 (2)	−631 (3)	3275 (1)	39 (1)
C(10)	8450 (2)	−178 (3)	4045 (1)	49 (1)
C(11)	7065 (2)	262 (3)	4122 (1)	51 (1)
C(12)	5979 (2)	−648 (2)	3967 (1)	41 (1)
C(13)	4712 (2)	−177 (2)	4010 (1)	40 (1)
C(14)	4482 (2)	1219 (3)	4195 (2)	40 (1)
C(15)	5566 (2)	2127 (3)	4346 (2)	39 (1)
C(16)	6843 (3)	1654 (3)	4317 (2)	44 (1)
C(17)	3082 (3)	1726 (3)	4188 (1)	44 (1)
C(18)	2522 (2)	2701 (3)	3544 (2)	53 (1)
N(19)	2794 (2)	2085 (2)	2874 (1)	61 (1)
C(20)	3198 (2)	2827 (2)	2350 (1)	66 (1)
O(21)	6944 (2)	−1769 (2)	1986 (1)	67 (1)
O(22)	3093 (2)	4120 (2)	2275 (1)	45 (1)
O(23)	6238 (2)	−2017 (2)	3767 (1)	46 (1)
C(24)	5160 (3)	−2746 (3)	3320 (2)	35 (1)
O(25)	5303 (2)	3500 (2)	4527 (1)	35 (1)
C(26)	6291 (3)	4538 (3)	4505 (2)	51 (1)
H(2)	578 (2)	−11 (3)	70 (2)	76 (8)
H(4)	523 (2)	112 (2)	275 (1)	32 (5)
H(6)	287 (3)	262 (3)	85 (1)	73 (8)
H(8)	754 (2)	107 (3)	280 (1)	68 (8)
H(91)	952 (2)	−47 (3)	320 (2)	60 (7)
H(92)	834 (2)	−172 (3)	321 (2)	66 (7)
H(101)	878 (2)	−100 (3)	441 (2)	77 (8)
H(102)	906 (3)	69 (3)	420 (1)	71 (8)
H(13)	395 (2)	−84 (3)	389 (1)	50 (6)
H(16)	764 (2)	234 (2)	442 (2)	54 (6)
H(171)	305 (2)	225 (3)	466 (2)	51 (6)
H(172)	250 (2)	86 (2)	417 (2)	57 (7)
H(181)	152 (2)	279 (2)	350 (1)	51 (6)
H(182)	296 (2)	370 (3)	361 (1)	65 (7)
H(19)	277 (3)	117 (3)	284 (2)	66 (7)
H(241)	557 (3)	−357 (3)	308 (2)	81 (8)
H(242)	447 (3)	−310 (3)	360 (2)	73 (8)
H(243)	471 (3)	−208 (3)	290 (1)	79 (8)
H(261)	655 (3)	448 (4)	399 (2)	121 (11)
H(262)	715 (3)	433 (4)	497 (2)	133 (12)
H(263)	586 (2)	548 (3)	465 (2)	86 (8)
(*b*) DHPP				
N(1)	2653 (2)	6120 (5)	444 (1)	47 (1)
C(2)	3317 (2)	7173 (6)	834 (1)	47 (1)
C(3)	3032 (2)	9021 (5)	1092 (1)	41 (1)
C(4)	1973 (2)	10086 (5)	952 (1)	44 (1)
C(5)	1243 (2)	8501 (5)	622 (1)	38 (1)
C(6)	1597 (3)	6695 (6)	374 (1)	46 (1)
C(7)	3747 (3)	9875 (6)	1544 (1)	50 (1)
N(8)	3484 (2)	11960 (5)	1724 (1)	58 (1)
C(9)	3861 (3)	12748 (9)	2243 (2)	87 (2)
C(10)	3086 (3)	14330 (9)	2439 (2)	85 (2)
C(11)	1957 (3)	13699 (7)	2247 (2)	58 (1)
C(12)	1493 (3)	11637 (6)	2373 (1)	59 (1)
C(13)	504 (3)	11000 (6)	2135 (1)	56 (1)
C(14)	−62 (3)	12391 (6)	1772 (1)	55 (1)
C(15)	370 (3)	14492 (6)	1665 (1)	64 (1)
C(16)	1363 (3)	15132 (6)	1893 (1)	64 (1)
C(17)	−1092 (3)	11433 (8)	1475 (2)	80 (2)
C(18)	−1154 (3)	11567 (7)	915 (2)	68 (1)
N(19)	−166 (2)	10971 (5)	749 (1)	52 (1)
C(20)	102 (2)	8831 (6)	599 (1)	43 (1)
O(21)	4514 (2)	8761 (5)	1746 (1)	73 (1)
O(22)	−545 (2)	7284 (4)	469 (1)	63 (1)
C(23)	3027 (3)	4315 (6)	130 (1)	53 (1)
C(24)	3422 (2)	5238 (6)	−335 (2)	46 (1)
C(25)	3926 (3)	7367 (7)	−347 (1)	63 (1)
C(26)	4288 (3)	8091 (7)	−788 (1)	73 (1)
C(27)	4156 (3)	6725 (8)	−1209 (1)	74 (1)
C(28)	3671 (3)	4619 (9)	−1200 (2)	85 (2)
C(29)	3295 (3)	3885 (7)	−765 (1)	70 (1)
H(2)	404 (3)	639 (6)	92 (1)	64 (9)
H(41)	198 (2)	1160 (6)	78 (1)	72 (10)
H(42)	168 (3)	1047 (5)	129 (1)	57 (9)
H(6)	110 (2)	561 (5)	13 (1)	53 (8)
H(8)	292 (3)	1277 (7)	155 (2)	93 (13)
H(91)	457 (3)	1328 (7)	228 (1)	99 (13)
H(92)	377 (4)	1128 (9)	252 (2)	169 (19)
H(101)	322 (3)	1444 (7)	284 (2)	103 (13)
H(102)	333 (4)	1629 (10)	231 (2)	198 (23)
H(12)	188 (3)	1060 (7)	262 (1)	93 (12)
H(13)	22 (3)	943 (6)	222 (2)	87 (12)
H(15)	−4 (3)	1551 (7)	140 (2)	107 (14)
H(16)	168 (3)	1665 (7)	179 (2)	93 (12)
H(171)	−120 (4)	931 (9)	152 (2)	154 (18)
H(172)	−168 (3)	1255 (7)	156 (2)	101 (13)
H(181)	−133 (3)	1341 (8)	85 (2)	133 (16)
H(182)	−172 (3)	1057 (6)	73 (2)	83 (12)
H(19)	40 (3)	1212 (7)	82 (2)	109 (14)
H(231)	239 (3)	303 (7)	3 (1)	99 (13)
H(232)	364 (3)	343 (6)	36 (1)	78 (11)
H(25)	406 (3)	828 (7)	−3 (2)	100 (13)
H(26)	470 (3)	965 (7)	−79 (2)	99 (13)
H(27)	444 (3)	723 (7)	−155 (2)	101 (13)
H(28)	357 (3)	352 (9)	−150 (2)	143 (18)
H(29)	282 (3)	236 (8)	−77 (1)	111 (14)

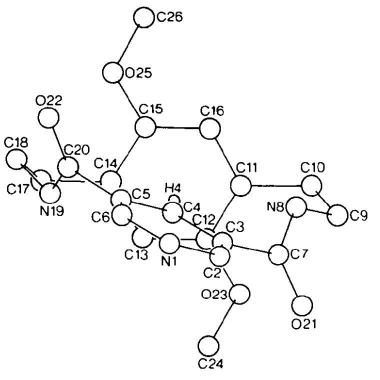
Introduction

The title compounds (hereafter referred to throughout as PP for the pyridinophane and DHPP for the dihydropyridinophane) have been synthesized by Rob, van Ramesdonk, Verhoeven, Pandit & de Boer (1980) in the course of a study of the shielding of 1,4-dihydropyridine in bridged dihydropyridines which might mimic the situation in various NAD(P)H dehydrogenase complexes. The crystal-structure determinations were undertaken to assist in the interpretation of the NMR data. The intensities were measured on a Nonius CAD-4 single-crystal diffractometer using graphite-monochromatized Cu $K\alpha$ radiation. Only reflexions with intensities above the 2σ level were treated as observed. No absorption correction was applied. The structures were solved by means of the symbolic addition program system *SIMPEL* (Overbeek

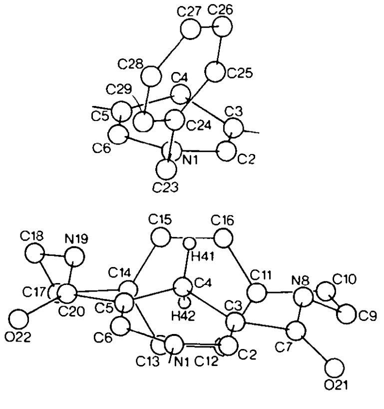
& Schenk, 1978). Refinement proceeded by means of block-diagonal least-squares calculations, anisotropic for C, N and O, isotropic for H. The H atoms were located in ΔF syntheses. The final R values were 0·041 for PP (2519 observed reflexions) and 0·048 for DHPP (2704 observed reflexions). The final coordinates are listed in Table 1.*

Discussion

Diagrams of the molecular geometries and the atomic numberings are given in Fig. 1. The bond distances and angles are normal and are listed in Table 2. As can be seen from Fig. 1 in both structures one H atom of the (dihydro)pyridine ring is approximately above the centre of the cyclophane benzene ring, the corresponding H–C(benzene) distances ranging from 2·80 to 3·11 Å in PP and from 2·94 to 3·18 Å in DHPP. The conformations of two ring-connecting chains in PP are very similar as can be seen in the Newman projections of Fig. 2(*a*). The two chains in DHPP have



(*a*)



(*b*)

Fig. 1. Numbering of the atoms and geometry of the molecule. (*a*) PP; (*b*) DHPP.

Table 2. *Bond distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

(*a*) PP			
N(1)–C(2)	1·343 (3)	C(11)–C(16)	1·394 (4)
N(1)–C(6)	1·344 (4)	C(12)–C(13)	1·394 (4)
C(2)–C(3)	1·381 (3)	C(12)–O(23)	1·385 (3)
C(3)–C(4)	1·385 (3)	C(13)–C(14)	1·394 (4)
C(3)–C(7)	1·504 (3)	C(14)–C(15)	1·390 (4)
C(4)–C(5)	1·383 (3)	C(14)–C(17)	1·514 (4)
C(5)–C(6)	1·377 (4)	C(15)–C(16)	1·398 (4)
C(5)–C(20)	1·503 (4)	C(15)–O(25)	1·379 (4)
C(7)–N(8)	1·336 (3)	C(17)–C(18)	1·535 (4)
C(7)–O(21)	1·236 (3)	C(18)–N(19)	1·459 (5)
N(8)–C(9)	1·460 (3)	N(19)–C(20)	1·336 (3)
C(9)–C(10)	1·534 (3)	C(20)–O(22)	1·230 (3)
C(10)–C(11)	1·517 (3)	O(23)–C(24)	1·426 (4)
C(11)–C(12)	1·393 (3)	O(25)–C(26)	1·417 (4)
C(2)–N(1)–C(6)	117·4 (2)	C(11)–C(12)–C(13)	120·8 (2)
N(1)–C(2)–C(3)	123·1 (2)	C(11)–C(12)–O(23)	116·2 (2)
C(2)–C(3)–C(4)	118·1 (2)	C(13)–C(12)–O(23)	123·0 (2)
C(2)–C(3)–C(7)	122·9 (2)	C(12)–C(13)–C(14)	121·5 (2)
C(4)–C(3)–C(7)	118·9 (2)	C(13)–C(14)–C(15)	117·7 (2)
C(3)–C(4)–C(5)	119·7 (2)	C(13)–C(14)–C(17)	120·3 (2)
C(4)–C(5)–C(6)	118·0 (3)	C(15)–C(14)–C(17)	122·0 (3)
C(4)–C(5)–C(20)	118·0 (3)	C(14)–C(15)–C(16)	121·1 (3)
C(6)–C(5)–C(20)	123·8 (2)	C(14)–C(15)–O(25)	116·1 (2)
N(1)–C(6)–C(5)	123·5 (2)	C(16)–C(15)–O(25)	122·7 (3)
C(3)–C(7)–N(8)	114·3 (2)	C(11)–C(16)–C(15)	121·0 (3)
C(3)–C(7)–O(21)	120·7 (2)	C(14)–C(17)–C(18)	113·8 (3)
N(8)–C(7)–O(21)	124·9 (2)	C(17)–C(18)–N(19)	109·3 (2)
C(7)–N(8)–C(9)	123·1 (2)	C(18)–N(19)–C(20)	124·2 (2)
N(8)–C(9)–C(10)	111·7 (2)	C(5)–C(20)–N(19)	113·9 (2)
C(9)–C(10)–C(11)	115·0 (2)	C(5)–C(20)–O(22)	121·2 (3)
C(10)–C(11)–C(12)	122·7 (2)	N(19)–C(20)–O(22)	124·8 (2)
C(10)–C(11)–C(16)	119·2 (2)	C(12)–O(23)–C(24)	116·1 (2)
C(12)–C(11)–C(16)	118·0 (2)	C(15)–O(25)–C(26)	117·7 (3)
(*b*) DHPP			
N(1)–C(2)	1·379 (4)	C(12)–C(13)	1·387 (6)
N(1)–C(6)	1·393 (5)	C(13)–C(14)	1·373 (5)
N(1)–C(23)	1·462 (5)	C(14)–C(15)	1·375 (5)
C(2)–C(3)	1·346 (5)	C(14)–C(17)	1·541 (6)
C(3)–C(4)	1·495 (4)	C(15)–C(16)	1·383 (5)
C(3)–C(7)	1·483 (4)	C(17)–C(18)	1·488 (8)
C(4)–C(5)	1·493 (4)	C(18)–N(19)	1·463 (5)
C(5)–C(6)	1·347 (5)	N(19)–C(20)	1·351 (5)
C(5)–C(20)	1·484 (4)	C(20)–O(22)	1·231 (4)
C(7)–N(8)	1·350 (5)	C(23)–C(24)	1·513 (6)
C(7)–O(21)	1·231 (5)	C(24)–C(25)	1·385 (5)
N(8)–C(9)	1·465 (6)	C(24)–C(29)	1·373 (6)
C(9)–C(10)	1·508 (7)	C(25)–C(26)	1·400 (5)
C(10)–C(11)	1·516 (6)	C(26)–C(27)	1·358 (5)
C(11)–C(12)	1·390 (6)	C(27)–C(28)	1·361 (7)
C(11)–C(16)	1·388 (5)	C(28)–C(29)	1·396 (7)
C(2)–N(1)–C(6)	118·7 (3)	C(12)–C(13)–C(14)	121·5 (3)
C(2)–N(1)–C(23)	121·1 (3)	C(13)–C(14)–C(15)	117·6 (3)
C(6)–N(1)–C(23)	120·0 (3)	C(13)–C(14)–C(17)	118·6 (4)
N(1)–C(2)–C(3)	122·7 (3)	C(15)–C(14)–C(17)	123·5 (3)
C(2)–C(3)–C(4)	120·6 (2)	C(14)–C(15)–C(16)	121·5 (3)
C(2)–C(3)–C(7)	119·3 (3)	C(11)–C(16)–C(15)	121·3 (4)
C(4)–C(3)–C(7)	120·0 (3)	C(14)–C(17)–C(18)	113·7 (4)
C(3)–C(4)–C(5)	118·8 (3)	C(17)–C(18)–N(19)	112·6 (3)
C(4)–C(5)–C(6)	121·5 (3)	C(18)–N(19)–C(20)	125·5 (3)
C(4)–C(5)–C(20)	111·8 (3)	C(5)–C(20)–N(19)	113·9 (3)
C(6)–C(5)–C(20)	119·6 (3)	C(5)–C(20)–O(22)	123·5 (3)
N(1)–C(6)–C(5)	121·4 (3)	N(19)–C(20)–O(22)	122·6 (3)
C(3)–C(7)–N(8)	114·9 (3)	N(1)–C(23)–C(24)	114·4 (3)
C(3)–C(7)–O(21)	122·8 (3)	C(23)–C(24)–C(25)	123·3 (4)
N(8)–C(7)–O(21)	122·3 (3)	C(23)–C(24)–C(29)	118·7 (3)
C(7)–N(8)–C(9)	122·9 (3)	C(25)–C(24)–C(29)	118·0 (4)
N(8)–C(9)–C(10)	111·9 (3)	C(24)–C(25)–C(26)	120·2 (4)
C(9)–C(10)–C(11)	113·7 (4)	C(25)–C(26)–C(27)	120·8 (4)
C(10)–C(11)–C(12)	123·6 (4)	C(26)–C(27)–C(28)	119·4 (4)
C(10)–C(11)–C(16)	119·4 (4)	C(27)–C(28)–C(29)	120·4 (5)
C(12)–C(11)–C(16)	116·8 (4)	C(24)–C(29)–C(28)	121·1 (4)
C(11)–C(12)–C(13)	121·1 (3)		

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36216 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

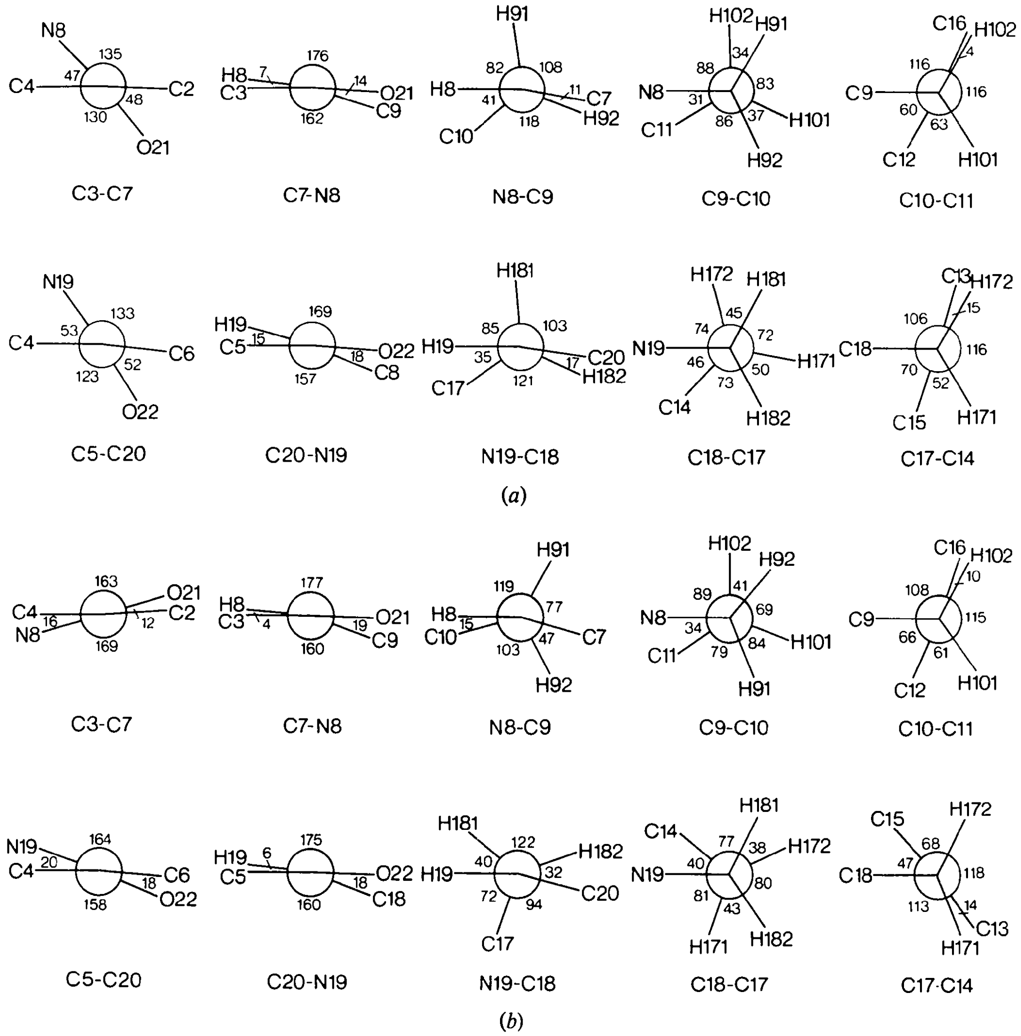

Fig. 2. Newman projections along the bonds of the ring-connecting chains. (*a*) PP; (*b*) DHPP. (Angles in degrees: e.s.d.'s ~0·2 and 0·3° for PP and DHPP respectively.)

Table 3. *Distances* (Å) *from various planes*

(I) N(1)···C(6) (PP), (II) C(11)···C(16) (PP), (III) C(2),C(3),C(5),C(6) (DHPP), (IV) C(11)···C(16) (DHPP), (V) C(24)···C(29) (DHPP).

	I		II		III		IV		V
N(1)	0·002 (2)	C(11)	−0·002 (2)	C(2)	0·006 (3)	C(11)	−0·020 (4)	C(24)	0·000 (4)
C(2)	−0·019 (2)	C(12)	−0·005 (2)	C(3)	−0·006 (3)	C(12)	0·015 (3)	C(25)	0·003 (4)
C(3)	0·016 (2)	C(13)	0·007 (2)	C(5)	0·006 (3)	C(13)	0·005 (3)	C(26)	−0·001 (4)
C(4)	0·002 (2)	C(14)	−0·002 (3)	C(6)	−0·006 (3)	C(14)	−0·021 (3)	C(27)	−0·004 (4)
C(5)	−0·018 (3)	C(15)	−0·004 (3)	N(1)	−0·119 (3)	C(15)	0·016 (3)	C(28)	0·007 (5)
C(6)	0·017 (2)	C(16)	0·007 (3)	C(4)	−0·207 (3)	C(16)	0·004 (3)	C(29)	−0·005 (4)
C(7)	0·027 (2)	C(10)	−0·088 (2)			C(10)	−0·202 (5)	C(23)	0·030 (3)
C(20)	0·050 (2)	C(17)	−0·082 (3)			C(17)	−0·214 (5)		
		O(23)	−0·031 (2)						
		C(24)	−0·600 (3)						
		O(25)	−0·014 (2)						
		C(26)	−0·355 (3)						

different conformations which also differ from those in PP (Fig. 2*b*). Judging from the deviations from the ideal conformations around the individual bonds, there is considerable strain in all four chains. The Newman projections along C(7)—N(8) and C(20)—N(19) in both compounds, for instance, reveal marked deviations from the ideal planar conformation for the amido group.

In Table 3 the deviations from the best planes through the various rings are given for the ring atoms and for a number of adjacent atoms. In PP the benzene ring is planar; the adjacent atoms C(10) and C(17) are displaced by about 0·08 Å towards the pyridine ring. The pyridine ring is slightly twisted about an axis perpendicular to the line N(1)—C(4). The two rings are at an angle of 77°. In DHPP the benzene ring C(11)—C(16) shows significant deviations from planarity, C(11) and C(14) being displaced by about 0·02 Å towards the dihydropyridine ring. The adjacent atoms C(10) and C(17) are displaced by about 0·2 Å in the same direction. Apparently this benzene ring is under greater stress than the corresponding one in PP. The dihydropyridine ring is in a boat conformation with C(2), C(3), C(5) and C(6) coplanar and N(1) and C(4) at 0·12 and 0·21 Å respectively from the plane of the first four atoms. The benzene ring C(24)—C(29) in DHPP is planar with C(23) at 0·03 Å. The N and O atoms of the amido groups in PP are involved in hydrogen bonding with O and N respectively of amido groups of adjacent molecules along the screw axes. The lengths of the two hydrogen bonds are 2·993 Å for N(8)···O(21) ($\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$) and 2·938 Å for N(19)···O(22) ($\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$). The hydrogen bonds interconnect the molecules to form sheets parallel to (001). These sheets can be clearly seen in the projection along [010] of Fig. 3. Benzene rings of adjacent sheets are overlapping across centres of symmetry (Fig. 4) with a perpendicular ring-to-ring separation of 3·43 Å.

No hydrogen bonds are found in DHPP, the packing of which shows no noticeable features.

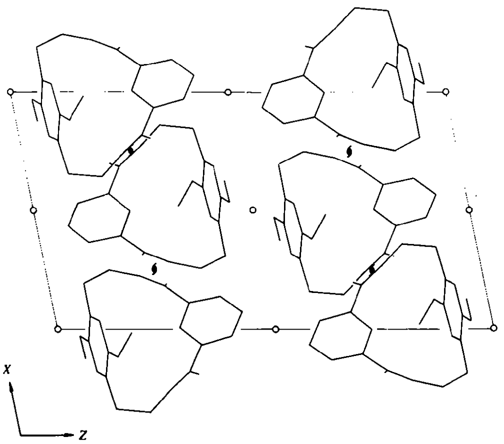

Fig. 3. Projection of the structure of PP along [010].

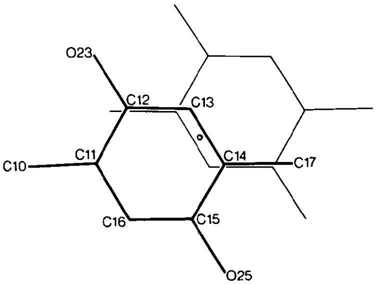

Fig. 4. Overlap of benzene rings across a centre of symmetry in PP. Projection perpendicular to the benzene rings.

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