Table 3. *Torsion angles* (°)

C(2*A*)–C(1*A*)–O(1*B*)–C(12*B*)	67·1	C(11*B*)–C(10*B*)–C(6*B*)–C(5*B*)	−46·0	O(1*A*)–C(12*A*)–C(11*A*)–C(10*A*)	172·0
C(9*A*)–C(1*A*)–O(1*B*)–C(12*B*)	−114·7	C(11*B*)–C(10*B*)–C(6*B*)–C(7*B*)	67·6	C(12*A*)–C(11*A*)–C(10*A*)–C(6*A*)	−150·9
C(1*A*)–O(1*B*)–C(12*B*)–C(11*B*)	69·2	C(2*B*)–C(1*B*)–O(1*A*)–C(12*A*)	177·3	C(11*A*)–C(10*A*)–C(6*A*)–C(5*A*)	−49·7
O(1*B*)–C(12*B*)–C(11*B*)–C(10*B*)	69·1	C(9*B*)–C(1*B*)–O(1*A*)–C(12*A*)	−4·4	C(11*A*)–C(10*A*)–C(6*A*)–C(7*A*)	64·9
C(12*B*)–C(11*B*)–C(10*B*)–C(6*B*)	−166·8	C(1*B*)–O(1*A*)–C(12*A*)–C(11*A*)	−72·2		

(torsion angles are given in Table 3). The molecule does not have the compact *ansa* shape of the centrosymmetric dimer, nor does it have twofold symmetry (which would be possible since both quaternary C atoms have the same chirality). It is possible to build models with planar anisolic groups and no unfavourable intramolecular contacts, so it is unclear why the conformation is so irregular.

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N,*N*′-Diphenylterephthalamide (DPTP)*

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Abstract. $C_{20}H_{16}N_2O_2$, monoclinic, $P2_1/n$, a = 6·912 (3), b = 21·462 (5), c = 5·323 (3) Å, β = 107·20 (5)°, Z = 2. The crystal structure was solved by direct methods and all H atoms were located: R_w = 4·9%. The structure contains planar phenyl rings which are rotated with respect to the plane of the amide group due to steric hindrance. The molecules are connected by hydrogen bonds.

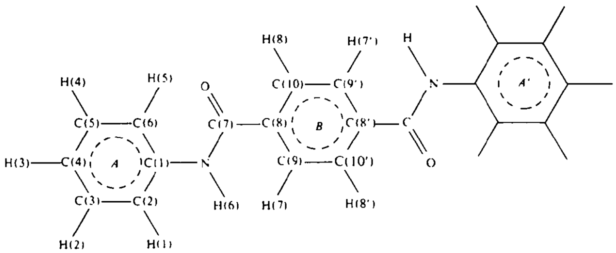

Fig. 1. Atomic arrangement of DPTP.

Introduction. The present investigation is part of a series on the structures of model compounds of aromatic and aliphatic–aromatic polyamides (Harkema & Gaymans, 1977). In this paper the crystal structure of DPTP (Fig. 1) is reported.

DPTP was prepared as described by Gaymans & Harkema (1977). Recrystallization from dimethylacetamide yielded suitable crystals. Intensities were collected at 293 K on a Philips PW 1100 diffractometer with graphite-monochromated Mo $K\alpha$ radiation (λ = 0·7107 Å). Reflexions up to θ = 30° were measured with the ω–2θ scan mode. The number of reflexions measured was 1912 and all were used in the refinement. No absorption correction was applied. The structure was solved by direct methods with *MAGIC* (Dewar, 1970). Details of the weighting scheme, scattering factors and the refinement procedure are given in Harkema & Gaymans (1977). The final value

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Table 1. *Fractional atomic coordinates* (×10⁴)

	x	*y*	*z*
C(1)	3643 (2)	6344 (1)	1581 (3)
C(2)	3384 (2)	6755 (1)	−507 (3)
C(3)	1681 (2)	7131 (1)	8758 (3)
C(4)	238 (2)	7101 (1)	77 (3)
C(5)	504 (2)	6691 (1)	2150 (3)
C(6)	2201 (2)	6308 (1)	2918 (3)
C(7)	6418 (2)	5734 (1)	4625 (3)
C(8)	8263 (2)	5355 (1)	4740 (3)
C(9)	8425 (2)	4984 (1)	2666 (3)
C(10)	9848 (2)	5367 (1)	7074 (3)
N	5391 (2)	5958 (1)	2210 (2)
O	5918 (2)	5837 (1)	6611 (2)
H(1)	4394 (25)	6769 (7)	−1434 (34)
H(2)	1497 (25)	7404 (8)	−2698 (37)
H(3)	−911 (24)	7355 (8)	−443 (33)
H(4)	9485 (23)	6653 (7)	3080 (31)
H(5)	2366 (22)	6023 (7)	4412 (32)
H(6)	5972 (23)	5905 (8)	1009 (34)
H(7)	7327 (20)	4961 (7)	1022 (31)
H(8)	9719 (21)	5631 (7)	8458 (30)

of R_w was 4·9%.* As the number of molecules in the unit cell is half the number of equivalent positions of the space group, the molecule has to be on a center of symmetry.

Discussion. Final atomic positions are given in Table 1, the numbering of the atoms in Fig. 1. Bond distances and angles are in Table 2. Best planes have been fitted to different groups of atoms (Table 3).

It can be seen that both phenyl rings including H atoms are planar within experimental error. However, the deviation of C(7) and N from the plane of the rings to which they are attached is significant. Furthermore the H atom of the amide group is not in the plane of the heavy atoms, giving a pyramidal arrangement of bonds around N. A similar effect occurs in *N,N'*-(*p*-phenylene)dibenzamide (PPDB) (Harkema & Gaymans, 1977).

The phenyl rings are rotated with respect to the plane of the amide group, the angles of rotation being 30·4 and −30·6° for rings *A* and *B* respectively. The angle between the two planes of the phenyl rings is 60·7°.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34043 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å) *and angles* (°)

C(1)–C(2)	1·389 (2)	C(8)–C(10)	1·393 (2)
C(1)–C(6)	1·387 (2)	C(9)–C(10')	1·384 (2)
C(1)–N	1·421 (2)		
C(2)–C(3)	1·385 (2)	C(2)–H(1)	0·97 (2)
C(3)–C(4)	1·381 (2)	C(3)–H(2)	0·95 (2)
C(4)–C(5)	1·380 (2)	C(4)–H(3)	0·94 (2)
C(5)–C(6)	1·392 (2)	C(5)–H(4)	0·98 (2)
C(7)–N	1·359 (2)	C(6)–H(5)	0·98 (2)
C(7)–O	1·226 (2)	C(9)–H(7)	0·98 (2)
C(7)–C(8)	1·499 (2)	C(10)–H(8)	0·95 (2)
C(8)–C(9)	1·392 (2)	N–H(6)	0·86 (2)
C(6)–C(1)–N	122·4 (2)	C(5)–C(6)–H(5)	119 (2)
C(2)–C(1)–N	117·3 (2)	C(8)–C(7)–N	115·5 (2)
C(2)–C(1)–C(6)	120·3 (2)	C(8)–C(7)–O	121·1 (2)
C(1)–C(2)–C(3)	119·6 (2)	N–C(7)–O	123·4 (2)
C(1)–C(2)–H(1)	119 (2)	C(7)–C(8)–C(9)	123·1 (2)
C(3)–C(2)–H(1)	121 (2)	C(7)–C(8)–C(10)	117·5 (2)
C(2)–C(3)–C(4)	120·7 (2)	C(9)–C(8)–C(10)	119·4 (2)
C(2)–C(3)–H(2)	119 (2)	C(8)–C(9)–C(10')	120·1 (2)
C(4)–C(3)–H(2)	120 (2)	C(8)–C(9)–H(7)	121 (2)
C(3)–C(4)–C(5)	119·4 (2)	C(10')–C(9)–H(7)	119 (2)
C(3)–C(4)–H(3)	120 (2)	C(8)–C(10)–C(9')	120·4 (2)
C(5)–C(4)–H(3)	121 (2)	C(8)–C(10)–H(8)	118 (2)
C(4)–C(5)–C(6)	120·9 (2)	C(9')–C(10)–H(8)	121 (2)
C(4)–C(5)–H(4)	121 (2)	C(1)–N–C(7)	126·8 (2)
C(6)–C(5)–H(4)	118 (2)	C(1)–N–H(6)	117 (2)
C(1)–C(6)–C(5)	119·2 (2)	C(7)–N–H(6)	116 (2)
C(1)–C(6)–H(5)	121 (2)		

Table 3. *Distances* (Å) *of the atoms to the different planes in the molecule*

Plane 1: plane fitted to the C atoms of phenyl ring *A* (Fig. 1)

$$0.20054x + 1.39875y + 0.25135z = 1$$

Plane 2: plane fitted to C(7), N and O of the amide group

$$0.30047x + 1.40576y + 0.00242z = 1$$

Plane 3: plane fitted to the C atoms of phenyl ring *B* (Fig. 1)

$$0.35210x + 1.54358y - 0.24777z = 1$$

	Plane 1	Plane 2	Plane 3		Plane 1	Plane 2	Plane 3
C(1)	−0·002 (2)	−0·020 (2)	–	N	0·033 (2)	0·000 (2)	–
C(2)	0·000 (2)	–	–	O	–	0·000 (2)	–
C(3)	0·001 (2)	–	–	H(1)	0·01 (2)	–	–
C(4)	0·000 (2)	–	–	H(2)	0·02 (2)	–	–
C(5)	−0·001 (2)	–	–	H(3)	0·01 (2)	–	–
C(6)	0·002 (2)	–	–	H(4)	0·03 (2)	–	–
C(7)	–	0·000 (2)	0·038 (2)	H(5)	−0·01 (2)	–	–
C(8)	–	−0·028 (2)	−0·001 (2)	H(6)	–	−0·12 (2)	–
C(9)	–	–	0·001 (2)	H(7)	–	–	0·02 (2)
C(10)	–	–	0·001 (2)	H(8)	–	–	−0·02 (2)

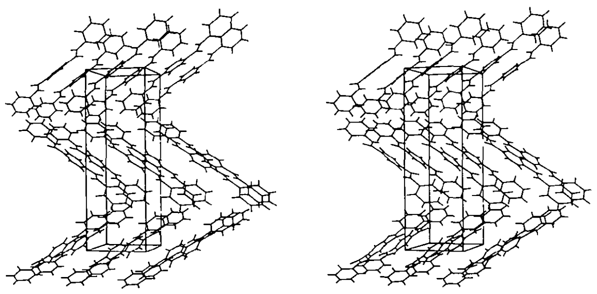

Fig. 2. A stereoscopic view of the packing.

Significant differences exist with twist angles observed in related compounds. The value of 30·4° observed here can be compared with the 17·6 in acetanilide (Brown, 1966) and 35·9° in PPDB. The corresponding values of the angle 30·6° are 24·6 in benzamide (Blake & Small, 1972) and 29·1° in PPDB.

The molecules of DPTP are linked by N—H···O hydrogen bonds of length 3·118 (2) Å. As in PPDB each molecule is hydrogen bonded to two other molecules. The molecules connected in this way are related to each other by translation along *c*. The hydrogen-bonding scheme found in both DPTP and PPDB contrasts with that found in a second polymorph of PPDB (Adams, Fratini & Wiff, 1978) in which each molecule is hydrogen bonded to four others.

A stereoscopic view of the crystal structure prepared by *POP*1 (van de Waal, 1978) is given in Fig. 2.

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Trifluoroacetic Acid*

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Abstract. $C_2HF_3O_2$, monoclinic, $P2_1/c$, $Z = 4$, $a = 8{\cdot}060\,(1)$, $b = 4{\cdot}762\,(1)$, $c = 9{\cdot}959\,(1)$ Å, $\beta = 107{\cdot}64\,(1)°$, $D_x = 2{\cdot}079$ Mg m^{-3} at 83 K, m.p. 257·9 K. Intensities were recorded at 83 K. Refinement with 524 observed data gave $R(F) = 0{\cdot}047$, $R_w(F) = 0{\cdot}060$. The structure is composed of hydrogen-bonded centrosymmetric dimers packing with normal van der Waals separations. The O—H···O bond is 2·648 (3) Å.

Introduction. The present investigation was undertaken to study the geometry of the CF_3COOH molecule and its bonding in the solid state. Formic and acetic acids have been found to form infinite chains in the crystalline state (Nahringbauer, 1978, 1970) whereas the chloro-substituted acetic acid (Jönsson & Hamilton, 1972) and higher carboxylic acids (Strieter, Templeton, Scheuerman & Sass, 1962) occur as dimers. The preference of the dimeric form to the chain form might be a steric effect due to the substitution of the CH_3 group by the larger CCl_3 or more bulky aliphatic groups. However, the substitution of only one H atom by F can give the dimeric form. The monofluoroacetic acid structure is composed of centrosymmetric dimers formed by carboxyl-group coupling (Kanters & Kroon, 1972). The size of the CF_3 group is intermediate between those of CH_3 and CCl_3; the structure determination of trifluoroacetic acid is thus a natural extension of the previous studies.

Crystals were grown by zone melting from commercially available CF_3COOH (*pro analysi*) sealed in thin-walled glass capillaries. Cell dimensions and intensities

* Hydrogen Bond Studies. CXXXV. Part CXXXIV: Lundgren, Tellgren & Olovsson (1978).

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