Acta Cryst. (1977). B**33**, 2449–2454

The Crystal and Molecular Structures of *p*-Aminoacetanilide and *p*-Methylacetanilide

By Masao Haisa, Setsuo Kashino, Yosuke Matsuzaki, Ryoichi Kawai and Koji Kunitomi

Department of Chemistry, Faculty of Science, Okayama University, Tsushima, Okayama 700, *Japan*

(*Received* 13 *October* 1976; *accepted* 24 *January* 1977)

The crystal structures of *p*-aminoacetanilide (PAAA), and the monoclinic [PMAA (*M*)] and orthorhombic [PMAA (*O*)] dimorphs of *p*-methylacetanilide have been determined from visually estimated Cu $K\alpha$ data. The unit cells are: *Pcab*, a = 11·98 (2), b = 17·44 (2), c = 7·37 (1) Å, Z = 8 for PAAA; $P2_1/c$, a = 11·74 (2), b = 9·59 (2), c = 7·56 (1) Å, β = 106·0 (2)°, Z = 4 for PMAA (*M*); and $Pna2_1$, a = 9·899 (5), b = 12·956 (6), c = 6·541 (4) Å, Z = 4 for PMAA (*O*). The structures were refined by block-diagonal least-squares calculations to R values of 0·084, 0·084 and 0·088 for 1161, 1328 and 767 non-zero reflexions, for PAAA, PMAA (*M*) and PMAA (*O*) respectively. In PAAA two kinds of hydrogen bonds [3·088 (4) Å, NH_2 donates H to O=C; 3·050 (4) Å, NH_2 accepts H from amide NH] form molecular sheets parallel to (001), in a similar manner to that found in the orthorhombic form of *p*-hydroxyacetanilide. The sheets are stacked along **c**. In PMAA (*M*) the molecules related by a twofold screw axis are linked together by the C=O···HN hydrogen bond [2·923 (3) Å], while in PMAA (*O*) those related by an *a* glide plane are O···N [2·904 (8) Å]. A disordered structure mirrored by an *n*-glide plane with an occupancy factor of 0·25 was found in PMAA (*O*). Torsion angles about the N(amide)–C(ring) bond vary from 8·3° for PMAA (*O*) to 32·2° for PAAA.

Introduction

As part of a study of molecular stacking and overlapping in the crystals of acetanilide derivatives, we have already determined the crystal structures of dimorphs of *p*-hydroxyacetanilide {orthorhombic [PHAA (*O*)] and monoclinic [PHAA (*M*)] forms (Haisa, Kashino & Maeda, 1974; Haisa, Kashino, Kawai & Maeda, 1976}. The present work has been undertaken to examine the effect of *para* substituents, p-XH_m (X = O, N, C for m = 1, 2, 3 respectively), on the hydrogen-bond system and on the crystal structure. The present paper reports the structures of *p*-aminoacetanilide (PAAA) and of the monoclinic [PMAA (*M*)] and orthorhombic [PMAA (*O*)] dimorphs of *p*-methylacetanilide, and the appearance of a disordered structure in PMAA (*O*).*

Experimental

All the crystals were grown by slow evaporation from ethanol solutions as transparent single crystals. Crystals of PMAA (*O*) were grown from a solution of relatively low saturation. Intensities were estimated visually on equi-inclination Weissenberg photographs and were corrected for Lorentz and polarization factors, and for spot shape. The data were put on an approximately absolute scale by Wilson's plot. The Weissenberg photographs of PMAA (*O*) exhibited remarkable diffuse streaks for the reflexions with $h = 2n$ and $k + l = 2n + 1$; the streaks were elongated along **c*** and **a***. Crystal data and experimental details are summarized in Table 1.

Structure determination and refinement

The structures of PAAA and PMAA (*M*) were solved by the symbolic addition procedure, as summarized in Table 2. The E maps revealed all the non-hydrogen atoms. Block-diagonal least-squares refinements with anisotropic thermal parameters reduced R values to 0·12 for PAAA and 0·11 for PMAA (*M*). Difference Fourier maps revealed all the H atoms. Including all the atoms, further refinements were carried out with the weighting scheme: $w = 1{\cdot}0$ for $0 < |F_o| \le F_{\max}$, $w = (F_{\max}/|F_o|)^2$ for $|F_o| > F_{\max}$. The values of $F_{\max}$ were chosen to be 7·0 for PAAA and 4·0 for PMAA (*M*). The final R values for PAAA and PMAA (*M*) were 0·084 and 0·084 for 1161 and 1328 non-zero reflexions respectively. In the case of PAAA, the six strongest reflexions were corrected for extinction according to the formula $I_{\rm corr} = I_{\rm obs}(1 - 1{\cdot}88 \times 10^{-5}\, I_{\rm obs})$.

The structure of PMAA (*O*) was solved with the parameters for *p*-bromoacetanilide (Andreetti, Cavalca, Domiano & Musatti, 1968), which was considered to be isomorphous. Block-diagonal least-squares calculations reduced the R value to 0·185. However, a difference Fourier map at this stage had hydrogen-atom peaks and residual electron densities (Fig. 1) which

---

* The structure of PMAA (*M*) determined from diffractometer data by Maeda, Kamijyo & Fukui (1976) agrees well with the present result from photographic data, but the structure of PMAA (*O*) shows some differences, as discussed in the text.

Table 1. *Crystal data and experimental details*

	p-Aminoacetanilide	p-Methylacetanilide	
	$C_8H_{10}N_2O$, M_r = 150·2	$C_9H_{11}NO$, M_r = 149·2	
Crystal system	Orthorhombic (PAAA)	Monoclinic [PMAA (*M*)]	Orthorhombic [PMAA (*O*)]
Morphology	Light-red needles elongated along **c**	Colourless plates developed on (100)	Colourless prisms elongated along **c**
M.p. (°C)	165–166	147–148	151–152
Space group	*Pcab*	$P2_1/c$	$Pna2_1$
Systematic absences	0*kl*, *l* odd *h*0*l*, *h* odd *hk*0, *k* odd	*h*0*l*, *l* odd 0*k*0, *k* odd	*h*0*l*, *l* odd 0*kl*, *k* + *l* odd
a (Å)	11·98 (2)	11·74 (2)	9·899 (5)
b (Å)	17·44 (2)	9·59 (2)	12·956 (6)
c (Å)	7·37 (1)	7·56 (1)	6·541 (4)
β (°)	–	106·0 (2)	–
V (Å^3)	1540 (4)	818 (2)	839·0 (8)
Z	8	4	4
D_x (g cm^{-3})	1·295	1·211	1·181
D_m (g cm^{-3})	1·27	1·19	1·19
Flotation mixture	KI–H_2O	KI–H_2O	Cyclohexane–CCl_4
Dimensions of specimens used (mm)	0·10 × 0·10 × 0·60 0·27 × 0·10 × 0·15	0·38 × 0·50 × 0·52 0·32 × 0·50 × 0·40	0·28 × 0·18 × 0·60 0·55 × 0·12 × 0·35
Layers photographed	*hk*0 to *hk*5 0*kl* to 9*kl*	*hk*0 to *hk*5 *h*0*l* to *h*7*l*	*hk*0 to *hk*5 0*kl* to 7*kl*
Non-zero reflexions	1161	1328	767
Per cent accessible	68·0	72·0	74·1
B (Å^2) from Wilson's plot	3·4	4·1	5·0

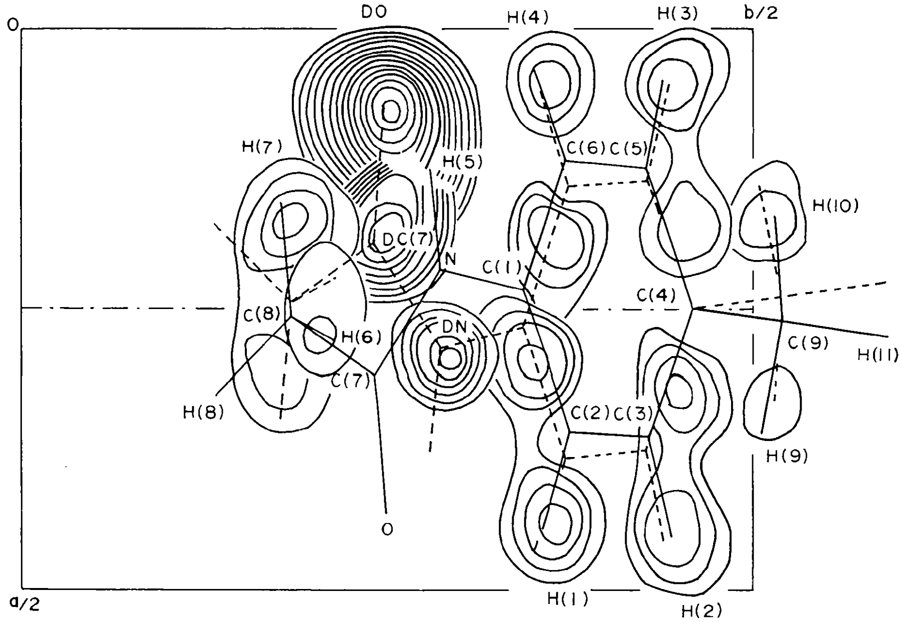

Fig. 1. Difference Fourier map for PMAA (*O*) at the stage of *R* = 0·185, showing the disorder of the molecule. Contours are at intervals of 0·1 e Å^{-3} starting at 0·3 e Å^{-3}. The molecular frames are based on the final positional parameters.

Table 2. *Details of the symbolic addition procedure*

Starting set of phases

PAAA h	k	l	$\|E\|$	Phases	PMAA (M) h	k	l	$\|E\|$	Phases
4	7	8	2·85	0	8	9	2	3·34	0
9	10	0	2·86	0	1	8	2	3·18	π
12	9	3	3·49	0	0	5	5	2·28	0
1	14	1	3·58	A	8	8	0	3·96	A
6	8	4	3·57	B	1	11	−4	3·73	B
10	10	1	3·20	C	7	7	1	3·60	C

Number of reflexions determined by the Σ_2 relationships

52 out of 119 with $|E| > 1{\cdot}8$ 50 out of 128 with $|E| > 1{\cdot}8$

Minimum value of Karle's R after the application of the tangent formula

0·211 for $A=C=0$ and $B=\pi$ 0·219 for $A=B=C=0$

Number of terms used for computing the E map

203 with $|E| > 1{\cdot}5$ 230 with $|E| > 1{\cdot}5$

Table 3. *The final positional parameters* ($\times 10^4$) *of the non-hydrogen atoms with standard deviations in parentheses*

For the disordered atoms the occupancy factor is 0·25, and their respective atomic coordinates are $\frac{1}{2}-x, y, z$.

	x	y	z
(*a*) PAAA			
O	1436 (2)	4854 (1)	3517 (4)
N(1)	2671 (2)	3921 (1)	2802 (3)
N(2)	13 (2)	1329 (1)	1291 (4)
C(1)	1941 (2)	3292 (1)	2494 (3)
C(2)	896 (2)	3367 (2)	1696 (4)
C(3)	264 (2)	2720 (2)	1296 (4)
C(4)	662 (2)	1987 (2)	1687 (3)
C(5)	1697 (2)	1918 (1)	2540 (4)
C(6)	2329 (2)	2565 (2)	2939 (4)
C(7)	2402 (3)	4641 (2)	3282 (4)
C(8)	3391 (3)	5167 (2)	3501 (5)
(*b*) PMAA (*M*)			
O	5212 (2)	2688 (2)	3391 (3)
N	4411 (2)	541 (2)	2684 (3)
C(1)	3245 (2)	760 (2)	2820 (3)
C(2)	2916 (2)	1862 (2)	3768 (3)
C(3)	1752 (2)	1970 (3)	3841 (4)
C(4)	886 (2)	1015 (3)	2993 (3)
C(5)	1235 (2)	−79 (3)	2054 (4)
C(6)	2391 (2)	−208 (2)	1969 (4)
C(7)	5302 (2)	1475 (2)	2958 (3)
C(8)	6436 (2)	915 (3)	2671 (4)
C(9)	−391 (3)	1148 (4)	3038 (5)
(*c*) PMAA (*O*)			
O	4304 (4)	2483 (4)	5585 (9)
N	2140 (4)	2870 (3)	4696 (9)
C(1)	2329 (4)	3436 (4)	2878 (9)
C(2)	3572 (5)	3743 (5)	2105 (11)
C(3)	3636 (5)	4297 (5)	299 (10)
C(4)	2494 (5)	4588 (4)	−763 (11)
C(5)	1250 (5)	4278 (5)	24 (11)
C(6)	1168 (5)	3729 (5)	1825 (11)
C(7)	3082 (5)	2419 (4)	5898 (10)
C(8)	2541 (5)	1842 (5)	7714 (13)
C(9)	2599 (6)	5213 (5)	−2724 (11)

Table 4. *The final parameters* ($\times 10^3$, *except* B) *of the hydrogen atoms*

	x	y	z	B (Å^2)
(*a*) PAAA				
H(1)	57 (3)	386 (2)	134 (4)	1·7 (7)
H(2)	−41 (3)	280 (2)	72 (5)	1·6 (7)
H(3)	201 (3)	136 (2)	282 (5)	1·9 (7)
H(4)	298 (3)	248 (2)	353 (4)	1·2 (6)
H(5)	333 (3)	387 (2)	263 (5)	1·2 (6)
H(6)	418 (6)	492 (4)	384 (8)	7·5 (17)
H(7)	355 (5)	543 (4)	245 (10)	7·3 (15)
H(8)	312 (5)	562 (3)	404 (9)	5·8 (14)
H(9)	54 (3)	86 (2)	117 (5)	2·2 (8)
H(10)	−38 (3)	140 (2)	33 (6)	2·8 (8)
(*b*) PMAA (*M*)				
H(1)	351 (3)	261 (4)	446 (5)	3·0 (7)
H(2)	153 (3)	280 (3)	448 (5)	2·4 (7)
H(3)	67 (4)	−85 (4)	157 (5)	3·9 (9)
H(4)	259 (4)	−97 (4)	138 (5)	3·2 (7)
H(5)	454 (3)	−30 (4)	237 (5)	2·4 (7)
H(6)	636 (4)	−5 (4)	244 (6)	4·6 (10)
H(7)	697 (7)	89 (7)	376 (10)	10·7 (20)
H(8)	657 (4)	143 (5)	166 (7)	5·3 (10)
H(9)	−74 (4)	187 (4)	219 (6)	5·0 (10)
H(10)	−37 (4)	160 (4)	424 (6)	4·8 (10)
H(11)	−66 (4)	22 (5)	294 (6)	4·9 (10)
(*c*) PMAA (*O*)				
H(1)	443	356	291	
H(2)	451	452	−28	
H(3)	44	440	−56	
H(4)	34	351	240	
H(5)	123	279	505	
H(6)	279	214	927	
H(7)	153	178	803	
H(8)	324	132	771	
H(9)	360	506	−326	
H(10)	168	515	−322	
H(11)	274	592	−245	

were interpreted on the assumption that the structure was disordered, with an additional mirror plane superposed on the *n*-glide plane. Space group *Pnam* was ruled out from a consideration of the molecular packing. The acceptable occupancy factor for the disordered structure was determined to be 0·25 by taking account of the variation of the R index, and thermal parameters and bond distances concerning the O, C(7), *D*O and *D*C(7) atoms. Further refinements of the parameters for the ordered non-hydrogen atoms (occupancy factor 0·75) reduced R to the final value of 0·088 for 767 nonzero reflexions.* For the H atoms and all the disordered atoms the isotropic thermal parameters $B=5{\cdot}0$ Å^2 were assumed and the positional parameters were kept fixed. The weighting scheme used was identical with that given above, but here $F_{\max}=5{\cdot}0$.

---

* Lists of structure factors and anisotropic thermal parameters for all three compounds have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32489 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

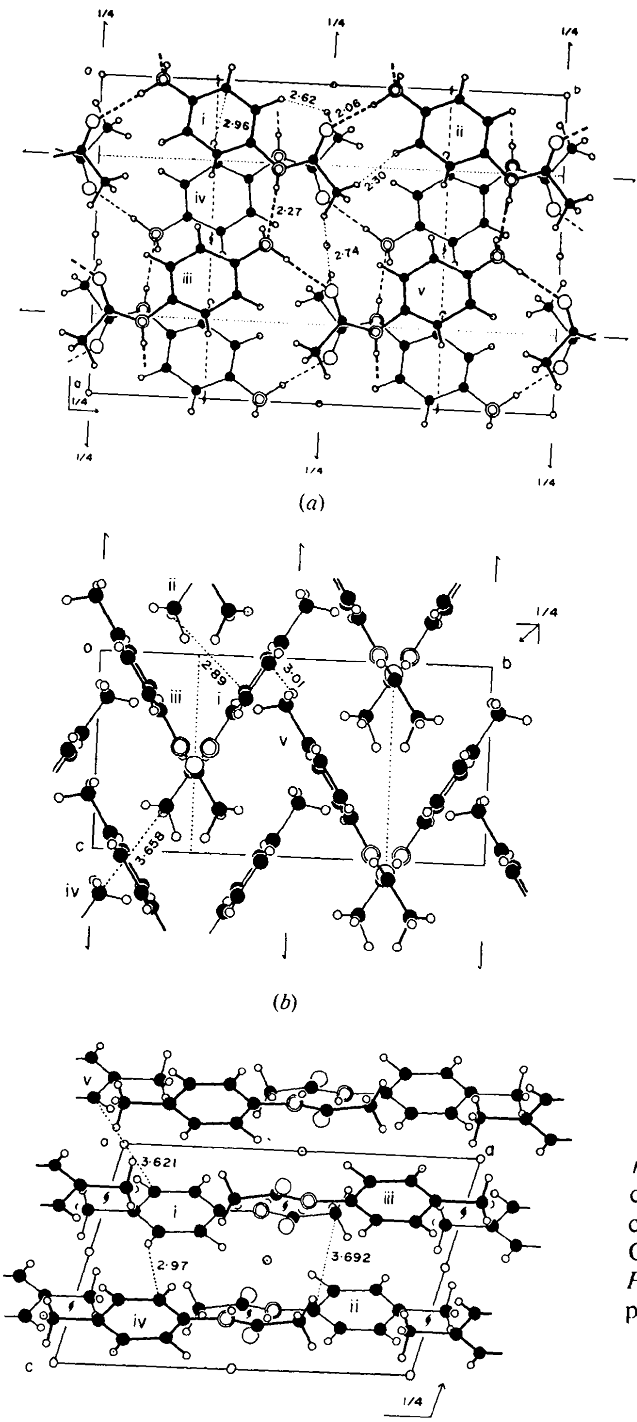

Fig. 2. Projections of the crystal structures. (*a*) PAAA viewed along **c**, (*b*) PMAA (*M*) viewed along **b**, and (*c*) PMAA (*O*) viewed along **a**. Symmetry code: for PAAA: (i) x,y,z; (ii) $x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, z$; (iv) $\frac{1}{2}-x, y, -\frac{1}{2}+z$; (v) $\frac{1}{2}+x, 1-y, z$; for PMAA (*M*): (i) x,y,z; (ii) $1-x, -y, 1-z$; (iii) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (v) $-x,-y,-z$; (vi) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; for PMAA (*O*): (i) x,y,z; (ii) $x, y, -1+z$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, z$; (iv) $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{3}{4}+z$; (v) $1-x, 1-y, \frac{1}{2}+z$; (vi) $-\frac{1}{2}+x, \frac{1}{2}-y, z$.

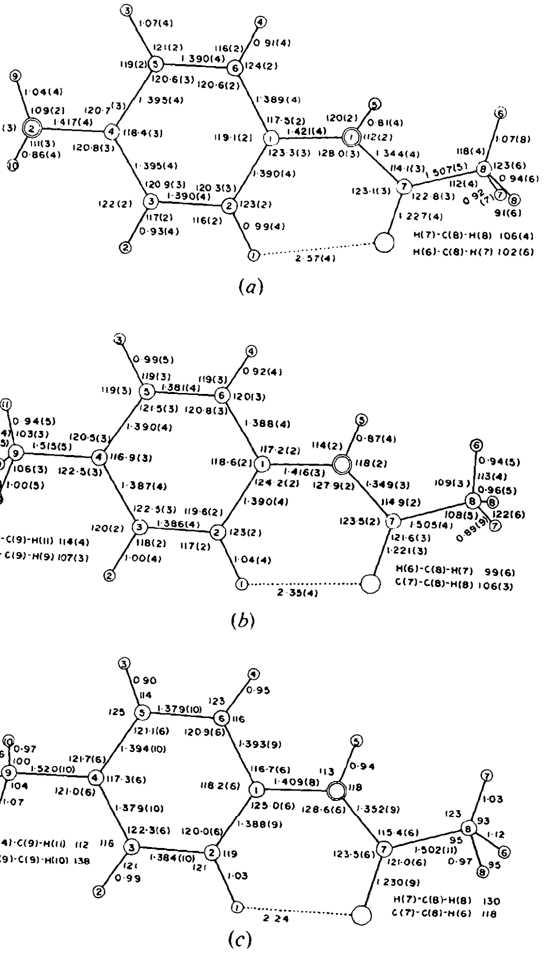

Fig. 3. Bond lengths (Å) and bond angles (°) for (*a*) PAAA, (*b*) PMAA (*M*) and (*c*) PMAA (*O*). Their e.s.d.'s are shown in parentheses.

Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1962). The computations were carried out on an NEAC 2200-500 computer at the Okayama University Computer Centre. The programs used were *SIGM*, *TANG*, *HBLS*-5 and *DAPH* (Ashida, 1973). The final atomic parameters are listed in Tables 3 and 4.

Description of the structures

The crystal structures projected along the crystal axes are illustrated in Fig. 2. The characteristic features of the crystal structures of p-XH$_m$ acetanilides are summarized in Table 5 under the items (*A*) to (*H*). The molecules related by (*A*) are linked together by the hydrogen bond C–O···H–(*B*) with dimensions (*C*) to form a chain along (*D*). The chains are held together by (*E*) between the molecules related by (*F*) to form a

Table 5. *A comparison of the crystal structure of p-XH$_m$ acetanilides*

	PAAA	PMAA (*M*)	PMAA (*O*)	PHAA (*O*)	PHAA (*M*)
p-XH$_m$	NH$_2$	CH$_3$	CH$_3$	OH	OH
Space group	*Pcab*	$P2_1/c$	$Pna2_1$	*Pcab*	$P2_1/a$
(*A*)	*b* glide	2_1	*a* glide	*b* glide	*a* glide + *c* translation
(*B*) *D*	N(amino)	N(amide)	N(amide)	O(hydroxy)	O(hydroxy)
(*C*) O···*D* (Å)	3·088 (4)	2·923 (3)	2·904 (8)	2·724 (5)	2·663 (3)
O···H (Å)	2·06 (4)	2·05 (4)	1·97	1·91 (5)	1·80 (4)
O···H–*D* (°)	167 (3)	178 (3)	174	171 (5)	165 (4)
C=O···H (°)	140 (1)	142 (1)	166	128 (1)	136 (1)
(*D*)	**b**	**b**	**a**	**b**	[102]
(*E*)	N(amino)···H–N (amide) hydrogen bond	Antiparallel molecular stacking	Parallel molecular stacking	O(hydroxy)···H–N hydrogen bond	O(hydroxy)···H–N hydrogen bond
(*F*)	*a* glide	Inversion	*c* translation	*a* glide	*a* glide
(*G*)	(001)	(100)	(010)	(001)	(010)
(*H*)	**c**	**a**	**b**	**c**	**b**

Table 6. *The least-squares planes and displacements* (Å) *of the atoms from the planes*

$X = ax + cz\cos\beta,\ Y = by,\ Z = cz\sin\beta.$

(I) Benzene ring

PAAA: $0{\cdot}4336X - 0{\cdot}0572Y - 0{\cdot}8993Z + 0{\cdot}9863 = 0$
PMAA (*M*): $0{\cdot}0105X + 0{\cdot}5498Y - 0{\cdot}8352Z + 1{\cdot}2781 = 0$
PMAA (*O*): $0{\cdot}0478X - 0{\cdot}8503Y - 0{\cdot}5241Z + 4{\cdot}6693 = 0$

	PAAA	PMAA (*M*)	PMAA (*O*)
C(1)*	0·0139	0·0008	0·0081
C(2)*	–0·0077	0·0005	–0·0065
C(3)*	–0·0066	–0·0014	0·0054
C(4)*	0·0147	0·0008	–0·0059
C(5)*	–0·0063	0·0005	0·0077
C(6)*	–0·0075	–0·0014	–0·0088
O	–1·0824	0·6940	0·2231
N(1)	0·1260	–0·0172	–0·0005
C(7)	–0·4034	0·3193	0·1288
C(8)	–0·0874	0·2125	0·1161
X	0·0050	0·0278	–0·0166

(II) Amide group

PAAA: $-0{\cdot}0641X + 0{\cdot}2543Y - 0{\cdot}9650Z + 0{\cdot}4594 = 0$
PMAA (*M*): $-0{\cdot}0426X + 0{\cdot}2573Y - 0{\cdot}9654Z + 1{\cdot}9472 = 0$
PMAA (*O*): $-0{\cdot}0449X - 0{\cdot}8325Y - 0{\cdot}5523Z + 4{\cdot}8839 = 0$

	PAAA	PMAA (*M*)	PMAA (*O*)
N(1)*	0·0002	0·0010	–0·0025
C(7)*	–0·0007	–0·0029	0·0077
O*	0·0003	0·0011	–0·0030
C(8)*	0·0002	0·0008	–0·0022
C(1)	–0·0036	0·0189	0·0354
Dihedral angle (°) between the planes (I) and (II)	34·4	18·7	5·7

* Atoms used for the calculation of the planes.

sheet parallel to (*G*). The sheets are stacked along (*H*) by van der Waals interactions.

Bond lengths and angles of PAAA, PMAA (*M*) and PMAA (*O*) are shown in Fig. 3, the corresponding values being very similar. The displacements of the atoms from the least-squares planes of the benzene ring and the acetamide group are listed in Table 6. It is noted that the benzene ring of PAAA takes a boat conformation as found in PHAA (*M*) and PHAA (*O*) (Haisa, Kashino, Kawai & Maeda, 1976; Haisa, Kashino & Maeda, 1974); the atoms C(1) and C(4) deviate by about +0·021 Å from the plane of the other atoms in the ring.

Discussion

Crystal structures

Two kinds of hydrogen bonds in PAAA are very similar to those in PHAA (*O*). That is, the amino group, as well as the hydroxy group of PHAA (*O*), donates one H atom to the carbonyl group [see (*C*) in Table 5] and accepts one H atom from the amide group [N(2^{iii})···N(1), 3·050 (4) Å; N(2^{iii})···H(5), 2·27 (4) Å; N(2^{iii})···H(5)–N(1), 163 (3)°]. This results in the similarity of the molecular arrangement in the two-dimensionally hydrogen-bonded sheets parallel to (001). In the sheet, H(5) is in contact with H(10^{iii}) (free from hydrogen bonding) at a distance of 2·34 Å. This contact increases the inclination of the long molecular axis of PAAA with **b** to 14·7°; the corresponding value in PHAA (*O*) is only 1·8°. The larger dihedral angle between the benzene ring and the acetamide planes in

Table 7. *Characteristic features of the molecular geometry of p-XH$_m$ acetanilides*

Bond lengths are in ångströms, angles in degrees.

	PAAA	PMAA (*M*)	PMAA (*O*)	PHAA (*O*)	PHAA (*M*)
p-XH$_m$	NH$_2$	CH$_3$	CH$_3$	OH	OH
C(1)–N	1·421	1·416	1·409	1·422	1·425
N–C(7)	1·344	1·349	1·351	1·341	1·340
C(7)=O	1·227	1·221	1·230	1·223	1·232
C(6)–C(1)–N	117·5	117·2	116·7	116·4	116·7
C(2)–C(1)–N	123·3	124·2	125·0	123·7	124·3
C(6)–C(1)–C(2)	119·1	118·6	118·2	119·8	119·0
C(3)–C(4)–C(5)	118·4	116·9	117·4	120·2	119·8
C(3)–C(4)–X	120·8	122·5	121·0	118·9	117·7
C(5)–C(4)–X	120·7	120·5	121·7	121·0	122·6
XH···C(3)	2·54	2·62	2·53	None	None
XH′···C(5)	2·53	2·51	2·44	2·42	2·44
τC(2)C(1)NC(7)	32·2	−19·6	−8·3	17·8	23·5
τC(1)NC(7)C(8)	179·8	181·0	181·7	181·2	177·6
τC(1)NC(7)O	−0·3	0·5	3·2	0·5	−2·3

PAAA is also an effect of this contact. The stacking of the sheets along **c** is somewhat different from that in PHAA (*O*): in PAAA the acetamide group lies near the *c*-glide plane, while in PHAA (*O*) the hydroxyl group does.

The dimorphic structures of PMAA are characterized by the directions of their long molecular axes with respect to the crystal axes {[100] for PMAA (*M*) and [012] for PMAA (*O*)}, the dihedral angles between the amide groups connected by the hydrogen bonds [29·8° for PMAA (*M*) and 67·3° for PMAA (*O*)], and the modes of molecular stacking [(*E*) in Table 5].

The disordered structure of PMAA (*O*), which gives rise to diffuse streaks for particular reflexions, may result from a misarrangement of molecules lying nearly parallel to the *n*-glide plane. Such a disorder has not been noted by Maeda, Kamijyo & Fukui (1976). The disorder effects have been reported for p-chloroacetanilide (Subramanian, 1966), which is isotypic with PMAA (*O*), but not for p-bromoacetanilide (Andreetti, Cavalca, Domiano & Musatti, 1968).

The density and the melting point of PAAA are close to those of PHAA, but higher than those of PMAA where the hydrogen-bonded sheet is missing.

Molecular structures

The characteristic features of the molecular geometry of p-XH$_m$ acetanilides are compared in Table 7. The maximum deviations of the C–C lengths in the benzene rings from the average values do not exceed 0·010 Å, which is contrary to the comment by Maeda, Kamijyo & Fukui (1976). All the C(6)–C(1)–C(2) angles are slightly smaller than the sp^2 angle. The C(3)–C(4)–C(5) angles for PAAA and PMAA are smaller than the sp^2 angle, but those for PHAA are close to it. It seems likely that the contacts of two H atoms in XH$_m$ for either PAAA or PMAA with C(3) and C(5) increase the two external angles at C(4) and hence decrease the inner angle. Such a contact for PHAA occurs only with C(5).

The torsion angles about the N–C(7) bond remain almost constant throughout, whereas the angles about the N–C(1) bond vary from 8·3 to 32·2°. This indicates that the twist around the N–C(1) bond without the loss of planarity of the acetamide group is responsible for the formation of the hydrogen bonding of the acetanilides.

References

Andreetti, G. D., Cavalca, L., Domiano, P. & Musatti, A. (1968). *Acta Cryst.* B**24**, 1195–1198.

Ashida, T. (1973). *The Universal Crystallographic Computing System – Osaka.* The Computation Centre, Osaka Univ.

Haisa, M., Kashino, S., Kawai, R. & Maeda, H. (1976). *Acta Cryst.* B**32**, 1283–1285.

Haisa, M., Kashino, S. & Maeda, H. (1974). *Acta Cryst.* B**30**, 2510–2512.

International Tables for X-ray Crystallography (1962). Vol. III, pp. 202–203. Birmingham: Kynoch Press.

Maeda, H., Kamijyo, N. & Fukui, K. (1976). *Cryst. Struct. Commun.* **5**, 129–134.

Subramanian, E. (1966). *Z. Kristallogr.* **123**, 222–234.