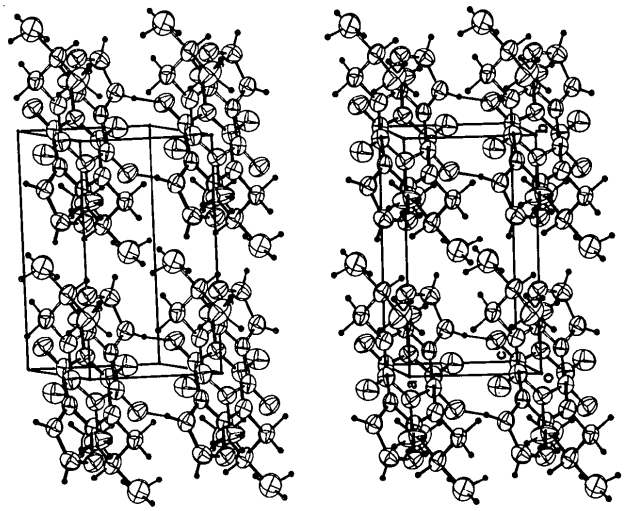

Fig. 2. A stereoscopic representation of the packing of the molecules in the unit cell showing the hydrogen-bonding details and the stacking of the xanthine bases in the crystal structure. Molecules of opposite hands are distinguished by open and filled bonds.

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Structure of Adenosine-5′-mononicotinate (AMN) Trihydrate: an Analog of NAD for Testing Intramolecular Stacking

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Abstract. $C_{16}H_{16}N_6O_5.3H_2O$, $M_r = 426{\cdot}4$, monoclinic, $P2_1$, $a = 9{\cdot}535$ (2), $b = 13{\cdot}932$ (2), $c = 7{\cdot}138$ (2) Å, $\beta = 93{\cdot}13$ (2)°, $V = 946{\cdot}85$ Å^3, $Z = 2$, $D_x = 1{\cdot}495$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 9{\cdot}93$ cm^{-1}, $F(000) = 428$, $T = 294$ K, $R = 0{\cdot}045$ and $wR = 0{\cdot}059$ for 1460 observed reflections [$I > 3\sigma(I)$]. The AMN molecules, unlike NAD or other model structures of NAD, are not charged and exhibit intra- as well as intermolecular stacking of pyridine ring over adenine ring. There is extensive hydrogen bonding in the crystal involving the pyridine and adenine rings and the three water molecules. Rather surprisingly, the ester carbonyl O atom is not involved in the hydrogen bonding.

Introduction. Solution NMR studies on the structure of NAD suggest an equilibrium existing between a folded, stacked conformation and an extended, unstacked one (Sarma, Ross & Kaplan, 1968). The shift towards an unfolded structure at acidic pH was attributed to the protonation of the adenine N1 atom. X-ray studies of a lithium salt of NAD (Reddy, Saenger, Muhlegger & Weimann, 1981) and the free acid form of NAD (Parthasarathy & Fridey, 1984) revealed only intermolecular stacking between the bases, though they showed different conformations of NAD. The absence of intramolecular base stacking was presumed to be due to the low pH (for the lithium salt of NAD: Reddy *et al.*, 1981) or to the charged bases (for the free acid form of NAD: Parthasarathy & Fridey, 1984). In previous years, there have been several structural reports on model compounds for NAD (Johnson, Frank & Paul, 1973; Johnson, Maier & Paul, 1973; Sakaki, Inoue, Senda & Tomita, 1978; Voet, 1973). These were either complexes containing adenine and nicotinamide rings (Sakaki *et al.*, 1978; Voet, 1973) or trimethylene-bridged adenine and nicotinamide rings (Johnson,

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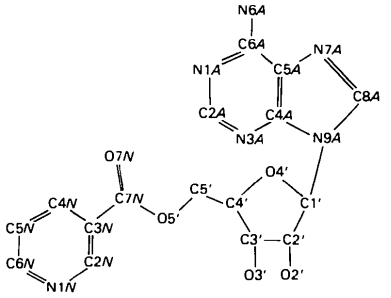
Frank & Paul, 1973; Johnson, Maier & Paul, 1973). Though the trimethylene-bridged analog would geometrically permit intramolecular overlap and stacking, such intramolecular interaction was not observed in that crystal structure. None of these models, however, has a sugar ring covalently linking the adenine and nicotinamide moieties.

Adenosine-5′-mononicotinate (AMN, 1) has a ribose ring linking the adenine and nicotinate moieties which are *endo* to the ribose ring. Therefore, AMN is structurally suited for intramolecular base stacking. It is also a good candidate for examining the effect of charges on stacking, since, unlike NAD or other model compounds, the nicotinate ring is not charged. We report here the structure of AMN which exhibits intra- as well as intermolecular stacking.



(1)

Experimental. The title compound was purchased from Sigma Chemicals and used without further purification; needle-shaped crystals obtained from water (pH 3·5) at room temperature; attempts to crystallize AMN from aqueous solutions at a lower pH range either produced uncharged AMN crystals or cleaved the ester bond to produce adenine dihydrochloride; crystal size: 0·35 × 0·30 × 0·25 mm; CAD-4 diffractometer; unit-cell dimensions from least-squares fit of 18 reflections ($20 < 2\theta < 52°$); for intensity data $2\theta_{max} = 154°$ for λ(Cu $K\alpha$); $\omega/2\theta$ scan; ω-scan width $(0{\cdot}95 + 0{\cdot}14\tan\theta)°$; aperture width $(3{\cdot}0 + 1{\cdot}2\tan\theta)$ mm; maximum time spent on any reflection 100 s; faster scan for strong reflections; three standards every hour of X-ray exposure; variation in intensity less than 2% during data collection; check on orientation matrix every 100 reflections; 2377 reflections measured (h: $-12\rightarrow12$, k: $0\rightarrow17$, l: $0\rightarrow9$), out of which 1460 were unique and significant [$I > 3\sigma(I)$]; $R_{symm} = 0{\cdot}018$; Lp correction applied; intensities of three reflections at $\chi \simeq 90°$ measured for different values of φ in the range from 0 to 360° in increments of 10° and the resultant curve of transmission as a function of φ used to calculate absorption for all reflections; max. and min. transmissions are 0·99 and 0·74 and average 0·87.

Initial attempts to solve the structure using direct-methods program *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) failed; partial structure from random generation of phases using *RANTAN* (Yao Jia-xing, 1981); complete structure from successive difference electron density maps; full-matrix refinement with anisotropic thermal parameters for non-H atoms led to an R of 0·060; H atoms from difference electron density map; the H atoms of one of the three water molecules (O3*W*) and of O2′ could not be located and were not included in the refinement; final cycle of refinement with anisotropic thermal parameters for non-H atoms and isotropic thermal parameter for H atoms; final $R = 0{\cdot}045$ and $wR = 0{\cdot}059$ for 1460 reflections; $S = 1{\cdot}87$; function minimized $\sum w(|F_o| - 1/k|F_c|)^2$ where $w = 1/[\sigma^2 + (0{\cdot}02F_o)^2 + 1]$ and $\sigma(I)$ is based on counting statistics, k is the scale factor; max. $\Delta/\sigma = 0{\cdot}03$; largest features in the final difference electron density map were 0·17 and $-0{\cdot}27$ e Å^{-3}. Programs from Enraf–Nonius *SDP* (Frenz, 1982); atomic scattering factors from *International Tables for X-ray Crystallography* (1974); drawings made by *ORTEP* (Johnson, 1976).

Discussion. The final atomic coordinates are given in Table 1.* The bond distances and angles are given in Table 2. A perspective view of the molecules showing the intramolecular stacking between the adenine and pyridine rings is shown in Fig. 1(*a*) and intermolecular stacking along the *c* axis is shown in Fig. 1(*b*). Both the pyridine and adenine rings are uncharged in the crystal structure of AMN and therefore exhibit intramolecular stacking whereas the NAD model compounds, *N*-[3-(aden-9-yl)propyl]-3-carbamoylpyridinium bromide (Johnson, Maier & Paul, 1973) and the dihydrobromide salt (Johnson, Frank & Paul, 1973), in which at least one of the rings is charged, do not exhibit intramolecular stacking. The bond distances and angles observed in the adenine ring of AMN agree well with the average values for 27 uncharged adenine rings (Taylor & Kennard, 1982*a*) except for N1*A*—C2*A*, C2*A*—N3*A* and C8*A*—N9*A* of 1·366 (6), 1·310 (6) and 1·386 (5) Å, respectively, which deviate by more than 3σ compared to the average values 1·338, 1·332 and 1·367 Å, respectively. Both the base rings are not strictly planar; several atoms deviate from the calculated least-squares plane by up to 0·0225 Å. Such slight deviations of ring atoms from calculated least-squares planes have been observed in many nucleosides and nucleotides and have been attributed to crystal packing forces (Voet & Rich, 1970). The two base rings are inclined at an angle of 7·3 (5)° and the ester group

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond lengths and angles involving H atoms, and torsional angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51193 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates with equivalent isotropic thermal parameters for non-*H *atoms (e.s.d.'s are given in parentheses)*

$B_{eq} = \frac{4}{3}[a^2B_{11} + b^2B_{22} + c^2B_{33} + ab(\cos\gamma)B_{12} + ac(\cos\beta)B_{13} + bc(\cos\alpha)B_{23}]$.

	x	*y*	*z*	B_{eq}(Å²)
N1*A*	−0·1011 (4)	0·2604 (3)	−0·0651 (7)	4·30 (9)
C2*A*	−0·0835 (5)	0·1631 (4)	−0·0624 (9)	4·6 (1)
N3*A*	0·0322 (4)	0·1132 (3)	−0·0733 (6)	3·79 (8)
C4*A*	0·1435 (4)	0·1710 (3)	−0·0888 (6)	2·72 (7)
C5*A*	0·1422 (4)	0·2697 (3)	−0·0925 (6)	2·59 (7)
C6*A*	0·0124 (4)	0·3158 (3)	−0·0816 (7)	3·12 (8)
N6*A*	−0·0034 (4)	0·4106 (3)	−0·0880 (6)	3·91 (8)
N7*A*	0·2774 (3)	0·3047 (2)	−0·1100 (6)	3·09 (7)
C8*A*	0·3556 (4)	0·2285 (3)	−0·1202 (7)	3·07 (8)
N9*A*	0·2810 (3)	0·1438 (2)	−0·1047 (5)	2·66 (6)
C1′	0·3268 (4)	0·0437 (3)	−0·1141 (6)	2·56 (7)
C2′	0·4852 (4)	0·0333 (3)	−0·1317 (6)	2·55 (7)
O2′	0·5061 (3)	−0·0594 (2)	−0·2043 (4)	3·15 (6)
C3′	0·5373 (4)	0·0374 (3)	0·0741 (6)	2·60 (7)
O3′	0·6743 (3)	0·0024 (2)	0·1134 (5)	3·52 (6)
C4′	0·4240 (4)	−0·0204 (3)	0·1675 (6)	2·71 (7)
O4′	0·2973 (3)	−0·004	0·0539 (4)	2·97 (5)
C5′	0·4003 (6)	0·0017 (4)	0·3681 (7)	4·3 (1)
O5′	0·3565 (3)	0·1012 (2)	0·3844 (5)	4·06 (7)
C7*N*	0·2217 (5)	0·1179 (3)	0·4173 (7)	3·49 (9)
O7*N*	0·1404 (4)	0·0555 (3)	0·4569 (6)	5·17 (8)
C3*N*	0·1867 (4)	0·2209 (4)	0·4086 (6)	3·12 (8)
C4*N*	0·0513 (5)	0·2505 (4)	0·4386 (7)	3·9 (1)
C5*N*	0·0208 (5)	0·3487 (4)	0·4304 (8)	4·4 (1)
C6*N*	0·1246 (6)	0·4101 (4)	0·3881 (8)	4·7 (1)
N1*N*	0·2562 (4)	0·3834 (3)	0·3597 (6)	4·21 (9)
C2*N*	0·2855 (5)	0·2898 (3)	0·3713 (7)	3·67 (9)
O1*W*	0·3391 (5)	−0·2238 (3)	0·8275 (9)	8·7 (1)
O2*W*	0·3575 (5)	−0·2468 (5)	0·3231 (9)	8·9 (2)
O3*W*	0·2640 (8)	−0·3625 (5)	0·580 (1)	10·9 (2)

Table 2. *Bond distances* (Å) *and angles* (°) *involving all non-*H *atoms (e.s.d.'s are given in parentheses)*

N1*A*	C2*A*	1·366 (6)		C7*N*	O7*N*	1·208 (6)	
C2′	C3′	1·526 (6)		C6*A*	N6*A*	1·330 (6)	
N1*A*	C6*A*	1·339 (5)		C7*N*	C3*N*	1·475 (7)	
C3′	O3′	1·408 (5)		N7*A*	C8*A*	1·301 (5)	
C2*A*	N3*A*	1·310 (6)		C3*N*	C4*N*	1·384 (6)	
C3′	C4′	1·530 (6)		C8*A*	N9*A*	1·386 (5)	
N3*A*	C4*A*	1·341 (5)		C3*N*	C2*N*	1·381 (6)	
C4′	O4′	1·435 (5)		N9*A*	C1′	1·464 (5)	
C4*A*	C5*A*	1·377 (5)		C4*N*	C5*N*	1·399 (7)	
C4′	C5′	1·494 (7)		C1′	C2′	1·529 (5)	
C4*A*	N9*A*	1·375 (5)		C5*N*	C6*N*	1·355 (7)	
C5′	O5′	1·454 (6)		C1′	O4′	1·415 (5)	
C5*A*	C6*A*	1·400 (5)		C6*N*	N1*N*	1·334 (7)	
O5′	C7*N*	1·339 (6)		C2′	O2′	1·410 (5)	
C5*A*	N7*A*	1·391 (5)		N1*N*	C2*N*	1·335 (6)	

C2*A*	N1*A*	C6*A*	118·3 (4)	O5′	C7*N*	C3*N*	112·2 (4)
O2′	C2′	C3′	110·0 (3)	C5*A*	N7*A*	C8*A*	104·8 (3)
N1*A*	C2*A*	N3*A*	128·9 (4)	O7*N*	C7*N*	C3*N*	124·3 (4)
C2*A*	N3*A*	C4*A*	111·1 (4)	N7*A*	C8*A*	N9*A*	113·1 (3)
C2′	C3′	C4′	101·5 (3)	C7*N*	C3*N*	C4*N*	119·6 (4)
N3*A*	C4*A*	C5*A*	126·5 (4)	C4*A*	N9*A*	C8*A*	105·5 (3)
O3′	C3′	C4′	113·6 (3)	C7*N*	C3*N*	C2*N*	122·0 (4)
N3*A*	C4*A*	N9*A*	127·2 (4)	C4*A*	N9*A*	C1′	123·6 (3)
C3′	C4′	O4′	105·3 (3)	C4*N*	C3*N*	C2*N*	118·4 (4)
C5*A*	C4*A*	N9*A*	106·4 (3)	C8*A*	N9*A*	C1′	130·7 (3)
C3′	C4′	C5′	117·2 (4)	C3*N*	C4*N*	C5*N*	118·6 (4)
C4*A*	C5*A*	C6*A*	117·7 (3)	N9*A*	C1′	C2′	113·0 (3)
O4′	C4′	C5′	110·0 (3)	C4*N*	C5*N*	C6*N*	118·3 (5)
C4*A*	C5*A*	N7*A*	110·1 (3)	N9*A*	C1′	O4′	109·8 (3)
C1′	O4′	C4′	110·7 (3)	C5*N*	C6*N*	N1*N*	124·2 (5)
C6*A*	C5*A*	N7*A*	132·2 (4)	C2′	C1′	O4′	105·5 (3)
C4′	C5′	O5′	109·4 (4)	C6*N*	N1*N*	C2*N*	117·3 (4)
N1*A*	C6*A*	C5*A*	117·5 (4)	C1′	C2′	O2′	106·0 (3)
C5′	O5′	C7*N*	117·5 (4)	C3*N*	C2*N*	N1*N*	123·2 (4)
N1*A*	C6*A*	N6*A*	119·0 (4)	C1′	C2′	C3′	100·9 (3)
O5′	C7*N*	O7*N*	123·4 (4)	C2′	C3′	O3′	115·4 (4)
C5*A*	C6*A*	N6*A*	123·5 (4)				

makes an angle of 1·7 (5)° to the pyridine ring. The intramolecular stacking distance is 3·007 (5) Å whereas the intermolecular distance is 3·170 (5) Å.

The sugar pucker is C2′-*exo*/C3′-*endo* ($^2T_3$). The orientation about the C4′—C5′ bond is + *gauche* (+ synclinal) [O5′—C5′—C4′—C3′ = 61·0 (6)°]. The torsion angle about the N9*A*—C1′ glycosidic linkage (O4′—C1′—N9*A*—C4*A*) is −62·5 (6)° exhibiting high-*anti* (−synclinal) conformation across this bond. The value of the furanose ring amplitude and the phase of the pseudorotation (Altona & Sundaralingam, 1972) are 40·2 (3) and 355·4 (4)°, respectively. Previous studies using molecular models and a crystal-structure survey of nucleosides suggested (Sundaralingam, 1969) that purine nucleosides with C2′-*endo* (^2E) pucker adopt both *syn* and *anti* conformations in nearly equal distribution but C3′-*endo* (^3E) pucker shifted the glycosidic orientation to *anti* (see also, de Leeuw, Haasnoot & Altona, 1980). It has been shown from quantum chemical methods that for *anti* purine nucleosides both sugar puckers are equally probable whereas the *syn* conformation correlates with C2′-*endo* pucker. A *syn* conformation with C3′-*endo* pucker was shown to correspond to 1–2 kcal (1 kcal ≡ 4·2 kJ) higher energy (for a summary see Saenger, 1984). Because the intramolecular stacking between the bases is predominant it can compensate for a high-energy conformation of the glycosidic bond in AMN. By adopting the *syn* conformation, the AMN molecule also avoids an otherwise steric overcrowding between the bases.

AMN crystallizes with three water molecules of hydration. The crystal structure consists of zigzag clusters of hydrophobic and adjacent hydrophilic regions; the water molecules are hydrogen bonded to the sugar hydroxyl groups as shown in Fig. 2. Each molecule of AMN is flanked between two clusters of three water molecules along the **a*** direction. Along the **c*** direction, the AMN molecules stack on top of each other. The geometrical parameters describing these and other hydrogen bonds in the structure are given in Table 3. It is interesting to note that of the three potential hydrogen acceptors in an uncharged adenine ring (N1*A*, N3*A* and N7*A*), in this structure N7*A* forms a stronger hydrogen bond than the other two as judged by the donor–acceptor distances (Table 3). The O4′ atom has been known to be involved in either a stacking interaction or in a weak hydrogen bond. In this structure, O4′ forms a weak hydrogen bond by accepting a hydrogen from N6*A*. Crystallographic studies have revealed that pyrimidine C6 and purine C8 are frequently at distances of only 3·1 to 3·3Å from

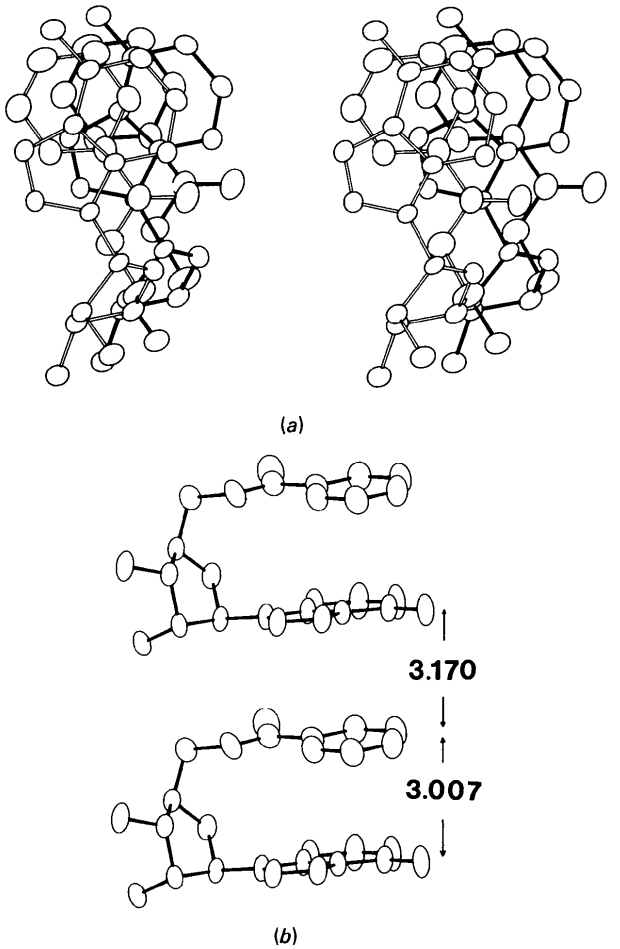


Fig. 1. (*a*) A stereoview of two AMN molecules showing the stacking of the bases. (*b*) Edge view of the stacking. The numbers indicate the interbase distances in Å.

Table 3. *Hydrogen bonds and* C—H···O *contact*

			Distance (Å)			Angle (°)
a	*b*	*c*	*a*—*b*	*a*···*c*	*b*···*c*	*a*—*b*···*c*
O3′	HO3′	N7*A*^{iii}	1·23 (14)	2·792 (4)	1·86 (14)	128 (15)
N6*A*	HN6*A*2	O4′^{iii}	0·91 (5)	3·065 (4)	2·18 (5)	164 (5)
O1*W*	H2O1*W*	O2′^{iv}	1·24 (9)	2·806 (5)	1·64 (9)	160 (7)
O2*W*	H1O2*W*	O3*W*^{i}	0·98 (4)	2·633 (10)	1·66 (4)	172 (3)
O2*W*	H2O2*W*	N1*A*^{vi}	1·47 (11)	2·981 (7)	1·54 (11)	164 (7)
C8*A*	HC8*A*	O2*W*^{vii}	0·95 (5)	3·183 (6)	2·42 (5)	138 (4)
O2′	—*	N1*N*^{iv}	—	2·698 (5)	—	—
O3*W*	—*	O1*W*^{i}	—	2·689 (9)	—	—

Symmetry code: (i) x, y, z; (ii) $-x, 0{\cdot}5+y, -z$; (iii) $1-x, y-0{\cdot}5, -z$; (iv) $x, y, -z$; (v) $x, y, 1+z$; (vi) $-x, y-0{\cdot}5, -z$; (vii) $1-x, 0{\cdot}5+y, -z$.

* H atoms attached to the donors were not located.

O5′ in *anti*-oriented bases with + *gauche* conformation about the C4′—C5′ bond (Taylor & Kennard, 1982*b*). Although the C4′—C5′ orientation in the AMN molecule is favorable for C8···O5′ hydrogen bonding, such a bond is not observed in the crystal structure

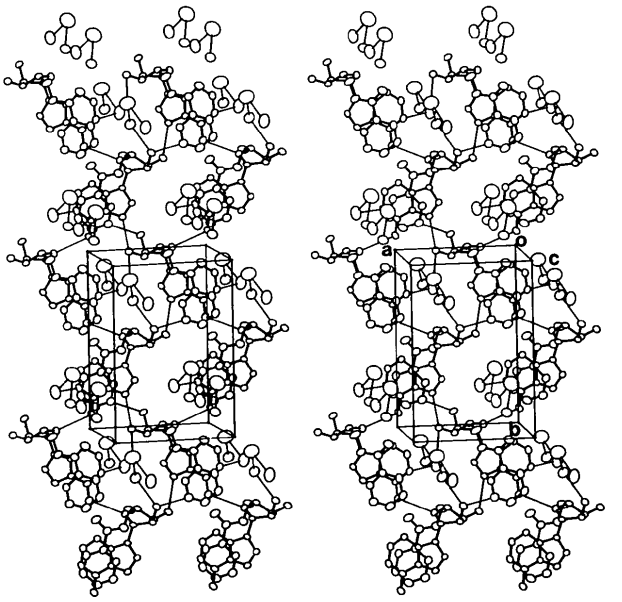


Fig. 2. Stereoview of the packing of the molecules. Hydrogen bonds are shown by thin lines. The figure includes c-translated water molecules to enhance the view of the flanking of bases by clusters of water molecules.

because the AMN molecule adopts a high-*anti* conformation. However, C8*A* is involved in a C—H···O type of interaction with the water molecule O2*W* (Table 3).

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Structure of N^1,N^2-Di(*p*-tolyl)acetamidine

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Abstract. $C_{16}H_{18}N_2$, $M_r = 238{\cdot}3$, orthorhombic, *Pbca*, $a = 24{\cdot}558$ (4), $b = 12{\cdot}534$ (3), $c = 9{\cdot}211$ (1) Å, $V = 2835{\cdot}2$ (9) Å^3, $Z = 8$, $D_m = 1{\cdot}10$, $D_x = 1{\cdot}12$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 0{\cdot}440$ mm^{-1}, $F(000) = 1024$, room temperature, $R = 0{\cdot}056$ for 1364 observed reflexions. The N^1—C and C—N^2 bonds are different [1·368 (4) and 1·283 (4) Å, respectively]. The N^1 atom and the *p*-tolyl substituent at the C=N^2 double bond are in a *trans* (*E*) configuration. The phenyl rings at N^1 and N^2 are twisted relative to the central amidine plane by 39·4 (4) and 88·1 (4)°, respectively. An intermolecular N^1—H···N^2 hydrogen bond joins the molecules into chains parallel to **c**.

Introduction. This work is part of a series of investigations carried out in this laboratory† to determine the changes induced in the geometry of the amidine core by its intra- and intermolecular environment. As the molecule belongs to the group of symmetrically substituted amidines with secondary amine nitrogen, which have two identical tautomeric forms, we expected the C—N bonds to be of equal length due to tautomerism and/or H-bond formation.

Experimental. The title compound was synthesized by Oszczapowicz, Orliński & Hejchman (1979). Plate-shaped crystals obtained from absolute ethanol; D_m by flotation; space group from Weissenberg photographs; crystal 0·15 × 0·20 × 0·45 mm; Syntex $P2_1$ diffractometer; cell parameters from least-squares treatment of setting angles of 15 reflexions with $16 \le 2\theta \le 22°$. No absorption correction. 1881 reflexions with $2\theta \le 115°$ measured in the range h: 0→+26, k: 0→+12, l: 0→+10; no significant intensity variation (±3·4%) for two standard reflexions (112, 4$\bar{1}$0) recorded every hour. Peak-profile analysis according to Lehmann & Larsen (1974); 1364 observed reflexions with $I \ge 2\sigma(I)$. Structure solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Phenyl H atoms and amine H atom from $\Delta\rho$ map, remaining H atoms calculated from methyl-group geometry and optimized with fixed U_{iso} (0·08 Å^2). Full-matrix least-squares refinement [function minimized: $\sum w(F_o - F_c)^2$] of anisotropic non-H atoms and isotropic H atoms found in $\Delta\rho$ map. F_c values multiplied by $(1 - xF_c^2/\sin 2\theta)$ where x is the empirical isotropic extinction parameter refined to 29 (9) × 10^{-7}. $R = 0{\cdot}056$, $wR = 0{\cdot}079$, $S = 3{\cdot}14$, $w = 1/[\sigma^2(F_o) + 0{\cdot}0003F_o^2]$, $(\Delta/\sigma)_{max} = 0{\cdot}1$, $(\Delta\rho)_{max} = 0{\cdot}19$, $(\Delta\rho)_{min} = -0{\cdot}28$ e Å^{-3}. Computer programs: *MULTAN*80 (Main *et al.*, 1980), *SHELX*76 (Sheldrick, 1976) and local programs (Jaskólski, 1982*a*). Molecular illustrations drawn using *PLUTO* (Motherwell & Clegg, 1978) and *ORTEP* (Johnson, 1976). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Atomic parameters are given in Table 1, bond lengths and angles in Table 2.†

An *ORTEP* stereodrawing showing the atom labelling system is presented in Fig. 1. The N(1)—C(1) and C(1)—N(2) bond lengths are significantly different. From a semiempirical correlation ($r = r_0 - 0{\cdot}18p$) between π-bond orders (p) and bond distances (r) where r_0 is a standard single-bond distance (1·458 Å for C—N

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† Previous paper: Ciszak, Gdaniec, Jaskólski, Kosturkiewicz, Owsiański & Tykarska (1989).

† Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51248 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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