Table 2. *Hydrogen-bond distances*

O(2)···N(7)^i	2·907 Å	N(10)···O(1)^{ii}	2·984 Å
N(6)···N(1)^{iii}	3·012	N(6)···O(2)^{iv}	3·207
O(2)···O(2)^{iv}	2·772	O(2)···O(2)^v	2·811
N(11)···N(3)^{vi}	3·064		

Symmetry code

(i)	x, y, z	(iv)	$-x, 1-y, 1-z$
(ii)	$x, y, -1+z$	(v)	$-x, 1-y, 2-z$
(iii)	$1-x, 1-y, -z$	(vi)	$2-x, -y, 1-z$

the amide groups. The water molecule O(2) forms hydrogen bonds with two water molecules, each O···O line passing through the centre of symmetry. Therefore, there must be disorder about one H atom of the water molecule which was not observed in the difference map. The other water H atom is donated to N(7) of adenine. At the same time, O(2) accepts an H atom from the amino group of adenine. Two adenine bases, related by the centre of symmetry at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, are paired by two N(6)H···N(1) hydrogen bonds. This type of hydrogen bonding is typical for crystals of adenine derivatives.

Furthermore, N(3) of adenine is hydrogen-bonded with N(11) of the indole. This mode of interaction is the same as that found in the 9-ethyladenine–indole complex (Kaneda & Tanaka, 1976). It may be

suggested that the N(3)···HN(indole) hydrogen bond is one of the typical interaction modes between adenine and tryptophane moieties. On the other hand, the intermolecular stacking presumed from spectroscopic studies (Brun, Toulmé & Hélène, 1975; Morita, 1974) is not observed in the present crystal.

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3-(9-Adenyl)propionyltyramine Dihydrate

By Minoru Ohki, Akio Takenaka, Hirotaka Shimanouchi and Yoshio Sasada

Laboratory of Chemistry for Natural Products, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo 152, Japan

Abstract. $C_{16}H_{18}N_6O_2 \cdot 2H_2O$, FW 362·39, monoclinic, $P2_1/c$, $a = 13·303$ (4), $b = 10·819$ (5), $c = 12·856$ (3) Å, $\beta = 107·57$ (2)°, $Z = 4$, $D_x = 1·364$, $D_m = 1·361$ g cm^{-3}, μ(Mo $K\alpha$) = 1·09 cm^{-1}. The structure was solved by the direct method using diffractometer data and was refined by a block-diagonal least-squares method. The final R value was 0·062 for 3642 reflexions. The molecule is fully extended. The adenine rings are related by a centre-of-symmetry overlap at a spacing of 3·35 Å. Water molecules participate in all the hydrogen bonds, except for N(6)H···N(3) between adenines.

Introduction. As part of a study of the elementary patterns of interaction between amino acids and

purine–pyrimidine bases, the title compound was synthesized from 9-β-carboxyethyladenine (Kondo, Miyata & Takemoto, 1971) and tyramine by the dicyclohexylcarbodiimide method, and the structure of a crystal of the hydrate was determined by X-ray analysis.

Prismatic crystals were grown from a methanol-water solution. The crystal density was measured by flotation in a mixture of cyclohexane and carbon tetrachloride. Weissenberg photographs showed systematic absences, $h0l$, $l = 2n + 1$ and $00l$, $l = 2n + 1$, indicating the space group $P2_1/c$. The precise unit-cell dimensions and the intensities of the reflexions were measured on a Rigaku four-circle automated diffractometer using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = $

0·71069 Å). The intensity data were collected up to 55° in 2θ from a crystal 0·18 × 0·24 × 0·37 mm. 4056 independent reflexions were obtained, 740 of which were zero-reflexions.

The structure was solved by the direct method (Karle & Karle, 1966). In the refinement by a block-diagonal least-squares method, the quantity minimized was $\Sigma w(|F_o| - |F_c|)^2$ with $w = 1/(\sigma_p^2 + qF_o^2)$, where σ_p is due to counting statistics and q is $1\cdot00 \times 10^{-5}$ (derived from the intensity variances of the monitored reflexions). In the present refinement, the zero-reflexions were included by assuming $|F_o| = F_{lim}$ and $w = w(F_{lim})$, where F_{lim} is 1·24, an observational threshold value. However, the zero-reflexions for which $|F_c| < F_{lim}$ were omitted. When the R value reached 0·12, a difference synthesis revealed all the H atoms. The refinement was terminated when the maximum shift of the parameters for the H atoms was less than 0·37σ. The final R value was 0·062 ($R = 0·054$ for $F_o \geq 3/\sqrt{w}$).* Atomic scattering factors used were taken from *International Tables for X-ray Crystallography* (1962). The positional parameters are given in Table 1.

Discussion. Bond lengths and angles involving non-hydrogen atoms are shown in Fig. 1, their standard deviations being 0·002 Å and 0·1–0·2° respectively. They are in good agreement with those found in related compounds.

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* Lists of structure factors, thermal parameters, bond lengths and angles involving H atoms, and atomic deviations from the least-squares planes through the adenine, phenol and amide moieties have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32727 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Final positional parameters (heavy atoms* ×10⁴; *hydrogen atoms* ×10³), *with their standard deviations in parentheses*

	x	y	z
N(1)	4619 (1)	7551 (1)	−710 (1)
C(2)	4699 (1)	7774 (1)	345 (1)
N(3)	4390 (1)	7071 (1)	1040 (1)
C(4)	3943 (1)	6018 (1)	559 (1)
C(5)	3800 (1)	5667 (1)	−511 (1)
C(6)	4172 (1)	6479 (1)	−1163 (1)
N(6)	4110 (1)	6255 (1)	−2208 (1)
N(7)	3311 (1)	4518 (1)	−718 (1)
C(8)	3179 (1)	4209 (1)	222 (1)
N(9)	3544 (1)	5071 (1)	1026 (1)
C(9)	3505 (1)	4991 (1)	2157 (1)
C(10)	2589 (1)	5737 (1)	2299 (1)
C(11)	2399 (1)	5465 (1)	3383 (1)
O(1)	2939 (1)	4732 (1)	4039 (1)
N(10)	1583 (1)	6074 (1)	3533 (1)
C(12)	1155 (1)	5873 (2)	4446 (1)
C(13)	1528 (1)	6847 (2)	5327 (1)
C(14)	884 (1)	6801 (1)	6124 (1)
C(15)	1154 (1)	6024 (2)	7028 (1)
C(16)	542 (1)	5965 (1)	7737 (1)
C(17)	−355 (1)	6688 (1)	7544 (1)
C(18)	−634 (1)	7472 (2)	6647 (1)
C(19)	−12 (1)	7517 (2)	5950 (1)
O(2)	−933 (1)	6607 (1)	8257 (1)
O(3)	3806 (1)	886 (1)	1159 (1)
O(4)	2639 (1)	1960 (1)	2315 (1)
H(2)	506 (1)	860 (1)	66 (1)
H(61)	432 (1)	686 (1)	−262 (1)
H(62)	390 (1)	552 (1)	−254 (1)
H(8)	286 (1)	341 (1)	33 (1)
H(91)	421 (1)	533 (1)	266 (1)
H(92)	339 (1)	410 (1)	228 (1)
H(101)	193 (1)	551 (1)	170 (1)
H(102)	272 (1)	662 (1)	222 (1)
H(10)	122 (1)	655 (2)	300 (1)
H(121)	135 (1)	497 (1)	473 (1)
H(122)	37 (1)	592 (1)	415 (1)
H(131)	147 (1)	769 (1)	497 (1)
H(132)	229 (1)	668 (2)	572 (1)
H(15)	179 (1)	548 (1)	720 (1)
H(16)	72 (1)	538 (1)	838 (1)
H(18)	−129 (1)	799 (1)	649 (1)
H(19)	−23 (1)	810 (1)	530 (1)
H(O2)	−155 (1)	716 (2)	805 (1)
H(31)	432 (1)	139 (2)	113 (1)
H(32)	346 (1)	69 (1)	49 (1)
H(41)	296 (1)	166 (2)	192 (1)
H(42)	288 (1)	155 (2)	296 (1)

Fig. 1. Bond lengths (Å) and angles (°).

Fig. 2. The crystal structure viewed along b.

Fig. 3. The hydrogen-bond arrangement in the crystal.

Table 2. *Hydrogen-bond distances and angles*

X H Y	$X \cdots Y$	$H \cdots Y$	$\angle X-H \cdots Y$
O(4)—H(41)$\cdots$O(3)^i	2·713 Å	1·90 Å	172°
O(2)—H(O2)$\cdots$O(4)^{ii}	2·662	1·68	180
O(3)—H(31)$\cdots$N(1)^{iii}	2·883	2·01	167
N(6)—H(62)$\cdots$O(3)^{iv}	3·069	2·24	152
O(4)—H(42)$\cdots$N(7)^{iv}	2·897	1·99	174
O(3)—H(32)$\cdots$O(1)^{iv}	2·703	1·84	171
N(6)—H(61)$\cdots$N(3)^v	2·999	2·10	161

Symmetry code

(i)	x, y, z	(iv)	$x, \frac{1}{2} - y, -\frac{1}{2} + z$
(ii)	$-x, 1 - y, 1 - z$	(v)	$x, \frac{3}{2} - y, -\frac{1}{2} + z$
(iii)	$1 - x, 1 - y, -z$		

The purine base is highly planar with a maximum shift of 0·011 Å for C(6) from the least-squares plane. The exocyclic atoms N(6) and C(9) deviate from the plane in the same direction. The phenol moiety, including O(2), is completely planar.

The molecule is fully extended. The torsions around the C(9)—C(10) and C(12)—C(13) bonds correspond to a staggered arrangement; the N(9)—C(9)—C(10)—C(11) and N(10)—C(12)—C(13)—C(14) torsion angles are 168·6 and 166·7° respectively. As shown in Fig. 2, the extended molecule lies nearly along $[-\frac{1}{2}, 0, 1]$. Two adenine bases related by the centre of symmetry at $(\frac{1}{2}, \frac{1}{2}, 0)$ are stacked at a spacing of 3·35 Å. The phenol groups come together around the 2_1 axes. The dihedral angle between the adenine and phenol rings in the molecule is 77·4°.

Hydrogen bonds found in the crystal are shown in Fig. 3, relevant distances and angles being listed in Table 2. The water molecules participate in all the hydrogen bonds, except for N(6)H$\cdots$N(3) between
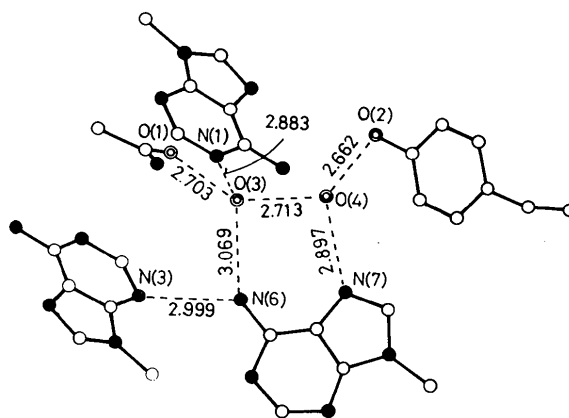
two adenines related by the c glide. One water molecule, O(3), donates H atoms to O(1) and N(1), and accepts from O(4) and N(6). The other water, O(4), is a hydrogen donor to O(3) and N(7) of adenine, and an acceptor from O(2) of phenol. Therefore, no direct interaction between adenine and phenol moieties exists in this crystal owing to the interposition of the water molecule.

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