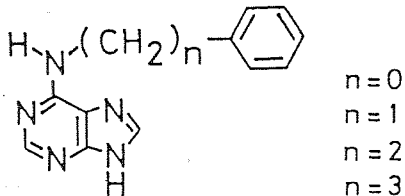


03.1-10 THE STRUCTURES OF  $\omega$ -PHENYLALKYL DERIVATIVES OF PURINE CYTOKININ. By H. Mizuno, Dept. of Molecular Biology, National Institute of Agrobiological Resources, Tsukuba Science City, Ibaraki 305, Japan and N. Nishikawa, Z. Kumazawa and N. Kashimura, Dept. of Agricultural Chemistry, Mie University, Tsu, Mie 514 Japan

N6-substituted purine is closely related to the plant growth hormone (cytokinin) which plays a major role in cell division and cell differentiation. We recently found an interesting alternation of cytokinin activity, depending on whether the number of methylene units is even or odd in N6-( $\omega$ -phenylalkyl) adenines (Nishikawa, Kumazawa, Kashimura, Nishikimi, Uemura, Agric. Biol. Chem., 1986, 50, 2243).



X-ray studies of such a series of adenine derivatives are thus appropriate for deducing structure-activity relationships of cytokinins. The structures of derivatives,  $n=0, 2$  and  $3$  were solved by MULTAN 84. The most interesting feature is an alternation of the values of interplanar angle between purine and phenyl ring system. Those angles in active derivatives ( $n$ -odd) are fairly close to  $90^\circ$  as observed in other active cytokinins, whereas about  $30^\circ$  in weakly active derivatives ( $n$ -even). This strongly suggests that the interplanar angle is closely related to cytokinin activity and can describe the activity alternation of the present molecules in terms of this angle. Another interesting feature is in intermolecular hydrogen bond scheme joining purine bases together in pairs. The derivative  $n=0$  has a unique hydrogen bond scheme which is allowed by the N7-H tautomer of purine. The other derivatives have the N6-H...N7 and N9-H...N3 hydrogen bonds which have commonly been observed in N6-substituted adenine structures.

n	a(Å)	b(Å)	c(Å)	$\beta$ (°)	Z	S.Gr.	R(%)
0	11.355	8.247	21.606		8	Pbca	8.3
2	24.103	11.619	8.958	110.64	8	C2/c	4.8
3	15.111	16.950	11.792	106.57	8	C2/c	8.4

n	$\omega$ (°)	Intermolecular hydrogen bonds	
0	30.1	N6-H...N9	N7-H...N3
1**	78.5	N6-H...N7	N9-H...N3
2	34.1	N6-H...N7	N9-H...N3
3	80.2	N6-H...N7	N9-H...N3

\*Angle between adenine and phenyl ring planes

\*\*Raghuathan, Sinha, Pattabhi, Gabe, Acta Cryst., 1983, C39, 1545.

03.1-11 THE CRYSTAL AND MOLECULAR STRUCTURE OF ALPHA AND BETA NALBUPHINE. By Stephen Z. Goldberg, Michael Insler and Robert E. Lippman, Department of Chemistry, Adelphi University, Garden City, New York, U.S.A.

The crystal structure of the title compounds, as free bases, have been determined from 3-dimensional single crystal X-ray data. The isomers crystallize in space groups  $P2_1$  ( $Z=4$ ) and  $P1$  ( $Z=2$ ) respectively.

The effect of the hydrogen-hydroxyl interchange on the structures of the two isomers will be discussed. Hydrogen bonding in the crystal has been found to be an important factor in the crystal structure.

The conformations of the ring systems and the spatial orientation of the  $-CH_2-C_6H_5$  substituent on nitrogen will be compared with those found in a series of related agonist and antagonist molecules. Possible implications for biological activity will be considered.

03.2-1 METASTABLE CRYSTALLINE STATE OF DISODIUM ADENOSINE 5'-TRIPHOSPHATE. By Y. Sugawara, T. Ito, N. Kamiya, and H. Iwasaki, RIKEN (The Institute of Physical and Chemical Research), Wako, Saitama, Japan and Y. Satow, KEK (National Laboratory for High Energy Physics), Tsukuba, Ibaraki, Japan.

Disodium adenosine 5'-triphosphate ( $Na_2ATP$ ) is known to take several crystal forms judging from the cell parameters. Previously, we reported crystal transformation from  $Na_2ATP \cdot 3H_2O$  (1) to  $Na_2ATP \cdot 2H_2O$  (2), which was caused by humidity condition of atmosphere (Authors, Acta Crystallogr., 1984, A40, C68). In this paper, we report the metastable crystal form of  $Na_2ATP \cdot xH_2O$  (3), which is thought to be in the intermediate stage between (1) and (2). Data collection was carried out using synchrotron radiation at Photon Factory in KEK. Cell parameters are listed in Table 1 (space group  $P2_12_12_1$ ). Refinement of (3) starting from the atomic parameters of (1) gave an R value of 0.14 for total 1723 independent reflections at the present stage. There are two ATP molecules, A and B, in an asymmetric unit. Electron densities around the pyrophosphate group of molecule A and the ribose group of molecule B are very diffuse. In these parts, structural differences between (1) and (2) are prominent. The disorder in (3) must be correlated with the crystal structures of (1) and (2).

Table 1.	(1)	(2)	(3)
a	30.349	27.565	29.274
b	20.826	21.067	20.896
c	7.026	7.086	7.043