Polymorphism of Inosine

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Two different forms of anhydrous inosine crystals have been found during the course of studies on the crystallization and purification of inosine. The crystal data of inosine dihydrate were reported by Bugg, Thewalt and Marsh,[1] but there is no report on the crystal data of anhydrous inosine. One inosine in orthorhombic system is usually crystallized with ease from aqueous solution above 20°C, as needles or long prisms elongated along the *b* axis. The other in the monoclinic system is crystallized as plates from the aqueous dimethylsulfoxide solution (about 70 v/v%). We call the former modification the α-form, and the latter the β-form.

X-ray diffraction studies were carried out on the two crystalline forms with CuK_α radiation. The space groups were obtained from equi-inclination Weissenberg photographs of zero and first layers about axes *a* and *b*. The unit-cell dimensions determined from precession photographs are shown in Table 1, with other data. Density was measured by flotation in a chloroform-tetrabromoethane mixture.

An interesting feature of the polymorphism is relatively large difference in density. A larger difference in density in the polymorphs was reported by Bugg & Marsh[2] in cytydilic acid b.

TABLE 1. CRYSTALLOGRAPHIC DATA OF ANHYDROUS INOSINE CRYSTALS

	α-Form	β-Form
System	Orthorhombic	Monoclinic
Space group	$P2_12_12_1$	$P2_1$
Unit-cell parameters	a=21.26 Å	a=10.925 Å
	b=8.09	b=4.84
	c=13.22	c=10.44
		β=90.6°
Density obsd	1.576 g·cm^{-3}	1.61 3 g·cm^{-3}
calcd	1.568	1.614
Number of molecules per unit cell	8	2
Melting point	218—220°C	212—214°C

TABLE 2. X-RAY POWDER DIFFRACTION DATA OF ANHYDROUS INOSINE CRYSTALS

α-Form			β-Form		
d (Å)	I/I_1[a]	hkl	d (Å)	I/I_1[a]	hkl
11.33	5	101	10.95	10	100
10.72	20	200	7.59	80	101, $\bar{1}$01
8.37	100	201	5.50	15	200
7.63	5	110	5.24	5	002
6.66	30	002	4.87	100	201, $\bar{2}$01
6.50	20	210	4.74	15	102, $\bar{1}$02
6.37	60	102	4.46	30	110
6.30	60	301	4.41	30	011
5.83	30	211	4.11	70	111, $\bar{1}$11
5.67	5	202	3.81	5	202, $\bar{2}$02
5.00	40	112, 311, 401	3.66	10	300
4.87	20	302	3.62	20	210
4.65	20	212	3.56	10	012
4.34	10	103	3.46	60	003, 301, $\bar{3}$01
4.24	20	411	3.42	10	211, $\bar{2}$11
4.08	20	501, 020	3.40	15	112, $\bar{1}$12
3.88	10	021	3.34	10	103, 103
3.83	20	121, 113	3.00	10	{302, $\bar{3}$02
3.79	20	510, 303			{212, $\bar{2}$12
3.66	30	221, 511, 213			
3.59	20	502			
3.56	20	600			
3.53	20	320			
3.41	30	403, 321, 122			
3.31	20	222			
3.29	20	104, 512			
3.23	20	420			
3.16	30	602, 413			

a) The scale is so chosen as to make the most intense line have the value 100.

The X-ray powder diffraction data of these two forms are shown in Table 2. The infrared spectra differ from each other in certain points.

The solubility data of inosine reported by Suzuki[3] were of α-form. Details of solubility data and crystallizing conditions of the β-form will be reported in the future.

1) C. E. Bugg, U. T. Thewalt and R. E. Marsh, *Biochem. Biophys. Res. Commun.*, **33**, 436 (1968).

2) C. E. Bugg and R. E. Marsh, *J. Mol. Biol.*, **25**, 67 (1967).

3) Y. Suzuki, T. Toki and T. Nakamura, Presented at 18th Annual Meeting of the Chemical Society of Japan, Osaka, 1965.