Two Crystalline Forms of DL-α-*Amino-n-butyric Acid*

By Masamichi Tsuboi, Yoichi Iitaka, Shigeko Suzuki and San-ichiro Mizushima

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In the course of our infrared studies on amino acids, we have found that there are at least two crystalline modifications in DL-α-amino-*n*-butyric acid,—one of which corresponds to the form already known (hereafter designated as A-form), while the other is a new form (B-form).

A-form is obtained as tabular crystals from the saturated aqueous solution on cooling. While, B-form is obtained as fibrous crystals from the aqueous solution (not necessarily saturated) by adding ethanol. The two forms give different

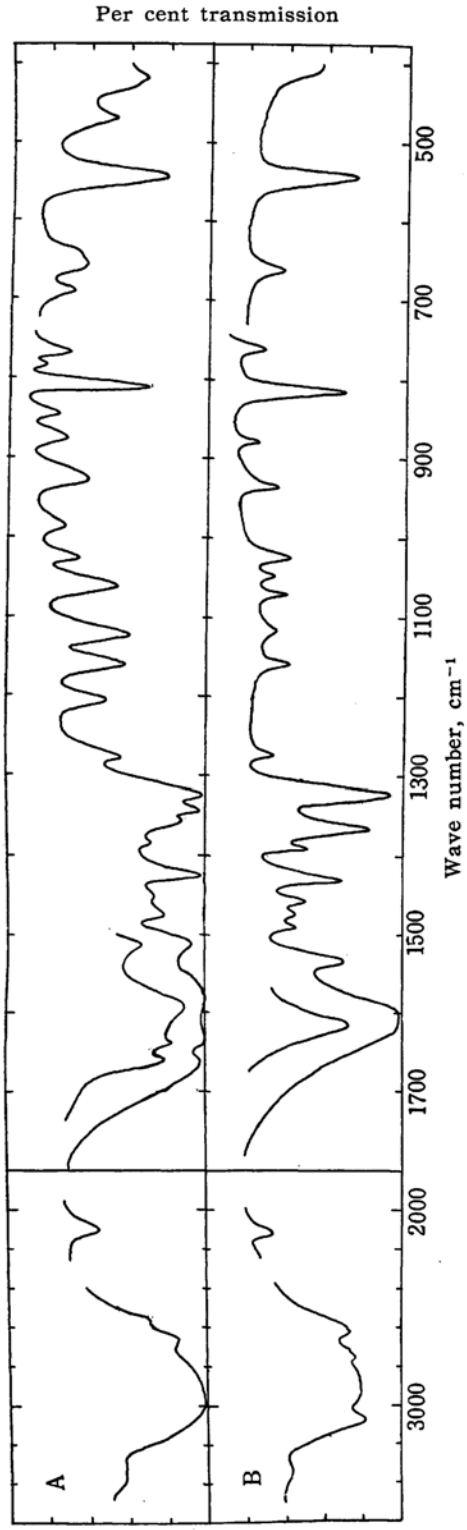

Fig. 1. Infrared absorption spectra of A- and B-forms of DL-α-amino-*n*-butyric acid.

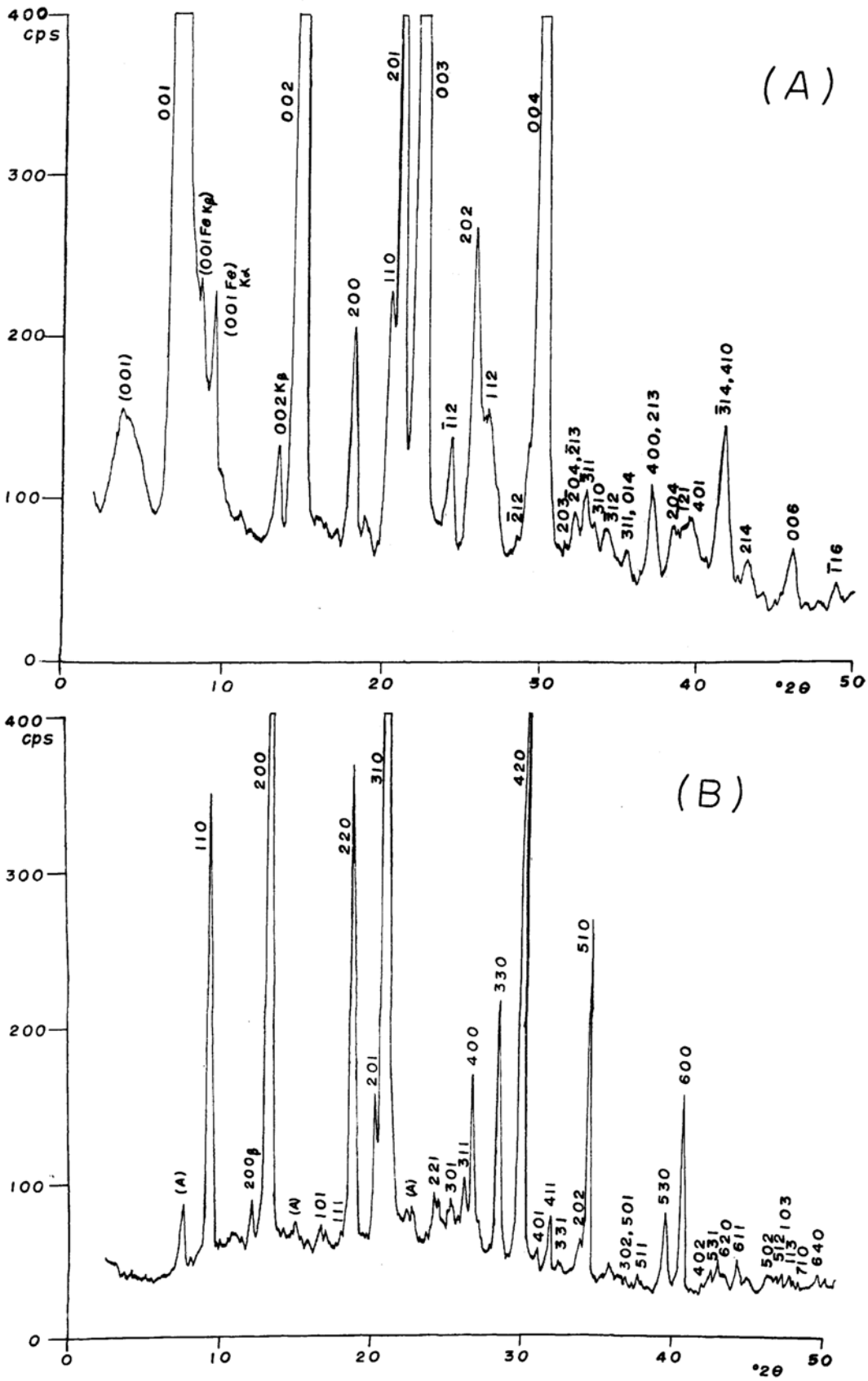

Fig. 2. X-ray powder patterns of A- and B-forms of DL-α-amino-n-butyric acid. Radiation used: CuK, 30 kV., 15 mA., Ni-filtered. (The diffused peak indicated as (0 0 1) for A-form is the continuous spectrum of the X-ray diffracted by the (0 0 1) plane.)

infrared spectra and X-ray powder patterns as shown in Figs. 1 and 2. From the measurements at different temperatures it was found that B-form is transformed into A-form at 195°C, whereas A-form remains unchanged from room temperature to 200°C. Therefore, at room temperature B-form is stable and A-form is metastable, but above 195°C this form becomes stable.

By our X-ray and infrared investigations, A-form is identified as the one, for which Dawson and Mathieson[1] gave the following constants: $P2_1/a$, $a=9.87$ Å, $b=4.80$ Å, $c=12.10$ Å, $\beta=101°$, $Z=4$, and Koegel et al.[2] observed infrared spectrum.

For B-form, it was found, from oscillation and Weissenberg photographs about the axis of the elongation (c-axis) and the axis perpendicular to it (a-axis), that the crystal is tetragonal, with the Laue symmetry of $4/m$, and with the unit cell dimensions: $a=13.38$ Å, and $c=5.85$ Å. Analysis of the photographs showed systematic absence of the reflections for ($h\,k\,0$) planes when $h+k$ is odd, and for ($0\,0\,l$) planes when l is odd; indicating the space group of $P4_2/n$.

As to the molecular configurations of A- and B-forms, it was found probable, from our infrared measurements with plane polarized radiation, that the two forms are rotational isomers to each other[3]. Furhther analysis of the X-ray photographs is now in progress, from which it is hoped to determine accurately the configurations of these isomers.

We wish to thank Sister Mary Marina, for her sending us the infrared spectra of a crystalline DL-α-amino-n-butyric acid which now turned out to be A-form.

Faculty of Science
The University of Tokyo
Hongo, Tokyo

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2) R. J. Koegel, R. A. McCallum, J. R. Greenstein, M. Winitz and S. M. Birnbaum, *Ann. N. Y. Acad. Sci.*, **69**, 94 (1957).
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