Acta Cryst. (1949). **2**, 260

The unit cell and space group of *N*-acetyl-L-tyrosylamide.*

By G. B. CARPENTER. *Gates and Crellin Laboratories of Chemistry, California Institute of Technology, Pasadena 4, California, U.S.A.*

(*Received 2 May* 1949)

The program of work in these laboratories on the structure of amino-acids and their derivatives includes a study of the structure of tyrosine. Since we had not obtained good crystals of tyrosine itself, we sought a crystalline derivative of tyrosine, preferably one in which the substituents would be similar to the immediate neighbors of a tyrosine residue in a polypeptide chain. To this end we examined crystals obtained by the crystallization of racemic *N*-acetyltyrosylamide to see if they might be suitable for use in a complete X-ray diffraction determination of the structure of tyrosine.

Clear crystals† of racemic *N*-acetyltyrosylamide and of *N*-acetyl-L-tyrosylamide were very similar and appeared to be tetragonal. Crystals of the inactive form were examined first in the hope that they might contain a center of symmetry. Laue photographs revealed that they are indeed tetragonal with a Laue symmetry of D_{4h}. Weissenberg photographs showed $h00$ present only for h even and $00l$ present only for l even; the absences are characteristic of the space group $P4_22_1$–D_4^6. This space group does not contain a center of symmetry; the general positions are eightfold.

Layer-line measurements on rotation photographs taken with a camera of 5 cm. radius using Ni-filtered Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ A.) gave the following axial lengths:

$$a_0 = 10{\cdot}84 \pm 0{\cdot}04, \quad c_0 = 20{\cdot}31 \pm 0{\cdot}05 \text{ A.}$$

Assuming eight molecules per unit cell leads to an X-ray density of 1·24 g.cm.$^{-3}$, which is not far from an experimental density of 1·19 g.cm.$^{-3}$ measured by the flotation method.

The space group could accommodate both D and L molecules in the unit cell only if there were at least sixteen of them, i.e. only if the asymmetric unit contained both a D and an L molecule; therefore it appeared that the racemate must resolve spontaneously on crystallization. This conclusion was verified by Laue photographs of *N*-acetyl-L-tyrosylamide, which proved to be identical with the corresponding photographs of the crystals from the racemate. The densities also appeared to be identical. Further, the melting-point of single crystals isolated from the racemate was found to be the same (224–226° C.) as that of the L material, whereas a powder of numerous crystals from the racemate melted around 198° C. (These melting-points were determined by Mr Robert MacAllister; they are corrected.)

Because of the large unit cell and the absence of a center of symmetry, an exhaustive determination of the structure of *N*-acetyl-L-tyrosylamide does not at present appear sufficiently profitable.

We wish to express our thanks to Dr Robert B. Corey who suggested this investigation.

* Contribution No. 1284 from the Gates and Crellin Laboratories. Aided by a grant from the National Foundation for Infantile Paralysis.

† Prepared by Mr Robert MacAllister of these laboratories.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Commission on Crystallographic Nomenclature

Members of the Commission on Crystallographic Nomenclature of the International Union of Crystallography (see *Acta Cryst.* (1948), **1**, 341) have now been nominated as follows:

Chairman:	W. L. BOND, Bell Telephone Laboratories, Murray Hill, N.J., U.S.A.
Other members:	J. D. H. DONNAY (U.S.A.)
	K. LONSDALE (U.K.)
	F. A. BANNISTER (U.K.)
	M. A. PEACOCK (Canada)
	H. BRASSEUR (Belgium)
	W. DE KEYSER (Belgium)

Crystallographers interested in the work of this Commission are cordially invited to make contact with the Chairman.

Optical crystals

Dan E. Mayers, 214 East 18th Street, New York 3, N.Y., U.S.A., announces the supply of optical calcite, quartz, zircon, beryl, topaz and fluorite (both natural and synthetic), and of tourmaline suitable for piezoelectric applications. The optical crystals are available in the form of blanks for lenses, windows and prisms. Inquiries should be addressed direct to the firm.

International Union of Crystallography

Notice of adhesion in Group IV, dated 2 June 1949, has been received from Spain through the Consejo Superior de Investigaciones Cientificas.