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

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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.

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† Prepared by Mr Robert MacAllister of these laboratories.

Notes and News

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