The Identity of Karrer and Gränacher's '2-Phenyl-5(4H)-imidazolone' and Hippuronitrile

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In the course of an investigation of various types of intramolecular anhydride formation in polypeptides Karrer and Gränacher 1 studied the reaction between hippuramide and phosphorus pentachloride in dry ether. From the reaction mixture they isolated in unstated vield a well crystallizing colorless compound melting at 141-3° with the analytical composition CoH2ON2. This finding in conjunction with the fact that the compound was hydrolyzed by acid to hippuric acid and small amounts of benzoic acid and that it possessed only weakly basic properties prompted Karrer and Gränacher (l. c.) to formulate it structurally as 2phenyl-5(4H)-imidazolone (I).

$$\mathbf{C_{6}H_{5} \cdot C}$$
 \mathbf{CO} \mathbf{I}

 ${\rm C_6H_5\cdot CO\cdot NH\cdot CH_2\cdot CN} \qquad {\rm II}$

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It was pointed out by the authors that (I) should be considered as a very simple representative of the poorly explored 5imidazolones. In the course of a study of these compounds in this laboratory it became imperative to repeat the preparation of the above mentioned phenylimidazolone for comparison. By following the procedure of Karrer and Gränacher (l. c.) there was isolated in 40 % yield a substance melting at 142°, giving the same analytical figures and showing further characteristics in accordance with the published data. However, a study of the ultraviolet spectrum revealed that the compound could not be represented by formula (I) because it showed in methanolic solution a typical benzamido-absorption with a peak at 228 m μ ($\varepsilon = 11700$) and not the split peak which will be shown in a forthcoming paper to be characteristic for this type of compounds.

A closer investigation of the presumed 2-phenyl-5(4H)-imidazolone rapidly disclosed that this compound is in fact simply hippuronitrile (II), a substance reported in the literature as early as 1902. The identity of the two compounds was secured by preparation of an authentic sample of hippuronitrile by benzovlation of aminoacetonitrile following the procedure of Klages and Haack 2. Analysis, spectroscopic data, melting point and mixed melting point of the two samples showed no discrepancies. Thus there can be no doubt that the compound claimed by Karrer and Gränacher as being the 2-phenyl-5(4H)-imidazolone is in fact hippuronitrile. As to the authentic phenylimidazolone it is quite certain from analogy considerations that its stability and chemical properties will differ quite widely from those here reported.

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