The Genometrical Structure of 3-β-Indolylacrylic Acid

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NMR-spectroscopy has proved to be a convenient tool in many fields of organic chemistry. One example is the determination of geometrical structures. Trans-compounds have larger spin coupling constants than cis-compounds; mean values of 17–18 cycles/sec for trans- and of 10–11 cycles/sec for cis-compounds are given.¹

In connection with studies on plant growth regulators it was of interest to investigate the geometrical structure of 3-β-indolylacrylic acid.² This acid was obtained by condensation of 3-formylindole with malonic acid.³ Condensation with malonic acid usually give trans-isomers,⁴ but in the present case no geometrical structure had been assigned to the product.

The NMR-spectrum of 3-β-indolylacrylic acid was recorded and compared with several known cis- and trans-isomers of α,β-unsaturated acids. The results are collected in Table 1. Both aliphatic and aromatic acids were investigated. Besides the spin coupling constants, aromatic acids show another difference between cis- and trans-isomers. The β-hydrogens of trans-acids have higher δ-values than the aromatic hydrogens, while the cis-acids have lower δ-values.

Both these features are in accordance with a trans configuration for the known 3-β-indolylacrylic acid. The latter has a coupling constant of 17.5 cycles/sec and the β-hydrogen doublet has a higher δ-value than the aromatic hydrogens.

Experimental. The NMR-spectra were recorded on a Varian Associates Model A 60 spectrometer. 3-β-Indolylacrylic acid. Commercial sample, Sigma Chemical Company, m.p. 192–194°C.

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The Effect of Sodium Salicylate on Hexosamine Synthesis in Eviscerated Mouse Fetuses

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Several anti-inflammatory drugs have been found to depress the synthesis of acid mucopolysaccharides in various tissues ⁵ and in addition, to produce eft-palate, as well as other skeletal and vascular malformations in mouse em-