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.

Table 1.

Acid	Spin coupling constants cycles/sec	
	cis-	*trans*-
$CH_3-CH=CH-COOH$	12	16.5
$C_2H_5-CH=CH-COOH$	12	—
$n\text{-}C_3H_7-CH=CH-COOH$	12	17
$iso\text{-}C_3H_7-CH=CH-COOH$	12	—
$BrCH=CH-COOH$	8.5	14
$ClCH=CH-COOH$	8.5	—
$C_6H_5-CH=CH-COOH$	13	17
$(4)ClC_6H_4-CH=CH-COOH$	13	17
$(3,4)Cl_2C_6H_3\ CH=CH-COOH$	13	—
$(3,5)Cl_2C_6H_3\ CH=CH-COOH$	13	17
$C_8H_7N-CH=CH-COOH$	—	17

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 [1,2] and in addition, to produce cleft-palate, as well as other skeletal and vascular malformations in mouse em-