

Hydrocinnamyl Nitrile in Cigar Smoke Condensate

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The presence of aliphatic nitriles in the gas phase of cigarette smoke has been reported recently by Keith and co-workers.¹ We report now the isolation and identification of hydrocinnamyl nitrile in cigar smoke condensate.

The neutral fraction of the cigar smoke condensate was partitioned between aqueous 90% methanol and hexane; the hexane fraction was concentrated *in vacuo* and then separated by chromatography on silicic acid. A fraction eluted with benzene contained at least 20 components as shown by gas-liquid chromatography on an SE-30 column (Fig.). The major components of this fraction were identified as phytol (peak 9), solanone (peak 6), and an unidentified high molecular weight ketone (peak 7). Two phenols, 3,5-dimethylphenol (peak 2) and a methyl-ethylphenol (peak 4) were also identified. Solanone² and 3,5-dimethylphenol³ have previously been isolated from cigarette smoke condensate. Rodgman and

Cook^{4,5} have isolated phytol in esterified form from cigarette smoke. Peak 8 actually contained three components which were resolved by rechromatography on a Carbowax 20M column. In fact, all chromatographic eluates were rechromatographed to obtain samples of a high degree of purity for meaningful spectroscopic and spectrometric data.

Peak 3 was identified as hydrocinnamyl nitrile by comparison of its infrared, ultraviolet and mass spectra, and gas chromatographic behaviour with a standard sample. This compound was shown not to be present in any of the solvents used in the isolation and, since only mild acid and base treatment was used, it seems unlikely that hydrocinnamyl nitrile could be an artifact of the isolation procedure.

We are now attempting to identify the remaining compounds isolated from this neutral fraction, some of which have been partially characterised.

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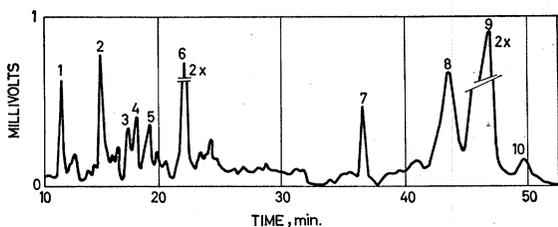


FIG.—Chromatogram of neutral fraction containing hydrocinnamyl nitrile (peak 3).

References

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