

Research & Development Establishment,  
British-American Tobacco Co. Ltd.,  
SOUTHAMPTON.

*Spare*  
Private & Confidential

Investigations on 3:4:9:10 - Dibenzpyrene

A sample of the above hydrocarbon was purified by repeated chromatographic fractionation of a benzene solution on alumina, until the optical extinction at a wavelength of 395  $m\mu$  was constant. The purified material was then characterised by determination of the ultra-violet absorption spectrum of solutions in cyclohexane.

Ten-fold serial dilutions were made of a stock solution in cyclohexane and the fluorescence spectra of these were recorded, using a Hilger Medium Quartz Spectrograph; exposures of three minutes were given, using Ilford HPS plates which were developed in Ilford PFP developer. A solution containing 10  $\mu\text{g}/\text{ml}$  of the hydrocarbon gave a fluorescence spectrum of 10 bands, only the five strongest of which were shown by a tenfold dilution (1  $\mu\text{g}/\text{ml}$ ). A further dilution (to 0.1  $\mu\text{g}/\text{ml}$ ) gave a fluorescence spectrum in which only a very faint indication of the strongest band could be detected. The same level of detection of 3:4-benzpyrene, under identical conditions, was given by a solution of 0.005  $\mu\text{g}/\text{ml}$  of the latter substance in cyclohexane, which

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showed a weak single band at 403 m $\mu$ . There was no indication of a fluorescent band spectrum with a solution of 0.01  $\mu$ g/ml of 3:4:9:10-dibenzpyrene.

Thus the smallest quantity of 3:4:9:10-dibenzpyrene which can be detected in this way is 20 times greater than that of 3:4-benzpyrene. The work of Bonnet and Neukomm has suggested that 3:4:9:10-dibenzpyrene, if it is present in cigarette smoke, is present in smaller quantities than is 3:4-benzpyrene. In these circumstances, a method of assay for 3:4:9:10-dibenzpyrene based upon that used for 3:4-benzpyrene viz., elution chromatography and detection by means of the fluorescence spectrum, is impracticable. No indication of the presence of 3:4:9:10-dibenzpyrene has been found in the course of examination of smoke fractions by fluorescence spectrography in routine assay of 3:4-benzpyrene.

No further work was undertaken on this compound.

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APPENDIX

(i) Ultraviolet Absorption maxima of 3:4:9:10-dibenzpyrene in cyclohexane solution ( $10 \mu\text{g/ml}$  and  $20 \mu\text{g/ml}$ ).

(Log  $E_{\text{max}}$  values in parentheses):

283 (4.51), 295 (4.71), 315 (4.25), 331 (4.16), 354 (4.13), 372 (4.65), 395 (4.81) and 419  $m\mu$  (3.03)

Inflexions at 237 and 403  $m\mu$ .

(ii) Fluorescence Spectrum of 3:4:9:10-dibenzpyrene in cyclohexane solution ( $10 \mu\text{g/ml}$ ).

Bands at 432, 459, 448, 437, 465, 491, 477, 453, 496 and 527  $m\mu$  (in order of decreasing intensity).

At  $1 \mu\text{g/ml}$ , only the five most intense bands are shown while at  $0.1 \mu\text{g/ml}$ , a weak band at 432  $m\mu$  is alone found.

These results are in good agreement with those subsequently reported by Muel, Hubert-Habart and Buu-Hoi (J. chim. phys. 1957, 54, 433).

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