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THE OCCURRENCE OF CAFFEINE IN THE AIR OF NEW YORK CITY

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Abstract—Caffeine was found to be a major constituent of the basic portion of organic particulate matter in New York City. The concentrations of caffeine in two composite samples collected in the period January to April, 1975 were 3.4 μg/1000 m^3 and 7.0 μg/1000 m^3 respectively. The ubiquity of coffee roasting plants in New York City and adjacent New Jersey may explain its abundance.

In our laboratory, we have been interested in the contribution of air pollution to the urban factor in lung cancer etiology (Wynder and Hammond, 1962). Present knowledge indicates that urban particulate organic matter (POM) contains at least two classes of compounds that are known animal carcinogens—the polynuclear aromatic hydrocarbons and the aza-arenes (Hoffmann and Wynder, 1976). This led us to an indepth chemical analysis of the basic portion of POM, which had elsewhere been shown to contain tumorigenic agents (Asahina *et al.* 1972). During the course of the characterization of a New York City POM sample we found, in addition to aza-arenes, a relatively large quantity of caffeine. To our knowledge, the occurrence of caffeine in POM has only been reported in the air of New Orleans by Tabor *et al* (1956), who identified the crystalline materials in crude benzene extracts of particulate matter as caffeine by means of i.r. and u.v. spectroscopy. Emissions from coffee-roasting plants in the vicinity of the sampling site were implicated as contributors. We confirmed this finding for New York City air and our data suggest that caffeine is indeed quite widely distributed in the air.

Quantitative analyses of two composite 100 filter samples, (ca. 1.8×10^5 m^3 air) collected at random sampling sites in the city during the period January–April 1975, showed concentrations of caffeine equivalent to 3.4 μg/1000 m^3 and 7.0 μg/1000 m^3, respectively. These concentrations are significantly higher than those of the aza-arenes (e.g., the concentrations of quinoline are 0.069 and 0.022 μg/1000 m^3 in the same samples), though apparently much lower than those samples from New Orleans.

To show that the caffeine in our composite samples did indeed come from ambient particulates and did not derive from a few sampling locations close to emission source, we conducted a subsequent study in which samples from six specific sampling sites were taken during March 1975 and analyzed. We found caffeine in all of these samples. Concentrations varied from 0.7–6.0 μg/1000 m^3 at these sites and higher concentrations are generally correlated with the locations of coffee roasting plants which cluster around South Manhattan, South Bronx and Long Island City in Queens (see Table 1). The membership list of the New York Coffee Roasters Association contains the names of 29 companies with locations in the city and we believe that emission from these roasters, plus contributions from roasters in adjacent New Jersey, could at least in part explain our ambient caffeine concentrations. This finding is of biological interest since a recent assay has revealed

Table 1. Concentrations of caffeine in various particulate samples in New York City

Sample	Sampling location	Sampling period	Equivalent concentration of caffeine in μg/1000 m^3
A	random	Jan–Mar 1975	3.4
B	random	Feb–Apr 1975	7.0
C	Bronx High School of Science	Mar 1975	6.0
D	Fort Schuyler, Bronx	Mar 1975	1.7
E	Mabel Dean Bacon High School, South Manhattan	Mar 1975	5.3
F	Greenpoint, Brooklyn	Mar 1975	5.3
G	PS 11, Queens	Mar 1975	1.0
H	Goethals Bridge, Staten Island	Mar 1975	0.7

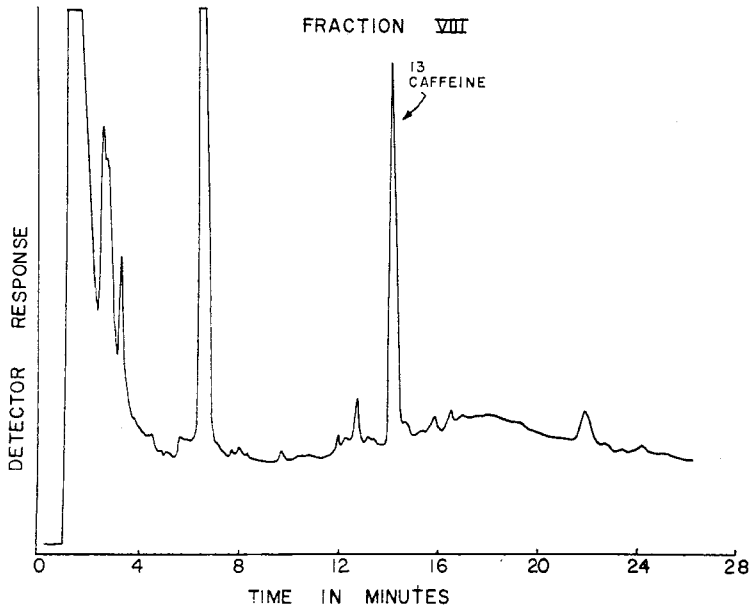

Fig. 1. Gas chromatogram of the caffeine fraction of sample A. (Chromatographic conditions: 160°C programmed to 300°C at 8°C/min. helium flow rate 30 ml/min, hydrogen pressure 20 psi, air pressure 30 psi. Column = 10 ft., 1/8″, 6% Dexsil 300 GC on Chromosorb W(HP), 80/100 mesh.

that caffeine can inhibit the carcinogenic activity of polynuclear aromatic hydrocarbons (Rothwell, 1974).

EXPERIMENTAL

The sampling procedure has been described in a previous publication (Dong *et al.* 1976). Suspended particulate samples were collected at various sites in New York City's Aerometric Network (operated by the New York City Department of Air Resources) on glass fiber filters, using high-volume samplers. POM was obtained by 8-hour soxhlet extraction with benzene/MeOH (4:1). The analytical scheme for the characterization of the basic portion of POM will be published elsewhere (Dong *et al.* 1977). The procedure for the isolation of caffeine can be summarized as follows. The basic organic portion was obtained in a procedure similar to that described by Sawicki *et al.*

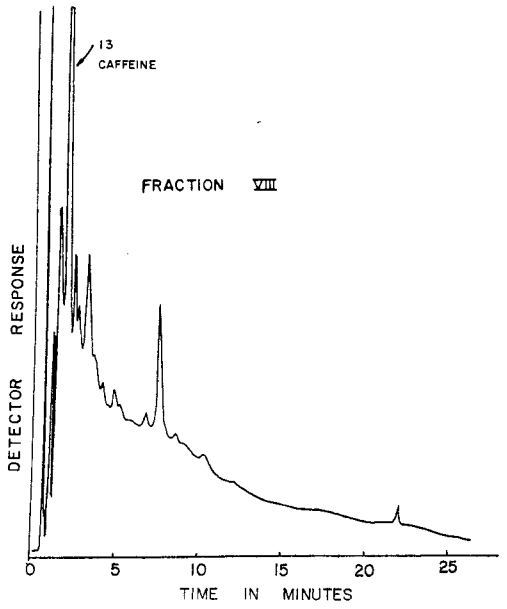

Fig. 2. Liquid chromatogram of the caffeine fraction of sample A. (Chromatographic conditions: 20% CH_3CN in H_2O programmed to 80% CH_3CN in H_2O at 4%/min at 3.0 ml/min flow rate; column: μ-Bondapak/C18.)

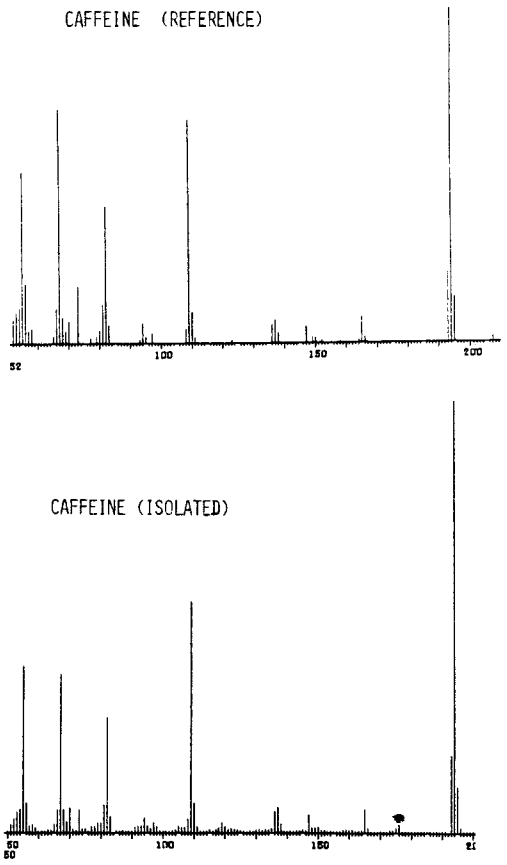

Fig. 3. Mass spectrum of caffeine isolated from sample A. Reference mass spectrum of pure caffeine is also shown.

(1965), involving acid extraction, basification, and back extraction. The basic portion was prefractionated by high pressure liquid chromatography (HPLC) on a Lichrosorb SI-60 silanized column. Eluents corresponding to the retention time of caffeine were collected, concentrated and analysed separately by gas chromatography–mass spectrometry (GC–MS) (Fig. 1) and reverse-phase HPLC (Fig. 2). Under these chromatographic conditions, the detection limit of caffeine was about 10 ng per injection in both systems. The u.v. and mass spectra (Fig. 3) of the isolated caffeine were virtually identical to those of the pure compound.

CONCLUSION

Emissions from coffee roasting seem to explain at least in part the relatively high concentration of caffeine in POM in New York City. This finding may be of biological interest since the carcinogenicity of POM can be modified by the presence of caffeine.

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