by extraction of the membrane lipids from isolated bacteria, followed by hydrolysis and methylation, and, finally, analysis with gas chromatography (GC). The resulting bacterial FAME profiles are diagnostic for the identification and differentiation of bacteria at the species level. A combination of a FOCUS autosampler and a Direct Thermal Desorption (DTD) interface was used to fully automated release fatty acids from the membranes of FC-sorted microbial cells, conversion into their methyl esters, and transfer into the GC column via an OPTIC injector. The DTD interface enables the use of the liner of the OPTIC injector as a sample and reaction container. Using a continuous culture, it was shown that the FAME yields compare favourably to the FAME yields obtained with the conventional off-line method, while the FAME profiles were identical. This method opened the way for direct analysis of FC-sorted raw lake water samples without tedious culturing of the limited amount of aquatic micro-organisms present. Future research will include coupling of this sample preparation method to GC–carbon isotope-ratio MS detection for elucidation of ecological and food chain related challenges.

83.

MEASUREMENT OF FREON-113 EXPOSURE DOSE IN EXHALED BREATH SAMPLES USING GC/MS WITH PRECONCENTRATION. *__Dennis J. Viscusi__, Ziqing Zhuang, and Ronald Shaffer Jr., Technology Branch, NIOSH/NPPTL, 626 Cochrans Mill Rd., Pittsburgh, PA 15236, Fax: 412-386-4070, dcv6@cdc.gov*

In previous work involving half-mask respirators, NIOSH found a correlation between fit factor (a quantitative measure of respirator performance) and total Freon-113 exposure dose (TFED), the amount of Freon-113 in a subject's end-exhaled breath measured 30 minutes after a simulated workplace test. Better detection methods for Freon-113 need to be developed in order to investigate the correlation for other classes of respirators. In this presentation we will describe improved strategies for measuring TFED using gas chromatography-mass spectrometry (GC-MS) with a preconcentration system. This presentation will describe column selection, detection limits, and precision of the analytical method. The effect of critical environmental parameters such as the background level of Freon-113 in the room will also be assessed. The use of GC/MS with preconcentration for exhaled breath analysis and trace detection may find suitability in other applications such as biomarker discovery, industrial hygiene and environmental monitoring.

84.

AEI: METHOD DEVELOPMENT FOR THE CHARACTERIZATION OF MAINSTREAM BIDI SMOKE BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY (GC-MS) AND INFRARED SPECTROMETRY (IR). *__Omobola A. Oladipupo__ and Ngee Sing Chong, Department of Chemistry, Middle Tennessee State University, 1301 East main Street, Murfreesboro, TN 37132-0001, Fax: 615-898-5182, oo2b@mtsu.edu*

The mainstream smokes of Indian cigarettes or bidis were analyzed by IR and GC-MS on a puff-by-puff basis and via continuous sampling of whole cigarettes. Hydrocarbons up to C5 and gaseous toxicants including CO and HCN were measured and compared to the smoke composition of American cigarettes. The CO concentration in bidi smoke decreased with increasing sampling flowrate, while the ethylene concentration initially decreased before increasing with increasing flowrate. GC-MS analysis of volatile carbonyl compounds were achieved with 2,4-dinitrophenylhydrazine-coated cartridges whereas volatile hydrocarbons were sampled with Carboxene or activated charcoal sorbent tubes. Compounds including pyridines, indoles, phenols, and sterols were detected in the particulate matter on filter pads. An undergraduate experiment derived from this research was designed to introduce the principles of gas-phase sampling and analysis using IR and/or GC instruments. The results pique the students' curiosity about cigarette smoke composition and more importantly, demonstrate key concepts in instrumental analysis.

85.

QUANTITATION OF CARBAZOLES IN CRUDE OIL AND ROCK EXTRACTS BY AMMONIA CHEMICAL IONIZATION GC-MS. *__Quan Shi__, Chunjiang Wang, and Tieguan Wang, State Key Laboratory of Heavy Oil Processing, University of Petroleum,China, Beijing 102200, China, Fax: 8610-69724721, sq@bjpeu.edu.cn*

Carbazoles were indentified and quantified by means of gas chromatograph and ammonia chemical ionization mass spectromitry(GC-NH3CIMS). NH3CIMS , compared with EI mass spectromitry, has higher sensitivity and selectivity on nitrogen compounds which usually interfered by polyaromatics. Nitrogen compounds could be quantified exactly even if with poor purrity or lower concentration. There were not fragments producted in NH3CI MS condition, and therefore, the quantification of carbazole compounds were not interfered by their larger molecular homologues.

86.

HIGH-THROUGHPUT FIELD DETECTION OF TOXIC CHEMICALS USING FAST GAS CHROMATOGRAPHY-MASS SPECTROMETRY. *__Frederick J. Cox Jr.__, Shannon B. Fox, and James C. Peterson, Battelle Eastern Science and Technology Center, 1204 Technology Drive, Aberdeen, MD 21001, Fax: 410-306-8420, coxfred@battelle.org*

Fast gas chromatography and time-of-flight mass spectrometers with high spectrum acquisition rates make possible GC/MS analysis of a well-defined, prepared sample from injection to end of run in less than a few minutes. However, implementation of the technique by itself for rapid analysis of large numbers of samples is difficult, because the total time for turnaround, including time for sample preparation from diverse sample matrices or GC oven cooldown, and other considerations ancillary to the GC run itself, is much longer. Additionally, a mobile environment limits the use of technologies possible in a fixed laboratory to increase throughput, such as cryogenic cooling. Here, practical strategies and technologies to overcome these limitations and reduce sample turnaround in a GC/MS mobile laboratory are discussed.

87.

THERMAL DECOMPOSITION OF T-BUTYL PEROXIDE IN A GAS CHROMATOGRAPHIC REACTOR: A COMPARISON OF KINETIC APPROACHES. *__Peter J. Skrdla__, Analytical Research, Merck & Co., Inc, P. O. Box 2000, RY818-A223, Rahway, NJ 07065, Fax: 732-594-3887, peter_skrdla@merck.com*

The thermal decomposition of t-butyl peroxide is investigated utilizing both the column and the injection port of a commercial gas chromatograph (GC) as chemical reactors. Using the injector liner as the reactor, the chromatographic peak areas of the reactant, measured at various injector temperatures, are used in the determination of the activation energy of the decomposition (Ea). With the column serving as the reactor, both the reactant peak areas and the product peak shapes are similarly utilized for this purpose. Values of Ea obtained using different mathematical treatments for each of the three approaches are found to range from 115 to 164 kJ/mol. Of these methods, the column reactor approach utilizing peak area measurements (referred to as PACR, for 'peak area, column reactor') is found to be far superior in terms of its speed, robustness and its accuracy in determining Ea. The PACR method's effectiveness can be largely attributed to the mathematical treatment that is described in the approach.

88.

SCALING RELATIONSHIP BETWEEN LEE AND KOVATS RETENTION INDICES. *__V.I. Babushok__, Bldg 221, room A111, NIST, Gaithersburg, MD 20899, Fax: 301-975-3670, babushok@nist.gov, and Peter J. Linstrom, Physical and Chemical Properties Division, NIST*

Retention indices are a generally accepted type of data for identification of chemical compounds in gas chromatography. The system of indices suggested by Kovats is a widely recognized system for accumulation of gas chromatographic data. However due to the different experimental features, convenience of analysis and measurements, several retention index systems are used in the practice. In this presentation we consider the conversion procedure of Lee retention indices into Kovats retention indices and vice versa based on the retention indices of reference compounds of Lee scale. The aim was to obtain relationship in a closed form between Kovats and Lee indices that takes into account temperature dependencies of retention indices. The results are limited to the commonly used dimethylsilicone stationary phases (OV-1,OV-101,DB-1,HP-1) and to isothermally derived retention indices. Based on numerous experimental data for dimethylsilicone stationary phase, parameters of linear temperature dependence of Kovats indices were estimated for reference compounds of Lee scale.

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ITEM INFORMATION

Abrev Title: Abstracts of Papers, 228th ACS National

Article Title: Measurement of Freon-113 exposure dose in exhaled breath samples using GC/

Author(s): Viscusi, Dennis J.; Zhuang, Zi

Volume/Issue: /	Year: 2004	CAN: 2004:655436
Page Range: ANYL-083	Total Pages: 1	Tech Report:
Coden: 69FTZ8	ISSN:	ISBN:
Source Reference: oc 3360246 Bennett, William		Po Type: OCLC

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