DOE/ER/60617-8

IONIZATION IN LIQUIDS
1993-1994 PROGRESS REPORT
and
REQUEST for 1994-1995 FUNDING
of the
1993-1996 RESEARCH PROGRAM
(November 1, 1993 - October 31, 1996)

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Submitted
July 29, 1994

To
The U. S. Department of Energy
Office of Health and Environmental Research
Washington, D. C. 20585

Grant No. DE-FG02-88ER60617

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FINANCIAL STATEMENT OF ESTIMATED COSTS

CASE WESTERN RESERVE UNIVERSITY

GRANT NO. DEFG2-88ER60617

November 1, 1992 to October 31, 1993

Estimated Total Costs this Contract Period	\$ 70,000.00
Support Costs for Contract Period	70,000.00
Cummulative Support Costs	384,838.00
Accumulative Support Ceiling	454,838.00
Amount of Free Support or Deficit	-0-

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SCOPE of 1993-1996 Proposed Research Program

The focus of efforts proposed in 1993 for the 1993-1996 project period was the full integration of results obtained in our interdisciplinary studies of electron and ion transport and reactions in liquids into a unified understanding of the well established correlation between the electrophilicity and carcinogenicity of chemicals. This goal was to be achieved through the coalescence of our three-pronged studies that clarify how excess charges interact with biological systems which complements radiation physics and chemistry in providing a better understanding of the biological effects of charges produced by ionizing radiation. Studies that involve the model charge acceptor fullerene and the ubiquitous environmental carcinogen radon were also proposed that contribute to the same goal.

SUMMARY of 1993-94 Progress

As in the 1990-93 project period that preceded the 1993 renewal of the "Ionization in Liquids" project, our goals were focused on and consistent with the goals of DOE's Medical Applications and Biophysical Research Division of the Office of Health and Environmental Research. These goals are: "...develop new concepts and techniques for detecting and measuring hazardous physical and chemical agents related to energy production..." and "...determine the physical and chemical mechanisms of radiation action in biological systems" [DOE, 1990]. Our commitment to continuing to contribute to these areas is evident from the following summary of our 1993-94 progress and the studies proposed for 1995-96.

Progress in 1993-94 was focused on two areas: (i) delineating how ions of the model nonpolar spherical solute Buckminsterfullerene interact differently with various nonpolar solvents than does the ellipsoidal fullerene analog C-70, and (ii) exposing a variety of new audiences to the electrophilicity-carcinogenicity relationship in order to obtain fresh insight into this relationship that may lead to elucidation of the role of electrons in carcinogenesis and thereby a better understanding of the biological effects of ionizing radiation. To achieve these goals a new collaboration was established with scientists at Oak Ridge National Lab who have unique facilities to characterize fullerene and its radiolytic products. Our work on the relationship between the electron attachment rate constant of a chemical and the carcinogenic properties of that chemical were presented in seminars to university students at seminars in two countries and in invited lectures at four major conferences, one of which included a symposium organized by the P.I. on the analysis of environmental biohazards. Publications from these lectures are appended and now summarized.

1993-94 DOE PROGRESS REPORT and REQUEST for 1994-95 FUNDING

I. MODEL SYSTEMS

A. Fullerene Solutions

1. *Introduction*

A significant fraction of our 1993-94 effort was directed toward unraveling several aspects of the various physico-chemical processes that were discovered in our cursory pulse-radiolysis studies of fullerene in 1992-93. In the earlier preliminary studies, the Stokes radii of the well characterized fullerene ions were measured in liquid hydrocarbons via time-of-flight measurements of the drift times of the ions using the Hahn-Meitner Institute (HMI) pulse conductivity system that we had used in numerous studies of electron mobilities [e.g. Bakale et al., 1992]. These studies were refined as was proposed in the 1993-1996 **"Ionization in Liquids" RESEARCH PROGRAM**; viz., solutions of highly purified (>99 mol%) C-60 were studied rather than fullerene known to contain >10-15 mol% of C-70 that was used in our initial studies. Further, fullerene C-70 having a purity of ~98% was also studied using the same HMI pulse conductivity system to determine if the ellipsoidal geometry of these ions significantly affected ionic interaction with the solvent. In addition, the drift time measurements of the C-60 and C-70 mobilities were extended from n-pentane (NPT) and cyclohexane (CHX) to the high viscosity solvent tridecane (TDC) for which the viscosity is 1.8 centi-Poise (cP) at 23 °C or ninefold greater than that of CHX. The fourth refinement done to delineate ion-solvent interaction in nonpolar solutions of fullerene was to measure the temperature dependence of the ion mobilities and thereby extend the viscosities studied over the range of 0.21 to 2.9 cP. A full description of these studies is given in the draft of the manuscript that is appended [Bakale et al., 1994c] and which is now summarized.

2. *Mobilities of C-60 and C-70 Ions*

The results obtained in our pulse-conductivity measurements of the temperature dependence of the mobilities of C-60 and C-70 ions are listed in Table I for the three solvents studied. These results are plotted in Figure 1 which illustrates the logarithmic dependence of the mobility on the solvent viscosity and the similar mobilities of the C-60 and C-70 ions. Also included in Fig. 1 is a single data point for the C-60 ion reported by the group of Albrecht [Lim et al., 1993] which is in reasonable agreement with the value that we report. The Stokes radii calculated for the ions in the three solvents are listed in Table I from which we conclude that the Stokes-Einstein equation is equally applicable to both spherical C-60 and ellipsoidal C-70 ions in nonpolar solvents; see the appended manuscripts [Bakale et al., 1993b, 1994c] for details that compares these radii with those that were also obtained at HMI using a photoionization technique [Katoh et al., 1994].

TABLE I. Summary of temperature dependences of viscosity, η , and mobility, μ , measured in fullerene solutions in n-pentane, c-hexane and tridecane before and after irradiation to 25 krad.

<u>Solvent</u>	<u>T(°C)</u>	<u>η(cP)</u>	<u>C-60</u>	<u>C-60+γ^a</u>	<u>C-70</u>	<u>C70+γ^a</u>
			<u>μ^b</u>	<u>μ^b</u>	<u>μ^b</u>	<u>μ^b</u>
n-Pentane	-78	0.72	2.1	1.0	1.7	1.2
	-32	0.37	4.0	2.2	3.7	2.4
	24	0.21	6.5	4.0	6.2	4.5
<u>Radius (Å)^c</u>		--	<u>5.3</u>	<u>10</u>	<u>5.4</u>	<u>9.2</u>
c-Hexane	7	1.3	--	0.62	0.9	0.61
	22	0.93	1.3	0.8	1.6	0.94
	42	0.68	1.5	--	--	--
	58	0.54	2.2	--	2.1	1.7
	63	0.51	--	1.45	--	--
<u>Radius (Å)^c</u>			<u>6.1</u>	<u>9.8</u>	<u>5.3</u>	<u>9.5</u>
Tridecane	0	2.9	0.46	0.23	0.60	0.25
	23	1.8	0.9	0.38	1.0	0.47
	58	0.98	1.8	0.72	1.6	0.91
<u>Radius (Å)^c</u>			<u>5.7</u>	<u>9.8</u>	<u>5.2</u>	<u>8.7</u>

LEGEND:

- Irradiated by gamma radiation to dose of 25 krad
- Units of ion mobility are $\text{cm}^2/\text{Vs} \times 10^4$
- Average Stokes radii from all values of mobility measured in each solvent.

Fig. 1. Dependence of mobility of C-60 (open symbols) and C-70 (closed symbols) ions on viscosity in n-pentane (squares), c-hexane (circles) and tridecane (triangles) solutions at 22 C. X-is data point of C-60 in n-hexane from Lim et al., 1993.

Fig.2. Dependence of mobility of C-60 (open symbols) and C-70 (closed symbols) ions on viscosity in n-pentane (squares), c-hexane (circles) and tridecane (triangles) solutions at 22 C irradiated to 25 krad. Dashed line is best fit of data in Figure 1.

3. Mobility and identification of radiolytic products of C-60

The most salient feature of our fullerene studies is illustrated in Fig.2 in which the mobilities of the C-60 and C-70 ions in gamma-irradiated solutions are compared with those reported in Fig.1. We hypothesized that the radiolytic products were dimers of C-60 or C-70 monomers based on the markedly lower mobilities of the observed ions, and we discussed these results with analytical chemists at CWRU and HMI in our attempt to identify the products. Initial mass spectral analysis of the products using fast atom bombardment mass spectrometry (FAB MS) at CWRU yielded inconclusive results which was presumed to be due to decomposition of the product during atom bombardment. A study by a group at the Oak Ridge National Laboratory (ORNL) who used small angle neutron and x-ray scattering (SANS and SAX, respectively) to measure the Van der Waals radii of C-60 and C-70 ions [Affholter et al., 1994] prompted us to seek collaboration with this group in order to identify the C-60 and C-70 radiolytic products. Drs. Compton, Henderson and Hettich of ORNL were contacted and agreed to use SAX and/or SANS as well as laser desorption MS to identify the fullerene radiolytic products. Solutions of degassed C-60 in CHX at $\sim 5 \mu\text{M}$ concentrations were irradiated at CWRU to doses of ~ 50 krad with cesium-137 gamma radiation, the solvent was removed by evaporation and the concentrated golden brown residue was sent to ORNL for analysis. A Van der Waals radius of the product of $\sim 6.5 \text{ \AA}$ was found by SAX which is $\sim$ twofold greater than that of the parent C-60 molecule [e.g., de Boer et al, 1994]. In addition, the molecular weight of the residue is 1514 which is more than twice the molecular weight of C-60 which is 720. The residual molecular weight of 74 (i.e. $1514 - [2 \times 720] = 74$) may be a partially hydrogenated molecule of the solvent which will be determined in duplicate analyses that are currently being conducted with high resolution MS. A significant product having a mass of 430 was also observed which may be C-36. This fullerene has a mass of 432 and has been predicted to be one of the more stable "small fullerenes" [Kroto and Walton, 1993].

Additional pulse-conductivity measurements of the mobilities of C-60 and C-70 ions and the radiolytic product ions are planned during the P.I.'s visit to HMI in August and September, and at this time a final draft of the appended manuscript will be prepared and submitted to the *Journal of Physical Chemistry*. Discussions of a manuscript in which the scattering and MS analyses of the C-60 radiolytic products will be reported have begun with the ORNL collaborators, and this manuscript may be submitted simultaneously with the manuscript in which the mobilities are reported. Submission of the CWRU-ORNL manuscript, however, is contingent upon the analyses that are currently underway which may indicate that additional product characterization studies are warranted.

4. Electron Attachment to C-60

In addition to the preceding studies of the fullerenes, considerable effort was directed toward measuring the rate constant of electron attachment, k_e , of C-60 and the dependence of k_e on the dose of gamma irradiation received by the C-60 solution. Considerable variation of the k_e dose dependence was observed in these studies which may be related to radiolytic conversion of the C-60 to a species having significantly different electron attachment properties than the parent molecule which caused the observed complex dose dependence of k_e . Although a reproducible dose dependence of k_e was not measured, the k_e of C-60 in unirradiated CHX was found to be $3.9 \times 10^{12} \text{ M}^{-1}\text{s}^{-1}$. This value is less than diffusion-controlled if the contribution of the induced dipole to the reaction radius which results from the anomalously high polarizability of C-60 is considered [Maltsev et al., 1993]. The implications of the measured value of k_e to the carcinogenicity of C-60 is discussed further in Section III.

5. Studies of Fullerenes projected for 1994-95

In addition to preparing and submitting for publication the manuscripts discussed in Section I.3, additional studies of the fullerenes are planned. The possibility of exploiting ionizing radiation to synthesize novel fullerene-based products is apparent from the studies being conducted in collaboration with ORNL and are particularly intriguing in view of the radiolytic C-60 product that appears to be a dumbbell of two C-60 balls connected by an unsaturated six-member carbon ring. This product suggests that two C-60s could be joined by various solvent molecules to yield a series of products in which the C-60s could be separated to the optimal distance to maximize the superconducting properties of the "dimer" [e.g., Enredi and Ladik, 1994]. The radiolytic method of linking C-60 molecules that we have discovered differs from conventional polymerization techniques [e.g., Fischer, 1994] and may thus yield a product having unique conductivity properties. A sample of the "dimer" product from C-60/CHX radiolysis will be prepared at CWRU and taken by the P.I. to HMI where a variety of techniques can be applied to characterizing the conductivity of the radiolytic product.

B. Electron Attachment in Mixtures

Our studies of electron transport in mixtures [Bakale and Schmidt, 1990; Bakale et al, 1992b] will be complemented by studies of electron attachment in the same mixtures that have been completed but not yet reported. These studies were conducted in collaboration with Dr. G. Beck at HMI, and completion of a manuscript now in preparation is anticipated during the P.I.'s visit to HMI in August-September, 1994.

II. BIOMIMETIC SYSTEMS

Our earlier study of electron attachment to the membrane-mimetic reversed micellar system Aerosol OT/H₂O in the solvents isooctane and tetramethylsilane [Bakale et al., 1992a] was recently presented to a group of radiation chemists [Bakale et al., 1994a]. The opportunity to do this arose when the P.I. was invited to lecture on electron attachment to carcinogens at the 1994 Gordon Research Conference on Radiation Chemistry. The motivation to present the published work on micelles was to arouse the conferees' interest in several aspects of the study that are pertinent to basic processes in radiation chemistry; these include the influence of water structure on electron solvation, the influence of induced dipoles on the electron attachment process, the influence of the residence time of the electron in the vicinity of the electron acceptor on the attachment rate, and other factors that are discussed in the condensed version of the poster that is appended. The P.I. drew the attention of Dr. Mozumder of Notre Dame to the poster at the conference in an effort to obtain the opinion of this noted theoretician on several of the hypotheses that had been proposed to explain the observed results. Dr. Mozumder viewed the materials presented in the poster and is currently reviewing our earlier AOT paper. Further discussions of electron attachment to Aerosol OT/H₂O micelles with Dr. Mozumder are anticipated.

The measurements of k_{e} s in micellar media that are more biomimetic than cyclohexane or isooctane which had been proposed in 1993 have not yet been initiated. Renovations to our laboratory in the Wearn Building of University Hospitals significantly interfered with pulse-radiolysis studies that could be conducted, particularly those that required use of the Van de Graaff generator. In addition, insufficient funds were available to obtain the transient digitizer that was to be used in conducting the proposed studies. Measurements of this type will be attempted in which equipment that is currently available will be used. In addition, studies of charge-carriers in these same micellar systems in which various biomolecules are encapsulated in pools of water will be attempted. A recent review of the latter system provides added incentive to conduct studies of this nature [Pileni, 1993].

III. ELECTRONS IN BIOLOGICAL SYSTEMS

The best indicator of progress in this area is the list of the P.I.'s 1993-94 activities pertinent to the "Ionization in Liquids" project which concludes this report. The presentations on the relationship between the electron attachment rate and the carcinogenic properties of a chemical at seminars, workshops, conferences and symposia provided an opportunity to expose new audiences to the carcinogen-screening technology that we have developed. The interdisciplinary nature of this technology is reflected in the variety of disciplines that were represented in the audiences which included physical, analytical, environmental and radiation chemists, chemical physicists, biochemists, biologists, toxicologists, medical

students as well as scientists from other disciplines. The publications that resulted from these presentations are appended and are now summarized.

A. *International Workshop on Predicting Chemical Carcinogenesis in Rodents*, (NIEHS, Research Triangle Park, NC, May 23-25, 1993).

The attention focused on this workshop is evident from the numerous reports on the workshop that appeared in various trade journals which included *Nature*, *Chemical & Engineering News*, *Environmental Health Perspectives*, *Environmental and Molecular Mutagenesis*, *Pesticide & Toxic Chemical News* and *Food Chemical News*. The purpose of the workshop was to compare the results of the predictions of ten different short-term screening tests that had been applied during the preceding two years to screen chemicals that were at that time being tested in rodent bioassays by the National Toxicology Program (NTP). The predictions of the carcinogenicity of these chemicals with the k_e test had been published earlier [Bakale and McCreary, 1992], and when the rodent results were disclosed at the Workshop, the k_e test predictions were the most accurate of all tests for which the test predictions had been previously published. The poor performance of the other screening tests that had been funded for years by NIEHS may have prompted the organizers to cancel plans for publishing the proceedings of the workshop, and attention was directed away from the short-term test results to the accuracy of the predictions of a "panel of experts". Since one of the purposes of short-term testing is to avoid the subjective nature of "panels of experts", it appears to the P.I. that the workshop failed in its alleged purpose to determine objectively which short-term test for carcinogens is most accurate.

The workshop concluded with a challenge from the NTP to the participants to begin applying their screening methods to the next set of chemicals that will be tested in NTP rodent bioassays. Efforts to obtain funding from the NTP to conduct k_e screening of these chemicals have been unsuccessful to this point; consequently, these chemicals will not be screened with DOE funds which is consistent with the objectives of the 1993-96 Proposed Research Program. Efforts will continue, however, to secure funding from the NTP, NIEHS, EPA and/or FDA to screen the 33 chemicals now being tested.

B. *NATO Advanced Study Institute on Linking the Gaseous & Condensed Phases of Matter: The Behavior of Slow Electrons*

The invited lecture entitled "A Carcinogen-Screening Test Based on Electrons" that was presented at this conference was aimed at motivating the attending physicists and chemists to extrapolate their knowledge of well defined basic processes in gases and liquids involving electrons and ions to the complexities of biological media. This challenge is repeated in the appended manuscript which also reiterates one of the points pertaining to

the biological effects of ionizing radiation that the P.I. attempted to make at the conference, viz., *since carcinogens are electrophiles and ionizing radiation is the most thoroughly characterized human carcinogen, should not more attention of radiation physicists and chemists be directed toward identifying the electrophilic component of ionizing radiation that effects biological damage?* The same question was discussed with several conferees including Dr. M. Inokuti who agreed that there appears to be a component of ionizing radiation that induces biological damage that has not been identified. This component is not simply the hydroxyl radicals on which radiation biologists have focused their attention for several decades. Both Dr. Inokuti and the P.I. agreed that the unknown electrophile could be a precursor of hydroxyl radicals, and studies to identify the unknown electrophile will be sought.

C. Symposium on "Analysis of Environmental Biohazards" Pittcon '94, Chicago, IL, February 27-March 4, 1994; Meeting Report in American Environmental Laboratory

The opportunity to organize a symposium at one of the world's major conferences on analytical instrumentation that focused on DOE OHER's goal of developing "...new concepts and techniques for detecting and measuring hazardous physical and chemical agents related to energy production..." was welcomed by the P.I. The objective of this symposium was to interface state-of-the-science chemical separation technology with state-of-the-science short-term carcinogen-screening techniques to illustrate how the analysis of environmental biohazards can be efficaciously conducted. The separation techniques that the P.I. selected to be described were solid-phase and supercritical fluid extractions which were followed by presentations on methods to assess the potential of complex mixtures to be biologically hazardous. The latter included a study to determine the significance of interactions of components in mixtures, a screening test that is based on DNA-adduct formation, and a device designed to probe the inherent electrophilicity of chemicals, which was the P.I.'s contribution to the symposium.

The first speaker was Craig Markell of 3M who demonstrated how solid-phase extraction (SPE) could be applied to the analysis of a spectrum of environmental samples that included air, water, foods, oil/grease and soil. Steven Hawthorne of the Energy & Environmental Research Center of the University of North Dakota followed the SPE presentation with a discussion of what SFE can and cannot do in the environmental laboratory, and how it does manyfold faster than conventional liquid-liquid extraction techniques those extractions to which it is applicable. The focus of the symposium then shifted from these separation technologies to bioassay-directed analysis. Lara Gundel of Lawrence Berkeley Laboratory reviewed recent progress in fractionation and chemical

characterization of polar organic material associated with airborne particles and then discussed a problem that is inherent to all complex mixtures but is rarely addressed, viz., the interactions of components in such mixtures. A new bioassay-directed analytical approach was then described by Joellen Lewtas of EPA's Health Effects Research Laboratory. In this test DNA-adduct formation serves as a biomarker to identify specific chemicals and exposures that result in alterations to DNA and may be hazardous to humans or other organisms in the environment. This genotoxicity-based end-point of DNA-adduct formation is somewhat related but also contrasts with the electron-based end-point used in the physico-chemical screening technique described in the concluding lecture of the symposium by the P.I. The focus of this lecture was on the pulsed electrophile detector that had been reported earlier [Bakale et al., 1993a], and the application of this detector to the analysis of complex mixtures such as cigarette smoke and dust from the homes of smokers and nonsmokers was described. The entire symposium is summarized in the Meeting Report that was the feature article in the most recent issue of *American Environmental Laboratory* which is appended [Bakale et al., 1994b].

D. Gordon Conference on Radiation Chemistry, Newport, RI., July 18-24, 1994.

The invitation to the P.I. by Dr. C. Jonah, Chairman of the 1994 Gordon Research Conference on Radiation Chemistry, to present a lecture at the Conference on electron attachment to chemical carcinogens is viewed by the P.I. as the highlight of progress in the past year. This invitation indicated that our research on chemical carcinogens has generated significant interest and provided the P.I. with an opportunity to convince a very special audience having expertise in all areas of electron reactions that the correlation between k_e and carcinogenicity has a sound theoretical basis. The degree to which this objective was achieved will best be measured by the influence that the lecture had as gauged by the audience's referring to the P.I.'s work in their future publications. A more direct effect will be the conferees' having access via the Notre Dame database to the values of k_e that have been measured; the k_e s will be entered into the database by Dr. Ross of Notre Dame who attended the Conference and oversees the database. From the number of reprint requests that the P.I. received from the audience, it is clear that most of the conferees were not familiar with the concept that their work had possible relevance to biological processes. Reprints that were distributed from journals such as *Carcinogenesis* and *Mutagenesis* may prompt some of the radiation chemists to take a more interdisciplinary approach to their research and to look beyond radiation chemistry for possible applications of their work.

E. University Presentations

Invited lectures to students at the Free University of Berlin and at Gannon University in Erie, PA contrasted strongly with the Gordon Conference in providing an opportunity to reach an audience that was eager for new ideas. The two audiences of students also contrasted with one another; those at the Free University were primarily chemical physicists whereas most of the students at Gannon were preparing for careers in medicine. This contrast in the audiences underscores the interdisciplinary nature of our research program.

F. Manuscripts in Preparation

In addition to those manuscripts that have been cited in the preceding sections as being in press or in preparation, the submission of two other manuscripts is imminent. Both manuscripts were appended to the 1990-93 "Ionization in Liquids" Progress Report but submission was delayed because the senior author, Dr. E. Zeiger of NIEHS, added the responsibility of editor of *Environmental and Molecular Mutagenesis* to his responsibilities at NIEHS. The revised cover page to that manuscript is appended, and our accompanying manuscript entitled "Comparison of k_e test electrophilicity and bacterial mutagenicity for 90 coded chemicals" is unchanged from the draft that was appended to the 1993 Progress Report. Another manuscript co-authored by Dr. F.K. Ennever of Wake Forest who collaborated in an earlier study [Ennever et al., 1992] is also in preparation. Another manuscript is planned in which the k_e of fullerene C-60 will be reported and the toxicological implications of this value will be discussed. Fullerene C-60 is receiving increased interest among biologists since it was reported to be an inhibitor of HIV protease [Friedman et al., 1993], and its conversion to derivatives that can be metabolized has intensified this interest [e.g., Scrivens, et al., 1994].

IV. RELATED STUDIES

The P.I.'s collaboration with Drs. H.H. Evans and P.S. Rao of the CWRU Radiology Department on the biological effects of radon on mammalian cells continues and was recently reported in two publications [Evans et al., 1993a,b]. These studies provide appreciation for the complexities of working with mammalian systems as well as recognition of the special problems associated with studying radon. This collaboration will be extended during the next year to studies that include *in vitro* irradiation of DNA which should complement the P.I.'s attempts to elucidate the mechanism of the biological effects of ionizing radiation.

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1993-1994 ACTIVITIES OF THE P.I. PERTINENT TO THE
IONIZATION IN LIQUIDS" PROJECT

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6/2-7/29/93
8/3-10/6/94

***Presentations, conferences, publications, etc. since submission of the
1993-96 Progress Report.***

*Bakale, G., and McCreary, R.D., "Synopsis of Prospective k_e Screening of Chemicals Tested by the NTP", in *Predicting Chemical Carcinogenesis in Rodents*, D. Bristol and J. Wachsman, eds., pp. 63- 65; 131-134 and presented at the *International Workshop on Predicting Chemical Carcinogenesis in Rodents*, (NIEHS, Research Triangle Park, NC, May 23-25, 1993).

Bakale, G., "An Electron-Based Carcinogen-Screening Test", invited lecture at the Freie Universitat Berlin, June 28, 1993.

*Bakale, G., Lacmann, K. and Schmidt, W.F. "Fullerene Ion Mobility in Liquid Hydrocarbons", *Proceedings of the Eleventh International Conference on Conduction and Breakdown in Dielectric Liquids*, J. Fuhr and P. Biller, eds., pp.131-134, (IEEE, Baden-Dattwil, Switzerland, 1993).

*Bakale, G., "A Carcinogen-Screening Test Based on Electrons", *NATO Advanced Study Institute on Linking the Gaseous & Condensed Phases of Matter: The Behavior of Slow Electrons*, (Patras, Greece, September 5-18, 1993); manuscript edited by L.G. Christophorou, W.F. Schmidt and E. Illenberger is in press (Plenum, New York).

Bakale, G., Katoh, R., Lacmann, K. and Schmidt, W.F. "Mobilities and Radii of C₆₀ and C₇₀ Fullerenes in Liquid Hydrocarbons, (poster) *ibid.*

*Bakale, G., Organized and presented lecture in Symposium on "Analysis of Environmental Biohazards" at Pittcon '94--Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Chicago, IL, February 27 - March 4, 1994

Bakale, G. "Screening Tests to Identify Environmental Biohazards" invited lecture at Gannon University, Erie, PA March 24, 1994.

*Bakale, G., Gundel, L., Hawthorne, S., Lewtas, J., Markell, C., Meeting Report in *American Environmental Laboratory*, 6, No. 6, pp. 1, 6, 8 (June, 1994).

Bakale, G., "Electron Attachment to Chemical Carcinogens", invited lecture at the 1994 Gordon Research Conference on Radiation Chemistry, Newport, RI., July 18-24.

*Bakale, G., Beck, G. and Thomas, J.K., "Electron Attachment to AOT/H₂O Reversed Micelles", Summary of poster presented at the 1994 Gordon Research Conference on Radiation Chemistry, *ibid.*

* Denotes appended material; see APPENDIX.

1993-1994 ACTIVITIES OF THE P.I. (CONTINUED)

Bakale, G., McCreary, R.D. and Ennever, F.K. "Response of k_e Test to NCI/NTP-Screened Chemicals. IV. Equivocal Carcinogens." (manuscript in preparation).

*Bakale, G., Lacmann, K. and Schmidt, W.F. "Mobilities and Stokes Radii of C_{60} and C_{70} Ions in Liquid Hydrocarbons", (manuscript in preparation).

Bakale, G. and McCreary, R.D. Comparison of k_e test electrophilicity and bacterial mutagenicity for 90 coded chemicals. (manuscript in preparation).

Evans, H.H., Menci, J., Bakale, G., Rao, P.S., Jostes, R.F., Hui, T.E., Cross, F.T., Schwartz, J.L. "Interlaboratory comparison of the effects of radon on L5178Y Cells: Dose contribution of radon daughter association with cells", *Radiat. Res.* 136, 48-56 (1993).

Evans, H.H., Menci, J., Hui, T.E., Ricanati, M., Homg, M.F., Di Salvo, C., Bakale, G., Rao, P.S. "Cytotoxic and mutagenic effects of radon and radon daughters on murine L5178Y lines differing in DNA repair", *Radiat. Res.* 136, 57-64 (1993).

Zeiger, E., Ashby, J., Bakale, G., Enslein, K., McCreary, R.D., and Rosenkranz, H.S., "Prediction of *Salmonella* Mutagenicity", (manuscript in preparation)

APPENDIX

PUBLICATIONS, ABSTRACTS OF PRESENTATIONS, AND MANUSCRIPTS IN PREPARATION THAT ARE PERTINENT TO THE "IONIZATION IN LIQUIDS" PROJECT.

Bakale, G., and McCreary, R.D., "Synopsis of Prospective k_e Screening of Chemicals Tested by the NTP", in *Predicting Chemical Carcinogenesis in Rodents*, D. Bristol and J. Wachsman, eds., pp. 63- 65; 131-134 and presented at the *International Workshop on Predicting Chemical Carcinogenesis in Rodents*, (NIEHS, Research Triangle Park, NC, May 23-25, 1993).

Bakale, G., Lacmann, K. and Schmidt, W.F. "Fullerene Ion Mobility in Liquid Hydrocarbons", Abstract in *Proceedings of the Eleventh International Conference on Conduction and Breakdown in Dielectric Liquids*, J. Fuhr and P. Biller, eds., pp.131-134, (IEEE, Baden-Dattwil, Switzerland, 1993).

Bakale, G., Lacmann, K. and Schmidt, W.F. "Mobilities and Stokes Radii of C_{60} and C_{70} Ions in Liquid Hydrocarbons", (manuscript in preparation).

Bakale, G., "A Carcinogen-Screening Test Based on Electrons", manuscript based on invited lecture presented at the *NATO Advanced Study Institute on Linking the Gaseous & Condensed Phases of Matter: The Behavior of Slow Electrons*, (Patras, Greece, September 5-18, 1993); edited by L.G. Christophorou, W.F. Schmidt and E. Illenberger (in press, Plenum, New York).

Bakale, G. and McCreary, R.D., "Application of a liquid-phase electron-capture detector to the analysis of environmental biohazards", Abstract of invited lecture presented in Symposium on "Analysis of Environmental Biohazards" at Pittcon '94—Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Chicago, IL, February 27-March 4, 1994;

Bakale, G., Gundel, L., Hawthorne, S., Lewtas, J., Markell, C., Meeting Report on "Analysis of environmental biohazards," *American Environmental Laboratory*, 6, No. 6, pp. 1, 6, 8.

Bakale, G., Beck, G. and Thomas, J.K., "Electron Attachment to AOT/ H_2O Reversed Micelles", Summary of poster presented at the 1994 Gordon Research Conference on Radiation Chemistry, Newport, RI., July 18-24 1994.

Zeiger, E., Ashby, J., Bakale, G., Enslein, K., McCreary, R.D., and Rosenkranz, H.S., "Prediction of *Salmonella* Mutagenicity", (Cover page of manuscript in preparation).

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