

# THE COUNCIL FOR NEAR-INFRARED SPECTROSCOPY



**NEWSLETTER issue #2**

*March 1987*

## **AT THE PITTSBURGH CONFERENCE:**

**ASTM E 13.03.03 NIR TASK GROUP MEETING, Monday, March 9, 7:00-10:00 PM, Caesar's Boardwalk Regency, Augustus room, all are invited (see agenda)**

**COUNCIL GOVERNING BOARD OPEN MEETING: Wednesday, March 11, 7:30-10:00 PM, Trump Plaza, Chelsea-A Room, all are invited**

## **ACTIVITIES OF THE COUNCIL FOR NEAR-INFRARED SPECTROSCOPY**

The Council for Near-Infrared Spectroscopy is a free standing entity, with its own constitution and by-laws, and nationwide membership. The Council has officially been accepted as an affiliate of the national Society for Applied Spectroscopy. SAS.

The Council met September 29, at the 1986 FACSS meeting in St. Louis to form committees and begin the programs stated in the objectives of the last Council newsletter.

### **Bibliography of NIR references**

Efficient and complete access to near-infrared literature is difficult and a problem because the references are spread over so many technical and trade publications representing many very different disciplines. It was agreed that the council would organize a bibliographic service to be made available at a nominal charge. A number of existing lists of NIR references were identified. David Honigs was appointed to chair the Bibliography Committee with the

assistance of Michael Lams, Jim Psotka, and Jerry Workman. David plans to have the bibliography operational in time for demonstration at this Pittsburgh Conference meeting. Those interested in helping should contact David Honigs, Department of Chemistry BG-10, University of Washington WA 98195, (206) 543-0713. We wish to thank Sam Gabriel for providing the newsletter with current Chemical Abstract citations.

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### Library of NIR Spectra

A library of digitized NIR spectra was the second major need identified at this meeting. The proposed JCAMP-DX format will be considered and, if necessary, extensions or modifications proposed to meet the needs of the NIR community. Standards for quality spectra must be established. It was agreed that the agricultural library of 450 spectra made available by Karl Norris must be expanded to include industrial and pharmaceutical chemicals. Those interested and able to develop formats, standards or provide reference quality spectra should contact Karl Norris, Instrumentation Research Laboratory, Beltsville Agricultural Research Center West, Beltsville, MD 20705, (301)344-3650.

### Bulletin Board

A computer bulletin board for the exchange of information among NIR practitioners is being set up. This BBS will serve as an information source and suggestion box for future Council activities as well as a question, answer and communication forum among members. Robert Lodder has agreed to spearhead this activity and is responsible for working out the technical details necessary for reserving a section of the SAS bulletin board for Council use. SAS has informed him that they expect to introduce a modification to their operating system in March. This system will then be compatible with many of our bulletin board needs. Plans are in progress to have the Council's BBS operational by April 15. At that time the Council will send a mailing to all members with instructions for its use. There is also a possibility that this modified system will have facilities for downloading bibliographic material. We hope that future improvements will further allow us to exchange spectra electronically.

*If you are interested in an electronic bulletin board for NIR use please express your interest to the representatives at the SAS booth. It is important that they be aware of our interest.*

Until April we can communicate with each other through the SAS bulletin board's electronic mail and on-line help facilities by using the following instructions:

1. The bulletin board can be accessed at 300 or 1200 baud, 8 bit, no parity, 1 stop bit, all hours (I think), max.20min.
2. On you first call you will be prompted to answer questions for new users and will be guided by menu driven help facilities.
3. The BBS telephone number is 1 (301) 694- 0697, press return when computer comes on line.

Anyone interested in information or helping Rob should contact Robert Lodder, Dept. of Chemistry, Indiana University, Bloomington, IN 47405, (812)335-7905.

International Affiliation - Discussions at the last meeting have not yet resolved how best to participate in the newly forming international association. Various pros and cons were presented but the actual direction is still under consideration.

### **ASTM TASK GROUP ON NEAR- INFRARED SPECTROSCOPY TO HOLD OPEN MEETING MONDAY EVENING, MARCH 9, CAESAR'S BOARDWALK REGENCY HOTEL, AUGUSTUS ROOM, 7:00 - 10:00 PM**

The ASTM E13.03.03 NIR Task Group, chaired by Council President, Edward Stark, is charged by the ASTM with the task of developing standards for the field of near-infrared spectroscopy. Everyone interested in NIRS is encouraged to come and participate in the discussions.

Monday evening the Task Group plans to complete its work on Standard Definitions of Terms and Symbols Relating to Near-infrared Spectroscopy. The document will be submitted for balloting through the ASTM. Definitions for accuracy, precision, bias, SEC, SEP, coefficient of determination, regular reflection, diffuse reflection, bulk reflection, transfection, spectral matching, intercorrelation, multiple correlation coefficient, transmission/reflection interaction, and more are being worked on.

The Task Group will also consider recommendations for revisions to the JCAMP-DX spectral data exchange format which are desirable for its use for NIRS data.

Several proposals have been made concerning NIR Instrument Test Procedures. The need for exceptional levels of instrument performance for modern NIRS makes this a particularly significant activity. In conjunction with test procedures, the Task Group will begin to consider standard and reference materials.

## **ASTM NIR TASK GROUP AGENDA**

### OLD BUSINESS

1. Committee Membership
2. Revised Standard Definitions of Terms and Symbols
3. JCAMP-DX Data Exchange Format
4. Location of Fall 1987 Meeting

### NEW BUSINESS

1. Standard and Reference Materials
2. Goals & Operation of NIR Task Group

## **ELECTION RESULTS**

President  
Edward Stark  
KES Analysis  
180 West End Ave.  
New York, N.Y. 10023  
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Beltsville, MD 20705

Treasurer (1987-89)  
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Silver Spring, MD 20910

Delegates: D.Burns, Technicon; D.Funk, Dickey-John; D.Wetzel Kansas State Univ.; Loi: Weyer, Hercules Inc.; P.Williams, Canadian Grain Commission

## **EDITORIAL SECTION**

The COUNCIL is now affiliated with the Society for Applied Spectroscopy, the number of submitted Near-IR papers at the Pittsburgh Conference (1987) has increased dramatically, and exciting meetings scheduled for the near future. The membership meeting at FACSS produced useful suggestions, not the least of which is David Honigs offer to do the job of Chief Bibliographer. The availability of technical information is critical for Near-IR to flourish as a technique. The titles brought to your attention in the NEWSLETTER are but a taste of current NIR or closely related topics published or presented yearly. It is, as all Council functions, an unpaid work of love. I urge everyone to aid David in this undertaking.

There is one small complaint that

I wish to register. "Pittcon" has two Near-infrared sessions scheduled for 1987; Monday afternoon, Near Infrared: I Trump Plaza, Ballroom A/C and Thursday afternoon, Near Infrared II: Atlantis, Ballroom B. On the one hand, I am happy that there are two sessions. On the other hand, I am distressed that the Conference Committee separated the two sessions by two whole days. Not all chemists can attend the conference for the entire week. This forces them to choose sessions. While I don't think this was done with any malice or forethought, I cannot imagine an other schedule which would force the conferees to miss half of the HPLC, IR, or GC papers. Since Pitcon is the premier analytical meeting in the world, its treatment of a particular topic can help

significantly affect the knowledge and attitudes of analytical chemists on that topic. Perhaps, if we all "suggested" that Near-IR be included as a keyword for the topic and subject area of the registration form for contributing authors, the session organizers would recognize NIR as a discipline and begin to group Near-IR papers more equitably. I have found myself in the position of being the co-author of two simultaneous papers (at two widely different sessions), only one of which I could attend (despite my size).

While many people have contributed to the successful launch of the Council for Near-IR Spectroscopy, none has done more than Ed Stark. He has taken a vision and made it come true. From outlining the Constitution and By-Laws to browbeating each of us into contribute something to the cause. I would like to wish him well in his role as the first president of the Council. With the excellent slate of officers elected, I'm sure this organization will become a very model of what a professional group should be. (P.S.: without Karen, Ed would merely be mortal).

#### Letters to the Editor

Since this NEWSLETTER is so new, there are no letters. In fact, if the idea of a computer network becomes, a reality, this column may become redundant. In the meantime, this column may be used to communicate with other members. If an epistle should be referred to a specific member (or non-member), I will do my best to forward it in a timely manner.

Please send correspondence to: Emil  
W. Ciurczak Newsletter  
Editor 6 Riverside Drive  
Denville, NJ 07834

#### **NIR ARTICLES PUBLISHED in 1986 or late 1985**

#### Review Articles:

CA:104(6) 45123z "Remote UV-VIS-NIR Spectroscopy Using Fiber Optic Chemical Sensing." Fitch, P., Gargus, A.G., Am. Lab., 17(12), 64(1985).

CA:104(8) 61093v "Sample Area Optimization in a Diffuse Reflectance Near-Infrared Spectrophotometer.", Hirschfeld, T., Appl. Spectrosc., 39(6), 1085(1985).

CA: 105(19) 107641 y "Chemical Sensing Using Near-IR Reflectance Analysis", Wetzel, D.L., ACS Symp. Ser., 5(6), 154(1986).

#### Pharmaceutical:

CA: 104(12) 95604c "Identification of Actives in Multicomponent Pharmaceutical Dosage Forms Using NIRA.", Ciurczak, E.W., Maldacker, T.A., Spectroscopy, 1(1), 36(1986).

CA: 105(10) 85080k "Determination of Particle Size of Pharmaceutical Raw Materials Using NIRA.", Ciurczak, E.W., Torlini, R.P., Demkowicz, M.P., Spectroscopy, 1(7), 36(1986).

#### Textiles/Polymers:

CA: 104(8) 51944J "NIRS Analysis of Cotton/Polyester Yarns.", Tincher, W.C., Luk, A., Text. Chem. Color., 17(10), 200(1985).

CA: 104(13) 10804u "Rapid Analysis of Packaging Laminates by Near-IR Spectroscopy.", Davies, A.M.C., Grant, A., Gravel, G.M., Steeper, R.V., Analyst (London), 110(6), 643(1985).

CA: 105(10) 79790a "Utilizing Zero Crossover Points in the Near-IR Reflectance Analysis of Industrial Polymers," Weyer, L.G., J. Appl. Polym. Sci., 31(8), 2417(1986).

#### Agriculture:

CA: 104(13) 107982q "Near-IR Analysis

in the Fourier Domain with Special Reference to Process Control," Davies, A.M.C., McClure W.F., Anal. Proc. (London), 22(11), 321 (1985).

CA: 104(21) 184969t "Near-IR Reflectance Analysis of Oil Concentration in an Emulsion: A Study of Oil and Water Migrations in a Mayonnaise-Based Salad.", Davies, A.M.C., Brocklehurst, T.F., J. Scie. Food Agric., 37(3), 310(1986).

CA: 105(7) 59532q "Near-IR Spectrophotometric Determination of Individual Sugars in Aqueous Mixtures," Giangiaco, R., Dull, G.G., J. Food Sci., 51 (3), 679(1986).

General:

CA: 104(12) 98367p "A Designed Experiment for the Examination of Techniques Used in the Analysis of Near-IR Spectra. Part 1: Analysis of Spectral Structure.", Cowe, I.A., McNicol, J.W., Cuthbertson, D.C., Analyst (London), 110(10), 1227(1985).

CA: 104(12) 98368q "A Designed Experiment for the Examination of Techniques Used in the Analysis of Near-IR Spectra. Part 2. Derivation and Testing of Regression Models", Cowe, I.A., McNicol, J.W., Cuthbertson, D.C., Analyst (London), 110(10), 1233(1985).

CA: 104(12) 101683w "Normalized Distances for Qualitative Near-IR Reflectance Analysis", Mark, H., Anal. Chem., 58(2), 379(1986).

CA: 105(2) 14978y "Plastic Optical Fibers for Near-IR Transmission", Kaino, T., Appl. Phys. Lett., 48(12), 757(1986).

CA: 105(4) 32115u "Method for Daily Check of Wavelength Accuracy in Near-IR Reflectance Spectrophotometers", Dzwinczyk, M., Mark, H., Spectroscopy. 1(6), 51(1986).

CA: 104(14) 122069r "Near-IR

Spectrophotometric Methods Development with a limited Number of Samples: Application to Carbonate in Geological Samples", Honigs, D.E., Hirschfeld, T.B., Heiftje, G.M., Appl. Spectroscopy, 39(6), 1062(1985).

CA: 104(23) 205615s "Effect of Repack on Calibrations Produced for Near-IR Reflectance Analysis", Mark, H., Workman, J., Anal. Chem., 58(7), 1454(1986).

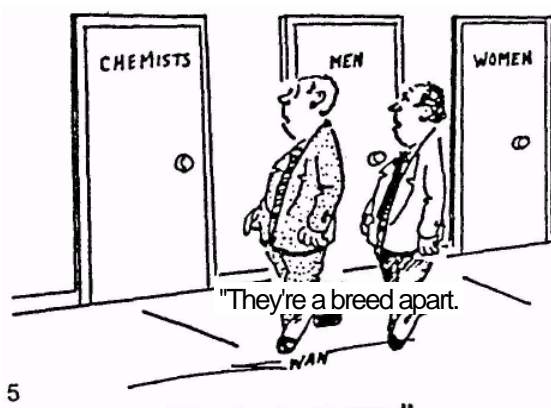
CA: 105(1) 5245e "Some Statistical Comments on the Errors in NIR Calibrations", Fearn, T., Anal. Proc. (London), 23(4), 123(1986).

### NEAR INFRARED SHORT COURSES

Near Infrared Reflectance Instrumentation. Feb. 10-11, 1987, Toronto, Ontario, sponsored by the American Association of Cereal Chemists. Faculty P. Williams, Wm.Hruschka, K.Norris & E.Stark, for information contact Dotty Ginsburg, AACC, (612) 454-7250 for future courses.

Near-IR Analysis: A New Industrial Tool. Mar. 7-8, 1987, Atlantic City, NJ, sponsored by ACS. Faculty D. Burns, D.Wetzel, contact Karen McIlvaine ACS, (202) 872-4508 for future courses.

Near Infrared Spectroscopy: An Overview Mar. 13, 1987, Atlantic City, NJ, sponsored by the Pittsburgh Conf. contact Mini-course registration (412) 797-7110 for future courses.



## FUTURE MEETINGS:

### **ACS National Meeting, April 5-10, 1987**, Executive Tower Inn, Denver, CO

Symposium on Near Infrared Analysis, April 8, organizer D. Honigs  
Papers will include the following topics: overview (David Honigs), oil and fat (R.B. Roy), silicone coating weights (C.M. Paralusz), on-line NIR techniques (LG. Weyer), Fourier self-deconvolution (P.R. Griffiths), Fourier transforms in NIR analysis (W.F. McClure), scatter-absorbance interactions (E.W. Stark), "Interactance" (K. Norris) discriminant analysis (H. Mark), spectral searching and matching (P.J. Cooper), the effects of wavelength search on calibrations (B. Tenge).

**SPECTROSCOPY ACROSS THE SPECTRUM, July 12-17, 1987**, Univ. of East Anglia, Norwich UK  
THE INTERNATIONAL COMMITTEE FOR NEAR INFRARED SPECTROSCOPY has organized the "First International Near Infrared Spectroscopy Conference" in association with the Royal Society of Chemistry - Analytical Division.

## SCIENTIFIC PROGRAMME

### Sunday 12 July

*Plenary lecture* K.H. Norris (USDA, Beltsville, USA)  
History, present status and future prospects for NIRS

### Monday 13 July—Combined Techniques

*Plenary lectures*  
Dr. J.G. Grasselli (SOHIO); Professor D. Games (UC Cardiff), Chromatography/MS; Professor L. Ebdon (Plymouth Polytechnic), LC/AS; Professor A.A. Fell (U of Bradford), LC/UV-vis; Professor P. Griffiths (Riverside, USA), Chromatography/FTIR.

*Parallel sessions*  
Near infrared Spectroscopy, infrared Spectroscopy, atomic Spectroscopy and UV/vis Spectroscopy. Speakers include:— Dr. K. Kaffka (Hungary), Dr. I. Murray, A.M.C. Davies, K.H. Norris (USA); Dr. J.G. Grasselli (USA), Dr. D.J. Gardener, Dr. H.J. Milledge, Dr. J.F. Alder; Dr. A.A. Brown, Dr. M. Thomsen, Dr. D. Littlejohn, Dr. P. Norman; Professor J. Miller, Dr. C. Burgess.

### Tuesday 14 July—Fourier Transformation Methods

*Plenary lectures*  
Professor N. Sheppard (JEA); Professor M.L. Gross (Nebraska), FTMS; Professor W.F. McClure (North Carolina), FTNIR; Dr. A. Thorne (Imperial College), FTAS

*Parallel sessions*  
Near infrared spectroscopy, Mass spectrometry, Nuclear magnetic Resonance, Process control methods. Speakers include:— Professor V. R. Krischenko (USSR), Dr. P. C. Williams (Canada), I.A. Cowe; Dr. J.A. Page, R. Self, Dr. A.L. Gray, Dr. M. Whitehouse, Dr. P. Farmer; Dr. W. Derbyshire, Dr. M.E. Cudby, Dr. T. Cholerton.

### Wednesday 15th July—Data Analysis

*Plenary lectures*  
Professor C.L. Wilkins (Riverside, USA); Dr. H. J.H. MacFie (Institute of Food Research), Chemometrics; Dr. E.W. Stark (KES Analysis, New York), NIRS data analysis; Dr. J.F. Tyson (U of T, Loughborough), Calibration methods.

*Parallel sessions*  
Near infrared Spectroscopy, Infrared Spectroscopy, Chemometrics. Speakers include:— Dr. E.W. Stark (USA), Dr. E.G. Osborne, Dr. L. Weyer (USA); Dr. M. Chesters, Professor H.A. Willis, I. Robertson, Dr. P.S. Belton; Dr. R. Tranter, Dr. D. Roberts, K.M. Wright, Dr. R. Spragg.

### END OF MAIN CONFERENCE: INIRS CONFERENCE CONTINUES

Thursday 16th July and Friday 17th July  
Practical Applications of Near Infrared Spectroscopy NIRS Workshops:— Sample Preparation, Calibration

ROYAL SOCIETY OF CHEMISTRY  
ANALYTICAL DIVISION  
East Anglia Region  
Atomic Spectroscopy and  
Automatic Methods Groups



## SPECTROSCOPY ACROSS THE SPECTRUM: Analytical Applications of Spectroscopy

12-15 July 1987

**Incorporating  
The First International  
Near Infrared Spectroscopy Conference**

(Organised by the International Committee (or  
Near Infrared Spectroscopy)

12-17 July 1987

University of East Anglia Norwich, UK

SECOND CIRCULAR

**EASTERN ANALYTICAL SYMPOSIUM Sept. 13-18, 1987, New York Hilton, NYC**  
program chairman Peter Keliher, (215) 645-4871

**FACSS XIV October 4-9, 1987, Cobo Hall Convention Center, Detroit**  
program chairman John Beaty, (617) 890-4300

NIRS TUTORIAL SERIES - The January and February issues of Spectroscopy contain the first two in a series of articles about statistics in spectroscopy. This series, by Howard Mark and Jerry Workman, began with basic concepts of the properties of random numbers and will extend to the analysis of variance, designed experiments; and the fitting of equations.

## **PAPERS OF INTEREST AT THE 1987 PITTSBURGH CONFERENCE**

### **SYMPOSIUM HONORING THE LATE TOMAS HIRSCHFELD**

Thursday Morning, Ballroom C, Atlantis

W.G.Fateley, Presiding

- (803) Reflections on Tomas Hirschfeld's Role in the Development of Micro-Raman Spectroscopy. E. Etz.
- (804) Hyphenated Instruments - A Problem Solver's Route S.A. Liebman.
- (805) The World of Industrial Spectroscopy - Before and After Tomas Hirschfeld. J.G. Grasselli, B.J. Bulkin, D.G. Cameron.
- (806) Hyphenated Infrared Spectrometry/ Chromatography for Elucidating Detailed Structures (Hirschfeld). P.R.Griffiths, S.L Pentoney Jr., D.J.J. Fraser.
- (807) FT-Raman. D.B. Chase.
- (808) Flames, Fibers, and Fourier Transforms - Interaction and Collaboration with Tomas Hirschfeld. G.M. Hieftje.
- (809) A Method of Treating a Consumable Product and Packaging for Consumable Products to Indicate Presence of Contamination. D.E. Honigs, J.H. Perkins, B.J. Tenge.

**Near Infrared I: Mon. afternoon, 1:30 PM papers 215-224, Ballroom A/C, Trump Plaza**

**Near Infrared II: Thurs. afternoon, 1:30 papers 1005-9, Ballroom B, Atlantis**

### **A LISTING OF SOME NEAR INFRARED PAPERS IN OTHER SESSIONS:**

- (485) Development of a Near Infrared, 4096 Channel Photodiode Array Emission Spectrograph with a Dual Port Random Access Memory Interface. J.M. Jatvis, E.E. King, R.C.Fry.
- (486) Comparison of Critical Design Features in Two NIRS Systems. A. Pietrantonio.
- (821) Near Infrared Spectral Matching for Qualitative Analysis. P.J. Cooper, T.H. Begley, K.M. Ronan.
- (831) Application of Near-Infrared Analysis to the Polymer Industry. F.A. DeThomas.
- (832) Characterization of Polymers Using Near Infrared Procedures. R.B. Roy, C.J. Kradjel.
- (833) Determination of the State of Epoxy Cure Advancement Using NIRA Procedures. R.B. Roy, C. Kradjel.
- (834) Near Infrared Measurements of Bisphenol-A-Epichlorohydrin Epoxide Resins Using an Indium Antimonide Detector. M.C. Paputa-Peck, R.O. Carter III.

**COUNCIL MEMBERSHIP APPLICATION:**

Because the Council For Near Infrared Spectroscopy is now affiliated with the Society of Applied Spectroscopy, SAS, the Council is providing a \$5.00 discount for combined Council and SAS membership fee. SAS membership includes a years subscription to the Journal of Applied Spectroscopy, as well as the SAS news bulletin published 4 times a year.

Please check the appropriate category:

Regular Membership - Council only [\$25 N.Amer./\$40 other] ( )  
discounted Council/SAS combined Membership [\$50 N.Amer./\$65 other] ( )

Student Membership - Council only [\$10] ( )  
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Sponsoring Membership [\$250] ( ) Name

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Company/School.

Area of Interest

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Patrick Cooper (treasurer)  
Pacific Scientific  
2431 Linden Lane Silver  
Spring MD 20910

We wish to thank the following instrument companies for becoming sponsoring members: Dickey John, Pacific Scientific and Technicon. A special thank you goes to Pacific Scientific for printing the first issue of our Council Newsletter and to Dickey-John, Pacific Scientific and Technicon for printing this issue. As a start-up venture we appreciate these acts of generosity.

**FOR FURTHER INFORMATION ABOUT SPECTROSCOPY ACROSS THE SPECTRUM**

contact or return this form to:

Dr. C.S. Greaser  
School of Chemical Sciences  
University of East Anglia  
Norwich NR4 7TJ, UK

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I would Like to present a poster titled ( )

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reductions: 2 days £80/£100; 1 day £50/£70