

## PROPOSED SPECIAL INTEREST GROUP ON NEAR INFRARED SPECTROSCOPY

### I. OBJECTIVE

To further the understanding and usage of near infrared spectroscopy.

### II. STRUCTURE

The proposed structure is to function as a special interest group of a larger scientific society which is associated with spectroscopy. The NIR-SIG should be organized at the national or International level rather than under any existing local or regional section. The two major possibilities seem to be ACS and SAS. Based on the difficulties in being recognized by the ACS encountered by the Vibrational Spectroscopy Topical Group of the NY-NJ Section, due to its "narrow" scope, it appears that SAS will be the more likely possibility. SAS maintains liaison with other organizations, such as Coblenz, FTS, American Iron and Steel, CESSE, CSI, and FACSS. There is an existing first class technical journal, Applied Spectroscopy, published eight times a year and a newsletter which appeared three times in 1985. SAS also sponsors a tour speaker program and a videotape library. The Pittsburgh Conference and FACSS meetings are the major conferences with which SAS is associated.

### III. PROPOSED FUNCTIONS A. Training

Operation of training programs can be a self-supporting activity, with perhaps some profit.

#### 1. Short courses:

There are now three short courses being run fairly regularly by D. Burns (ACS); D. Wetzel/T. Hirschfeld (FACSS/EAS); P. Williams/K. Norris (AACC); each with additional teachers. Cooperative effort and publicity could make each of these more effective and better attended. To achieve this, no change in sponsorship would be required or necessarily desirable, however cross-fertilization would be organized within the NIR-SIG.

#### 2. Workshop/seminars:

A workshop/seminar would cover a more specific area of NIR technology than a short course, and be directed to the more advanced user as opposed to the introductory level. Evening, half day, and full day sessions could be considered.

#### 3. Courseware:

The computer data processing is a major part of NIR methods development. Development of computer courseware (disks and workbook) covering various aspects of calibration,

validation and maintenance is a practical adjunct to and extension of short courses and workshop/ seminars. The ubiquitous IBM PC/XT/AT is commonly available so it would be an appropriate host. The host for courseware would not have to be the same as for operation, as long as the courseware covered the various formats of data presentation where necessary for clarity.

#### 4. Videotape:

SAS runs a videotape library with free distribution to members and sponsors (donation requested), rental (\$25/8 weeks to avoid waiting list), and purchase (\$60). Tapes are donated by authors, who retain rights for use involving remuneration (short courses, etc). Videotapes would cover both general introductory material and specifics, such as sample preparation, which are better covered by videotape than courseware.

### B. Libraries,

These library functions could also generate revenue.

#### 1. Bibliography and Reference Library:

Acceptance of NIR by the scientific community depends on a base of published literature. NIR work is spread over a remarkable breadth of sources, many of which are not commonly seen by spectroscopists. Efficient searches are difficult to design and expensive. A complete bibliography, maintained and updated by users as new material appears, would be valuable. Annotations, if possible, would increase the value. Furthermore, making copies of complete papers available (at a fee) would enhance the service. A start toward this has been made by the instrument companies and some individuals, however a cooperative effort would be much more effective.

#### 2. Software Library:

The common availability of IBM PC/XT/AT computers makes a general purpose software library a realistic possibility. This library would include utilities, new data analysis approaches, and data handling of results, etc. For users whose instruments utilize different computers, translation of data files either from disk, if possible, or by a communication link would allow them to use the IBM PC/XT/AT library programs. Programs specific to other computers could also be distributed if the originators were willing to generate copies. "Freeware" programs would be contributed by the authors and distributed by the NIR-SIG at a modest profit. Programs could also be leased or sold through the NIR-SIG with profits shared by the author and the NIR-SIG. This would require adequate program documentation and support by the author.

### 3. Spectral Library:

Until recently, spectral libraries were of little value in NIR. However, material identification is now becoming important and good digitized spectral libraries could become valuable. Selection or confirmation of analytical wavelengths is another possible value. The format and quality of spectra must be defined, and utility software provided to convert to files usable by the commercially available computers and software packages. Reference spectra must be included so that wavelength and absorption scales can be matched between instruments. Documentation of the sample preparation and presentation should also be provided. Spectral files would be contributed by users and the instrument companies. The NIR-SIG could sell these at a modest profit.

### 4. Application Library:

A library of applications information would be most valuable in expanding the use of NIR, because it would provide confidence to new users of existing or related applications as well as an indication of the limits attained to date in various applications. A standardized format should be generated for users input to the library. Confidentiality as to the source should be maintained where necessary. The problem of proprietary information must be addressed to achieve maximum availability of information.

#### C. Technical Publications and Meetings

The NIR-SIG would organize and sponsor meetings, symposia, and other opportunities for presentation and publication of technical results in the field of NIR spectroscopy.

##### 1. Symposia at Major Conferences:

The Pittsburgh Conference and FACSS now have regular symposia or sessions devoted to NIR. The EAS is organizing a data analysis symposium combining NIR-MIR. The NIR-SIG could help organize and publicize symposia at these and other appropriate meetings.

##### 2. Newsletter/Journal:

A NIR newsletter/journal is being organized by Emil Ciurczak of Sandoz. Given the backing of the NIR-SIG, this could be expanded and broadened in scope. Technical notes should include a breadth of material not suitable for publication in the refereed journals such as Applied Spectroscopy, Analytical Chemistry, and Cereal Chemistry. Coverage of all the other activities of the NIR-SIG would provide needed publicity. If possible, the NIR-SIG should also have a special column/page in the SAS newsletter and its activities should be included in the "Spectroscopists' Calendar" in Applied Spectroscopy.

### 3. Annual or Biannual NIR Conference:

A week long conference on diffuse reflectance spectroscopy has been successfully held at Wilson College in Chambersburg PA in 1982 and 1984 with a third scheduled for 1986. Instrument companies have also sponsored two and three day symposia both in the US and Europe. While it is recognized that the instrument companies will want to continue sponsoring meetings of their users, regular annual or biannual conferences attracting a broader cross-section of users and potential users should be arranged by the NIR-SIG. These might be an extension and continuation of the above diffuse reflectance conference.

### D. Other Activities

The NIR-SIG should look for other opportunities to expand the field of NIR spectroscopy.

#### 1. Education:

The NIR-SIG should encourage inclusion of NIR spectroscopy in the university curriculum, both undergraduate and graduate. Sponsorship of prizes by the SIG is one avenue. Provision of courseware, as mentioned above, would allow exposure to the technique without an investment in expensive hardware and the time and effort of preparing calibration sample sets. As the most used example of multivariate calibration, NIR spectroscopy should find acceptance as a teaching tool if properly promoted. Encouragement of graduate research in NIR is more difficult due to the cost of fellowships. The NIR-SIG could attempt to obtain multiple corporation support from users and instrument companies.

#### 2. Other Cooperative Efforts:

The NIR-SIG should look for opportunities to work with other organizations, such as the ASTM, AACC, AOCS, etc., to foster greater knowledge and use of NIR spectroscopy. Cooperation with international organizations, users, and manufacturers would add to the breadth of support available.

### IV. FINANCIAL SUPPORT

The NIR-SIG should be financially independent of the sponsoring society, such as the SAS, although it should pay the fair cost of any services obtained. These services might include office support staff, telephone, printing and mailing. Both individual memberships and corporate sponsorship are essential to make the idea viable. While support of the instrument companies is vital, major corporate users should be encouraged to find sponsorship attractive.