COMMUNICATIONS MATERIAL REVIEW FORM

Dat 3/17/87 Number of Paqes

From: TIS ADVERTISING DEPT.

Project Description article for NIR Council Newsletter

This material was prepared according to specific objectives. After reviewing it from the point of view of your responsibilities, please route it to the next department on the list. If you have any questions, call [illegible] ext. 6820

ROUTE TO:

	Signature	Date
Advertising Manager	Michelle Bryant	3/17/8
Market Manager		3/17
Director of Marketing		
Technical Review		3/18/87
Legal not necessary.	C. Maddi	
RA/QA		

RETURN TO: Arnold Kranzler, TIS Advertising, Dept. 14B,

by latest...earlier if possible

Report on JCAMP

Dr. Howard Mark
Technicon Industrial Systems
511 Benedict Ave.
Tarrytown, N.Y. 10901

As the appointed representative of the Council for Near-Infrared Spectroscopy I attended the meeting of the executive council of JCAMP on Tuesday, March 10, at Pittcon. JCAMP turns out to be considerably more than just a data-transfer standard.

The full name is "The Joint Committee on Atomic and Molecular Physical Data". It is a continuing committee of interested spectroscopists from all subdisciplines of spectroscopy, including IR, FTIR, NIR, mass spectroscopy, various X-ray spectroscopies, line spectra of the elements, Raman, etc. From time to time the committee takes on various projects as needed, which in the past have included: providing IR spectra to the Coblentz society, running a pilot study of generating class II spectra for the Coblentz society, writing specifications for Raman spectroscopy, writing specifications for mass spectroscopy. Formulation of a data-transfer standard happens to be simply their current project, which is nearly complete.

I reported the status of the NIR Council to the JCAMP executive committee, after which they voted to accept the Council as a sponsoring organization, contingent upon the Council's affirmative vote the next night, at the Council meeting.

Bob McDonald reported on the status of the data transfer standard, particularly as regards its extension to other spectroscopies and non-spectroscopic analytical methodologies. The standard is almost in its final form, ready to submit to Applied Spectroscopy for publication. Bob told the group that comments received within the next two weeks could be incorporated, but anything past that would be too late.

A second, open, meeting was held later on in the afternoon, to which Don Burns and myself were the only attendees from the NIR community. When the subject of the data transfer standard was discussed, representatives of the different spectroscopic communities who were in attendance were asked to present their views of it. Reporting for the NIR community, I told the group that we found it almost completely satisfactory, and the changes that we wished to see would be discussed with Bob McDonald at an ad hoc meeting scheduled for the next morning.

Bob told the group that he is preparing a test disk containing data written in JCAMP-DX format, to allow users of the standard to test the software that they design to read the data. This disk will be sold; the proceeds will be divided between JCAMP and Bob.

Bob also stated that he is writing subroutines for the IBM-PC in PASCAL, C, and BASIC (and maybe FORTRAN) to read JCAMP-DX formatted data. These subroutines will be put in the public domain.

John Coates of Spectra-Tech announced that he is on ASTM committee E13, Molecular Spectroscopy, and in that capacity is acting as liaison between ASTM and JCAMP.

At the ad hoc meeting mentioned above, Ed Stark, Dave Hopkins, Mark Lovik (newly hired at Dickey-John), Bob McDonald and myself discussed what we in the NIR community saw as the shortcomings of the current version of the standard. The major

change to the standard was the inclusion of a specification for a standard method of describing the constituent composition, which, unless Bob finds a reason that it is unsatisfactory, will be of the form:

##CONCENTRATIONS=<constitname#1;constitvalue#1;units> <constitname#2;constitvalue#2;units> ...

for as many constituents as is desired. The second semicolon and units specifier are optional.

Bob also agreed to change the definition of the specifier for naming samples, to include natural products, as none of the ones available were quite right. Some other minor points were also brought up, mostly Bob "decided not to decide": he made notes about our suggestions but in most cases he wanted time to think about them some more before coming to a conclusion as to how the points we made could best be handled within the context of what he was trying to do.

We also discussed the fact that, even within a subdiscipline within the field of spectroscopy, there will be incompatibilities between the way different workers use the standard. The standard is general enough to accommodate a wide variety of situations, and all of us at the ad hoc meeting agreed that the NIR community could work within the specifications of the standard.

There are two types of problems that arise: the first is to see that, within the confines of the standard, different people using the standard to do the same thing use the standard the same way. To this end, there must be agreement within the NIR community on how to use the standard (more on this later).

The second problem is that, even when all possible agreements are made, there are fundamental incompatibilities among the different users of the standard. An example of this would be the inability of the Technicon data file structure to accommodate Fred McClure's 1700-point spectra, or—Dickey-John's inability to deal with derivatives. Bob was adamant in insisting that problems of that nature, i.e., deciding what to do with the data once it was read, were up to the recipient of the data to deal with; the only requirement on the sender is that the recipient should be able to read the data according to the standard.

At the NIR Council meeting, Wednesday evening, I reported on the JCAMP activities (basically what appears above) and recommended that the NIR council agree to sponsor JCAMP. After some discussion, the council voted affirmatively on the motion to support JCAMP. The council then voted me as the official liaison with JCAMP; upon my recommendation it also voted Rob Lodder as a second liaison.

The council then discussed the JCAMP-DX standard itself; only a few people already had copies of the version 4.23, the latest version distributed by Bob McDonald. As discussed above,

the standard still leaves latitude for how it is to be implemented. I distributed copies of some recommendations I had prepared to help ensure that usage of the standard would be common throughout the NIR community (a copy of these recommendations is attached). The council deferred consideration of these recommendations until everyone could obtain a copy of the draft standard (available from Robert McDonald, 9 Woodside Drive, Burnt Hills, N.Y. 12027), as the recommendations were not comprehensible without having a knowledge of the standard within whose framework they were to be applied.

These recommendations, along with any others that may be proposed, will be taken up at the next meeting of the Council. Presumably, by then the JCAMP-DX data transfer standard will have been published, and will be the officially recommended data transfer standard of JCAMP.

RECOMMENDATIONS TO NIRA COMMITTEE FOR USE OF JCAMP PROTOCOL

by: H. Mark
1/10/87

Note: numbers referring to sections of the JCAMP-DX standard are taken from version 4.10 of the standard.

1. In order to avoid conflict with the use of the term ABSORBANCE to describe log(l/T) measurements, data from near infrared reflectance instruments converted to JCAMP-DX form should be reported either as:

A. Reflectance, in which case specify:

```
##SAMPLING PROCEDURE=DIFFUSE REFLECTANCE     $$(sec. 6.6.1)
```

B. Log(l/R), then specify:

```
##SAMPLING PROCEDURE= LOG(1/R)          $$(NOT ABSORBANCE)
```

C. Other form: ##SAMPLING PROCEDURE= should be as above, data transformations (e.g., derivatives) should be reported under ##DATA PROCESSING=

Other data transforms, e.g., Fourier transforms, might be describable in the same terms as interferograms: this needs to be investigated.

Preferably the ##YUNITS= specifier should match l.A. or 1.B., as appropriate.

2. Recommend that NIRA users convert to JCAMP as follows:

```
##DATA TYPE= NEAR INFRARED SPECTRUM $$ Sec 6.2.1; Bob MacDonald
$$ recommended NEAR INFRARED SPECTRUM rather than INFRARED
$$ SPECTRUM

##SAMPLING PROCEDURE= DIFFUSE REFLECTANCE  $$ Sec. 6.6.1
##SAMPLING PROCEDURE= TRANSMISSION         $$ as appropriate
```