CRIMINAL JUSTICE RESEARCH

For Forensic Science Laboratories: An Evaluation Study

U.S. DEPARTMENT OF JUSTICE
Law Enforcement Assistance Administration
National Institute of Law Enforcement and Criminal Justice

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Pilot Computerized Infrared Data File For Forensic Science Laboratories: An Evaluation Study

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PREFACE

The purpose of this project was to evaluate under operational conditions, the application of a commercially supplied computerized infrared data file and search system to the needs of forensic science laboratories.

The project plan called for the purchase of an infrared data search system and the use of this system by selected forensic laboratories operating within New York State.

This project could not have been completed without the cooperation and advice of personnel from the forensic science laboratories that tested the system. The author, therefore, extends his grateful appreciation to Captain Stark Ferriss of the New York State Police Scientific Laboratory and staff members Robert Ellis and Anthony Piscatelli and Dr. Charles Umberger of the New York City Medical Examiner's Toxicology Laboratory and staff members Dr. E. Bungaro and Carmen Bardi.

Appreciation is also extended to Dr. Duncan Erley of Dow Chemical Company who worked out the administrative details for obtaining the file and search program.

The author also wishes to thank Mr. Joseph Laden and Mrs. Virginia Pollock of the Division of Criminal Justice Services programming staff for their work in adapting the program to the Burroughs B-6500 computer system.

SUMMARY

A study was conducted to evaluate the operation of a pilot computerized remote access infrared data search and retrieval system for selected forensic science laboratories in New York State.

The fundamental premise of this study was that the infrared spectrophotometer can be an extremely useful instrument in the forensic laboratory. A secondary assumption was that infrared analysis is most likely an underutilized technique. We wished therefore to test the hypothesis that the availability of a computerized data file could provide the mechanism through which the true potential of infrared analysis could be realized within the operating context of a forensic science laboratory.

The major goals of the study were:

1. To demonstrate the utility of the central computerized data file concept for forensic science laboratories.

2. To provide data to enable the Criminalistics Research Bureau to make recommendations for further development of the central data file concept as applied to forensic science operations.

3. To provide an immediate, albeit developmental in nature, computerized data file service for selected forensic science laboratories.

If these goals were met, we anticipated that the project would directly impact operation in the cooperating laboratories in the following ways:

1. The efficiency and effectiveness in handling difficult identification problems involving infrared data would improve.

2. Identifications would be possible using the file which would not have been attempted due to time limitations or lack of available data.

3. The project would lead to an increased interest on the part of the laboratories in the development of more sophisticated types of data files and to the extension of the computerized data file concept to other analytical techniques.

Since this project was designed as a pilot operation, we planned to continuously evaluate our progress against the goals cited above. Specifically, we sought to answer the following types of questions:

1. Does the estimated or actual volume of search requests warrant a central data file?

2. Should the bench chemist be on-line to the computer? We expected that there would be a period of time when the laboratories would not have a terminal and therefore all search requests would be input through the terminal in CRB offices. This, of course, would give us the opportunity to test the system in both off-line and on-line modes.

3. Does existing data satisfy the needs of the user agency or would forensic files have to be developed in-house to be useful?

4. What types of systems, personnel, and technical problems would develop in a fully operational system?

5. What is the potential cost of providing the service to all forensic laboratories having a need and what types of financing arrangements are possible?

6. Will the time required to interpret infrared data be decreased by a significant amount because of the availability of a computerized system as opposed to a manual system?

We hoped to fulfill these objectives through actual operation of a pilot system.

The approach in conducting the project was relatively straightforward. We planned to purchase and implement a commercially available infrared data file and search system. This system would be installed in the Division of Criminal Justice Services (DCJS) central computer system in Albany, New York with the capability of access via data phone line from terminals located in the laboratories cooperating in the project.

The infrared (IR) spectrophotometer is a highly sophisticated analytical instrument capable of presenting complex, but extremely specific data to the analytical chemist. The instrument measures a chemical compound's absorption of light energy in the infrared region of the spectrum and records the data on graph paper for presentation to the analyst. Each sample absorbs energy at different wavelengths in the IR region and therefore the resulting spectrum is a unique representation for a chemical substance.

The IR spectrophotometer is potentially one of the most useful analytical tools in a forensic laboratory. There are several reasons for this. The fact that no two compounds have the same IR spectrum or "curve" makes the technique one of the most definitive ways to identify a substance. The IR technique provides data on the actual types of chemical bonding in the molecule. Thus, it is very specific.

Popular analytical techniques such as thin layer chromatography, or gas chromatography may be quicker and simpler techniques for certain kinds of samples. However, they rely on measurement of physical properties of the compounds and are subject to ambiguities in the interpretation of the data.

Infrared instruments are also within the budgetary range of most forensic operations. Whereas techniques such as neutron activation, mass spectrometry and nuclear magnetic resonance spectroscopy offer data potentially as useful or more useful for identification purposes, their cost is outside the range of most forensic laboratory budgets.

Operation of the instrument can be learned quickly by technicians or graduate chemists. Success in making identifications is dependent on experience rather than lengthy specialized training.

The amount of data present in an IR spectrum is enormous. However, there are only a limited number of methods of using this data for identification purposes. One is to make a determination of what types of bands are present in the IR spectrum by the use of functional group frequency correlations. This is basically a manual method and requires an analyst with substantial experience in infrared interpretation. Certain chemical groups such as the benzene ring, carbonyl, OH, N-H and methoxy have bands which are very common and easily recognized by the experienced chemist.

Figure 4 (p.23) is an example of the type of chart used in group frequency correlation. This technique provides the analyst with information about the substructure of the molecule, but does not indicate its total structure.

The foregoing implies that a computerized data file can potentially aid forensic science laboratories in the solution of some of their IR data handling problems. There are several reasons for this.

-- A data file can increase the efficiency of an individual IR analysis by eliminating the need for laborious manual correlation or interpretative techniques.

-- The current reliance on experience, manual selection of standards from files, or searches through reference books can be diminished.

-- The ability of a computer file to store and rapidly retrieve data from thousands of compounds will increase the probability of identifications.

After evaluating commercially available systems, we chose to implement a system that was being operated by the Dow Chemical Company for its installation in Midland, Michigan. This system was developed by Duncan Erley, a research chemist with considerable experience in infrared analysis and interpretation.

The system characteristics had been reported in the literature. This system fulfilled all of the criteria for use in the study in that the file used for searching is the American Society for Testing and Materials (ASTM) file of infrared data which contains more than 100,000 chemical compounds collected from commercial suppliers and the chemical literature; the search program was written for the B-5500 computer system and was designed for terminal operation by a chemist in his own laboratory environment; the negotiated price for obtaining the file and program was within the budget constraints imposed by the CRB and grant budget allocations for the program. We were able to execute a non-exclusive lease arrangement whereby Dow received compensation for program development and ASTM received a royalty fee for use of the data file.

Figure 7 (p.39) illustrates the system as it was configured for the pilot project.

Araangements for the telephone connections to the terminals were made through the New York State Office of General Services which coordinates the operation of a New York State agency tie-line network for telephone communications.

Table 4 (p.44) summarizes both the one time and on-going costs to operate the system in its current configuration.

It must be emphasized that the costs indicated in Table 4 are only illustrative of the typical elements of cost incurred in operation of this system. Actual costs for any specific implementation of the system would depend on the type of terminal used, the particular communications network utilized, and the specific mechanism used for obtaining the file. Of equal importance with the individual cost of the components of the system is the distribution of the costs among the users and the central agency.

The major questions to be answered in evaluating the program and file were:

a. Could a chemist make "hits" using the search argument?

b. Is the file responsive to forensic needs?

Based on more than six months operational experience we have come to the conclusion that the program in its present operating status is capable of making identifications of forensic samples. Tables 5 and 6 (p. 49 and p. 50) illustrate identifications made by each laboratory. These "hits" are unique compounds identified by the file. They are categorized by investigation type to illustrate the file and search program's responsiveness to samples across the full range of forensic cases.

These "hits" represent both routine and specialized cases. Some of the hits for the so-called routine cases provided unambiguous confirmation of an identification made by another technique. In these cases, the identification was made very rapidly with a minimum number of retrievals from the file.

The non-routine identifications represent cases that might not have been solved were it not for the availability of the computerized file. Indeed, the IR technique might not have been utilized were it not for the file.

The program has assisted many times in giving an indication that the unknown is a particular type or class of compound. While there is no positive identification, information concerning the type or class of the compound many times offers investigative leads in the solution of a case.

The operation of the State Police terminal gave us the opportunity to determine the likely volume of requests that the program would handle from a busy forensic laboratory. Table 7 (p. 60) summarizes operational experience relative to samples (cases) searched and total number of searches likely to occur per month.

The figures in Table 7 suggest that during any week we can expect that the State Police Laboratory will require the search program for about 50 searches requiring about ten minutes elapsed time per search. This indicates that approximately eight hours of elapsed computer time will be required per week.

There will be a random distribution of this time depending on caseload, sample preparation required and priorities concerning the type of case worked on in any one day. Computer usage will tend to level off at this amount for this laboratory unless there is an increase in personnel.

Actual central processor and input/output time used by a laboratory during a given time period is important from the perspective of the overall DCJS operating system. The current program requires approximately 1 min 44 central processor and 3 min 45 input/output time for a search of the entire file. Of course, the laboratories frequently search only a small portion of the file. We anticipate that the volume of searches generated by the potential maximum number of user laboratories will not hinder the operation of established DCJS information systems.

Both laboratories had the opportunity to evaluate whether the IR system is responsive to forensic needs from the standpoint of its ability to provide identifications. They also evaluated the ability of DCJS personnel to perform the necessary systems improvement tasks in a timely and an effective manner.

Appendices C and D contain complete evaluation reports prepared by the technical and administrative personnel of both the New York State Police and New York City Medical Examiner's Laboratories.

Based on the pilot operation of the IR system, we have formulated the following project conclusions:

1. The central data file concept for forensic science laboratories is not only feasible, but is a highly desirable addition to the laboratories' analytical capabilities.

2. The Infrared Data File search system in its present state of development is of definite assistance in infrared data interpretation connected with cases across the full range of forensic problems. The degree of assistance can be increased by the addition of forensic subfiles.

3. The existence of the IR data file search system has resulted in a definite increase in the utility of the IR spectrophotometer in the forensic laboratory.

4. To derive maximum benefits from the system, the chemist should be on-line to the computer system.

5. File and system update maintenance, and improvement should be performed by the central agency staff subject to the advice and counsel of the user agencies.

6. A system for providing standard "hard copy" spectra for final verification will increase the utility of the computer system.

7. The communications system is capable of handling the current amount of traffic generated by the two laboratories and the maintenance functions performed at the central level. However, as additional laboratories are added, a method for allowing searches by all laboratories simultaneously will be required.

Based on the project conclusions, we recommend the following courses of action with respect to the design and implementation of scientific data files for forensic science laboratories:

1. The IR system should continue to be operated for all laboratories who can share in the cost.

2. The data file should be expanded to include a forensic subfile containing standards contributed by as many forensic laboratories as possible.

3. The search program should be modified to a version (already commercially available) which would make it more "forgiving" when erroneous search data is entered. This should increase the utility of the system by raising the identification rate.

4. A study should be made of the alternative ways of providing "hard copy" standard spectra to each laboratory.

5. Based on the conclusion that scientific data storage and retrieval is a valuable asset to forensic work, additional files should be created to store data from the following techniques:

   a. Ultraviolet spectrophotometry.

   b. Gas-liquid and thin layer chromatography.

   c. Mass spectrometry.

   d. Color and crystal tests.

A correlated cross referenced type search procedure could then be developed using all the data in the file.

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I. BACKGROUND

Forensic science laboratories, in fulfilling their role as the scientific arm of law enforcement, are increasingly taking advantage of modern analytical instruments to aid in the identification and individualization of common evidence materials. As routine work volumes increase and as investigations become more sophisticated, laboratories have introduced instruments such as the gas chromatograph, the infrared spectrophotometer, and the mass spectrometer.

The use of analytical instruments can potentially aid forensic laboratories in several ways. First, smaller size samples may be analyzed. Second, analyses may be done more rapidly. Third, a greater quantity of data, and in many cases, more specific data may result from an instrumental analysis as opposed to a wet chemical technique. These advantages, however, are somewhat mitigated by several drawbacks.

For example, the increased volume of data available to the analyst may confuse the issue rather than lead to a definitive answer. In the context of overall laboratory operations, the use of instruments may lead to a general increase in the analysis time required for certain types of cases. This is because the lab can now perform analyses that were formerly not attempted.

Another problem made evident by the increased application of analytical instruments to forensic work is the shortage of trained analysts. This latter problem is particularly important since interpretation of the data from many analytical instruments is not an easy or straightforward task and requires experienced personnel.

A final problem is that analysis of instrumentally obtained data frequently takes far longer than the time required to obtain the data.

During the past several years, there have been numerous studies of crime laboratory operations. These studies were mainly directed at finding ways of improving these operations with respect to their efficiency and effectiveness in handling their caseloads in the face of vastly increased volumes of work and general increases in the difficulty of the cases which they have been asked to handle.

Reports prepared for the Office of Law Enforcement Assistance by John Jay College of Criminal Justice, for the New York State Office of Crime Control Planning by Cornell Aeronautical Laboratory, Inc., and for the New York State Identification and Intelligence System by Arthur D. Little, Inc.[1] are examples of three reports which have identified and quantified the current crises in the forensic science laboratories of the country with respect to volume of work, shortage of trained personnel, and inadequate instrumentation and data analysis capabilities.

Each of these reports recommends a strengthening of the existing laboratories through addition of manpower, and instrumentation. They have also clearly recognized the needs of forensic science operations in the area of information handling and have recommended that in addition to manpower and instruments, the laboratories should introduce the use of the computer in their operations.

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[1] O.L.E.A. Project No. 013, "Study of Needs and the Development of Curricula in the Field of Forensic Science," Dr. Alexander Joseph, John Jay College of Criminal Justice, the City University of New York; "Planning Study for Evaluation of Forensic Laboratory Services in Erie, Niagara and Wyoming Counties, New York," Cornell Aeronautical Laboratory, Inc., Grant from the New York State Office of Crime Control Planning; "Computerized Data Files for Forensic Science Laboratories: A Utility Study," Arthur D. Little, Inc., under contract to the New York State Identification and Intelligence System.

Arthur D. Little recognized several potential roles the computer could play in forensic science operations.

> "The benefits to be realized by utilizing the digital computer in conjunction with analytical-chemical measurement techniques include freeing valuable personnel from routine, time-consuming, manual instrument and data manipulations; increasing the accuracy and precision of the experimental data; and creating a capability for tasks which would otherwise be too complex to consider."[2]

Taking cognizance of the conclusions in the foregoing studies of forensic science operations, the New York State Division of Criminal Justice Services (DCJS) has pursued a program to provide computerized information services for the forensic science laboratories of the State. This is in keeping with the agency's role as a central information sharing agency for the criminal justice agencies of the State of New York.

In delineating the problem to be addressed by the Criminalistics Research Bureau (CRB), we identified several distinct types of computerized files that could potentially aid laboratories in their data analysis tasks. These files would apply to the use of analytical data as opposed to the more general types of computerized files such as inventory systems, literature search and retrieval systems and general accounting systems.

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[2]See Footnote 1, page 2.

The first type of analytical file would be designed to assist in the identification of unknown substances or in the verification of the identity of substances whose chemical composition is suspected through information received external to laboratory analysis. The analytical techniques mentioned above are generally powerful aids in the analysis and characterization of unknown materials. Their effectiveness could be greatly enhanced through interface with computerized data files.

Another potential computerized file could assist in determining the origin of common evidence materials. These files would contain data on the physical and chemical properties of materials frequently encountered as evidence. After statistical relationships were derived for the occurrence of these properties, the data could be used to evaluate the probability of a direct relationship between a piece of evidence material and a suspected source or origin.

A third type of file would aid in relating evidence found in connection with one crime to evidence on file from another crime. This is the classic procedure used with latent fingerprints. This same procedure also could be of use in determining patterns of distribution of illicitly manufactured dangerous drugs.

Although each of these types of files has potentially great benefits for forensic science operations, it was decided to limit initial CRB development efforts to the first mentioned. There were several reasons for this decision.

1. The CRB was working within funding constraints imposed by both the New York State Division of the Budget and the Justice Department's pilot grant program.

2. We desired to develop a service that would have high potential payoff in a short period of time.

3. We desired to focus development effort on a portion of the overall problem that could be handled given the staffing constraints in the CRB.

4. Preliminary investigations indicated that the industrial community had addressed this problem and therefore available technology could be directly transferred to forensic applications.

This project report represents an evaluation of the operation of a commercially supplied remote access computerized infrared data file and search system as applied to typical analytical problems of two of the major forensic science laboratories of the State of New York.

The fundamental premise of this study was that the infrared spectrophotometer can be an extremely useful instrument in the forensic laboratory. A secondary assumption was that infrared analysis is most likely an underutilized technique. We wished therefore to test the hypothesis that the availability of a computerized data file could provide the mechanism through which the true potential of infrared analysis could be realized within the operating context of a forensic science laboratory.

Section II delineates the specific objectives of the study.

II. OBJECTIVES

This project addressed the forensic science data analysis problems described in Section I by attempting to fulfill the following goals:

1. To demonstrate the utility of the central computerized data file concept for forensic science laboratories.

2. To provide data to enable the Criminalistics Research Bureau to make recommendations for further development of the central data file concept as applied to forensic science operations.

3. To provide an immediate, albeit developmental in nature, computerized data file service for selected forensic science laboratories.

If these goals were met, we anticipated that the project would directly impact operations in the cooperating laboratories in the following ways:

1. The efficiency and effectiveness in handling difficult identification problems involving infrared data would improve.

2. Identifications would be possible using the file which would not have been attempted due to time limitations or lack of available data.

3. The project would lead to an increased interest on the part of the laboratories in the development of the more sophisticated types of data files and to the extension of the computerized data file concept to other analytical techniques. These files would increase the effectiveness in determining the origin of evidence materials.

Since this project was designed as a pilot operation, we planned to continuously evaluate our progress against the goals cited above. Specifically, we sought to answer the following types of questions:

1. Does the estimated or actual volume of search requests warrant a central data file?

2. Should the bench chemist be on-line to the computer? We expected that there would be a period of time when the laboratories would not have a terminal and therefore all search requests would be input through the terminal in CRB offices. This, of course, would give us the opportunity to test the system in both off-line and on-line modes.

3. Does existing data satisfy the needs of the user agency or would forensic files have to be developed in-house to be useful?

4. What types of systems, personnel, and technical problems would develop in a fully operational system?

5. What is the potential cost of providing the service to all forensic laboratories having a need and what types of financing arrangements are possible?

6. Will the time required to interpret infrared data be decreased by a significant amount because of the availability of a computerized system as opposed to a manual system?

We hoped to fulfill these objectives through actual operation of a pilot system. Section III describes this approach in detail.

III. APPROACH

The approach in conducting the project was relatively straightforward. We planned to purchase and implement a commercially available infrared data file and search system. This system would be installed in the DCJS central computer system in Albany, New York with the capability of access via data phone line from terminals located in the laboratories cooperating in the project. It was originally planned to enlist the cooperation of one laboratory for the pilot project. However, due to circumstances developing shortly after project inception, we were able to obtain the cooperation of two of the largest laboratories in the State dealing with forensic problems.

There were several criteria with which the laboratories were judged with respect to their participation in the program.

1. Volume of Cases

   We desired to work with laboratories which potentially or actually had a large volume of cases that were amenable to infrared analysis.

2. Instrumentation

   A necessary condition for participation was the presence in the laboratory of an operational infrared spectrophotometer.

3. Personnel

We required the availability of an experienced chemist who had worked with infrared data in the past and was fully cognizant of the advantages and drawbacks of the technique.

4. Willingness to Participate in Evaluation

Since a major goal of the project was to obtain both objective and subjective data on the ability of the file to address forensic needs, we sought to work with laboratories that expressed a willingness to provide periodic reports evaluating the file's performance.

Two laboratories that met the above criteria were the New York State Police Scientific Laboratory in Albany, New York and the New York City Medical Examiner's Toxicology Laboratory. The choice of these laboratories also provided the added benefit that we could test the ability of a central agency staff to perform the necessary liaison tasks for both local and distant laboratories.

Table 1 indicates the types of personnel which were committed to the project by the Criminalistics Research Bureau and each of the cooperating laboratories.

TABLE 1

PERSONNEL ASSIGNED TO PROJECT*

Criminalistics Research Bureau

Research Criminalist
Statistics Clerk
Programmer
Clerical Support
Photographer

State Police Laboratory

2 Senior Chemists

New York City Medical Examiner's Laboratory

2 Chemists (Toxicology)

*The assignment of these personnel does not mean that they worked full time on project work. This table only indicates the types of personnel involved in the evaluation.

It is essential to place the computerized data file in context with the conventional methods of interpreting infrared spectra. Therefore, Section IV presents information on the theory and use of the infrared spectrophotometer as an aid in the identification of unknown substances. Section IV will also serve to give the reader an appreciation of the potential applicability of the infrared spectrophotometer to forensic work.

IV. THEORY AND USE OF THE INFRARED SPECTROPHOTOMETER[1]

The infrared (IR) spectrophotometer is a highly sophisticated analytical instrument capable of presenting complex, but extremely specific data to the analytical chemist. The instrument measures a chemical compound's absorption of light energy in the infrared region of the spectrum and records the data on graph paper for presentation to the analyst.

Each sample absorbs energy at different wavelengths in the IR region and therefore the resulting spectrum is a unique representation for a chemical substance.

The infrared spectrophotometer consists of an infrared radiation source, a sample holder, a monochrometer, a detector, an amplifier, and a recorder. Generally speaking, a double beam instrument is used. That is, the detector compares a sample and reference beam and then amplifies the resulting signal to drive a pen motor on the recorder. This type of operation tends to minimize the effect of the absorption of moisture in the air or of the solvent used for preparing the sample.

Figure 1 is a schematic diagram of a typical infrared instrument indicating the major components.

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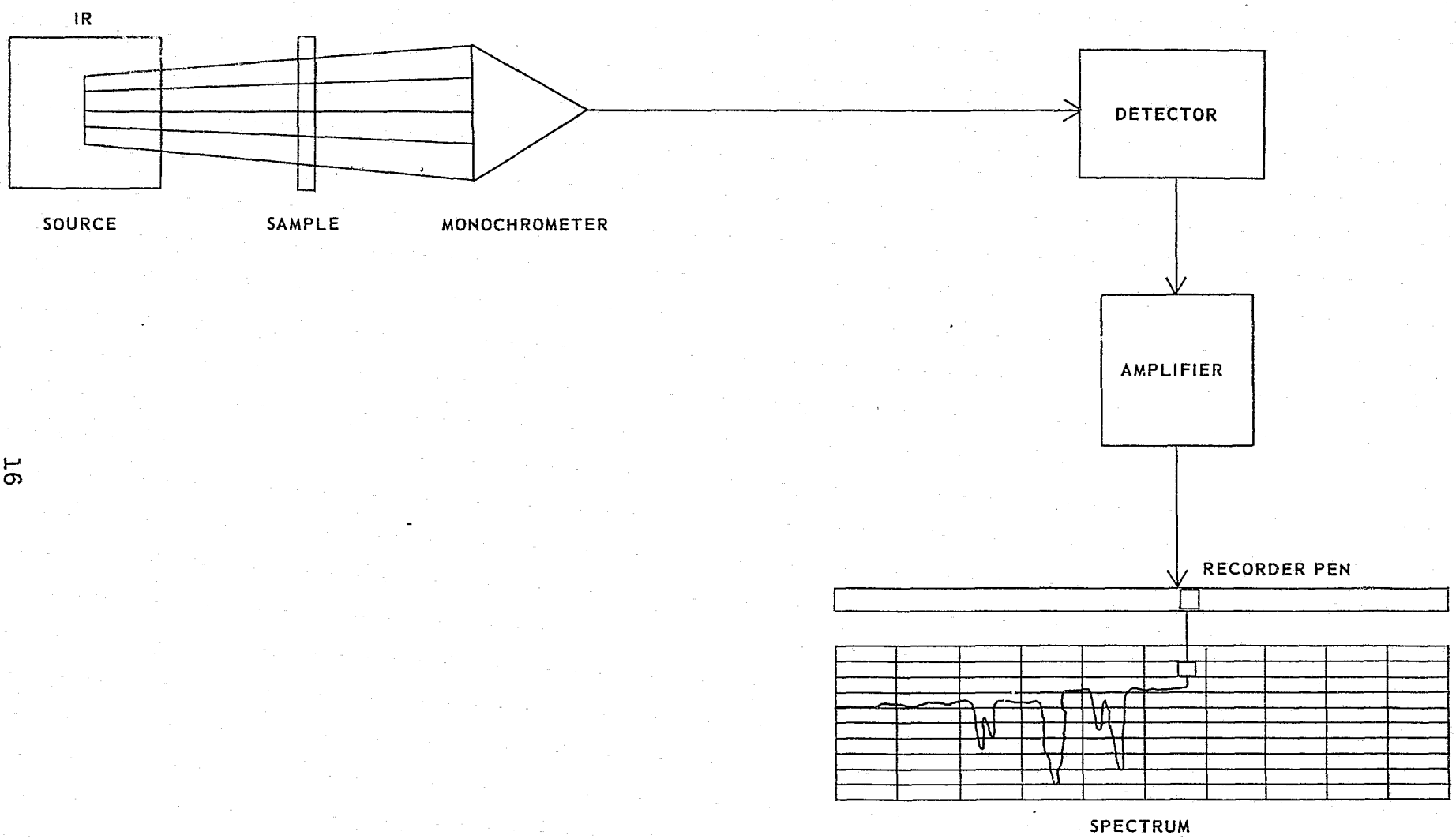
[1]Taken in part from Madrazo, F. G., Ellis, R., Bungaro, Dr. E., "Pilot Computerized Infrared Data File for Forensic Science Laboratories," presented at Project SEARCH International Symposium on Criminal Justice Information and Statistics Systems, October, 1972.



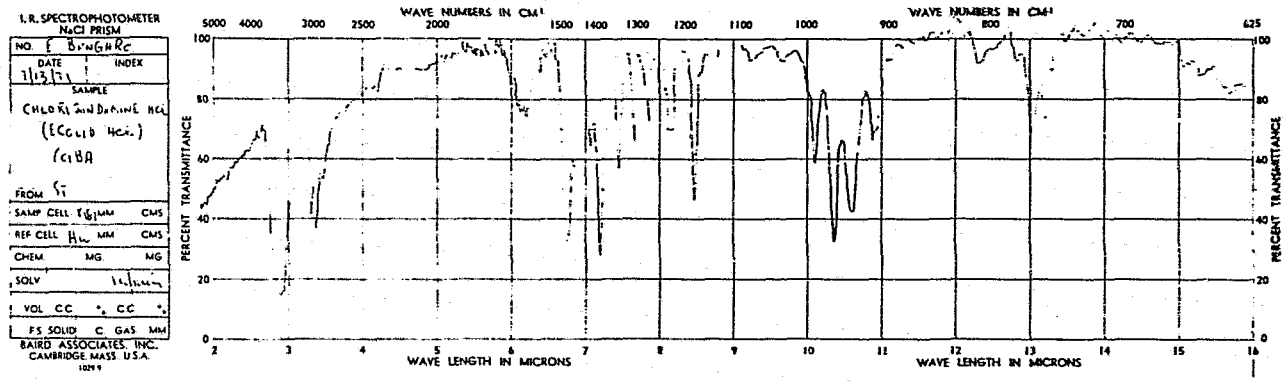
SCHEMATIC DIAGRAM OF AN IR SPECTROPHOTOMETER

Figure 1

Samples can be in the gas, liquid or solid state. However, the IR spectrum will vary depending on the state in which the sample is presented to the instrument. Due to the fact that glass absorbs IR radiation, the sample holder must be sodium chloride, potassium bromide or a similar salt. Most forensic samples are analyzed in potassium bromide pellets or between sodium chloride plates.

Figure 2 is an example of a typical spectrum of interest to the forensic community. An analyst identifies a compound by the wavelength locations, intensity and shape of the absorption bands. The comparisons made are similar to those made by fingerprint technicians.

The IR spectrophotometer is potentially one of the most useful analytical tools in a forensic laboratory. There are several reasons for this. The fact that no two compounds have the same IR spectrum or "curve" makes the technique one of the most definitive ways to identify a substance. The IR technique provides data on the actual types of chemical bonding in the molecule. Thus, it is very specific. Popular analytical techniques such as thin layer chromatography, or gas chromatography may be quicker and simpler techniques for certain kinds of samples. However, they rely on measurement of physical properties of the compounds and are subject to ambiguities in the interpretation of the data.



TYPICAL INFRARED SPECTRUM

FIGURE 2

Infrared instruments are also within the budgetary range of most forensic operations. Whereas techniques such as neutron activation, mass spectrometry and nuclear magnetic resonance spectroscopy offer data potentially as useful or more useful for identification purposes, their cost is outside the range of most forensic laboratory budgets.

Operation of the instrument can be learned quickly by technicians or graduate chemists. Success in making identifications is dependent on experience rather than lengthy specialized training.

Mention should be made of some of the drawbacks of infrared techniques so that a balanced picture can be presented of its potential usefulness in the forensic laboratory. These drawbacks are the primary reasons that the IR technique is possibly underutilized by the forensic community.

1. SAMPLE SIZES MUST BE QUITE LARGE TO OBTAIN USABLE SPECTRA WITHOUT RELIANCE ON BEAM CONDENSING OR MICROSAMPLING TECHNIQUES. The energy required for absorption is such that a sample size threshhold must be exceeded. This lessens the effect of inherent machine "noise" or the quality of the spectrum. Techniques of beam condensing and microsampling which are utilized quite widely in the industrial community for minute samples are less widely used in the forensic community.

2. THE SAMPLE OF INTEREST MUST EXHIBIT A HIGH DEGREE OF PURITY. The very fact that IR is so specific in nature works to its disadvantage if contaminants are present in the sample. Interactions take place in mixtures which can completely distort the spectrum and prevent an unambiguous identification from being made.

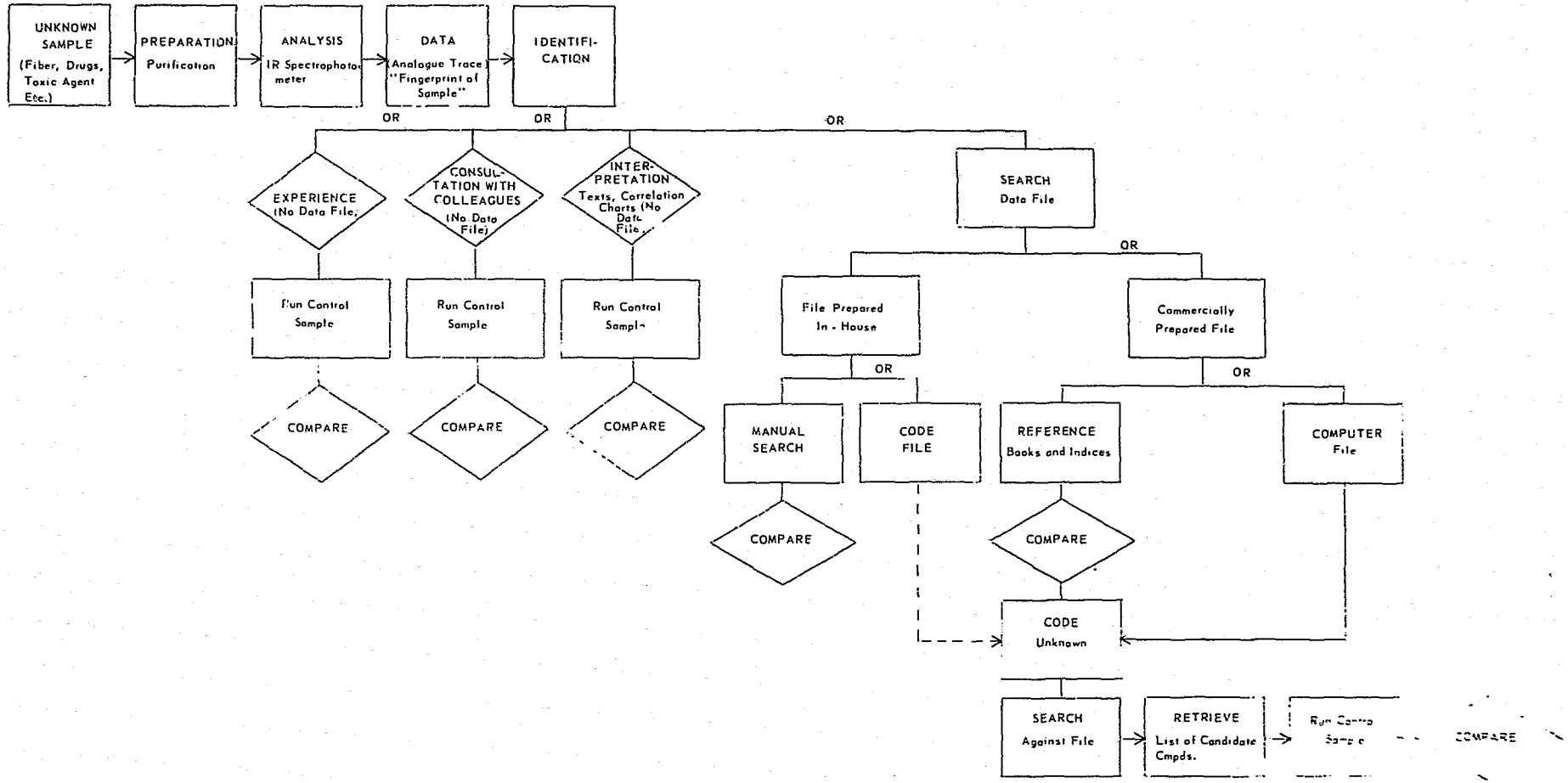
Serving to mitigate against this drawback are modern advances in separation techniques which have led to an increase in the types of samples amenable to IR characterization. The gas chromatograph, for instance, is capable of separating complex mixtures into their component parts. These components can then be collected for either IR or mass spectrometric characterization.

3. THE COMPLEXITY OF THE IR SPECTRUM CAUSES PROBLEMS IN THE INTERPRETATION OF THE DATA. As mentioned previously, the band location, intensity, and shape can be used to interpret an IR curve. Location and intensity can be represented quantitatively. However, band shape is a subjective feature.

Problems 1 and 2 can be overcome as implied above by modifying either the sample preparation procedures or by adding attachments to the basic IR instrument. Problem 3 must be addressed by modifying the interpretation procedures.

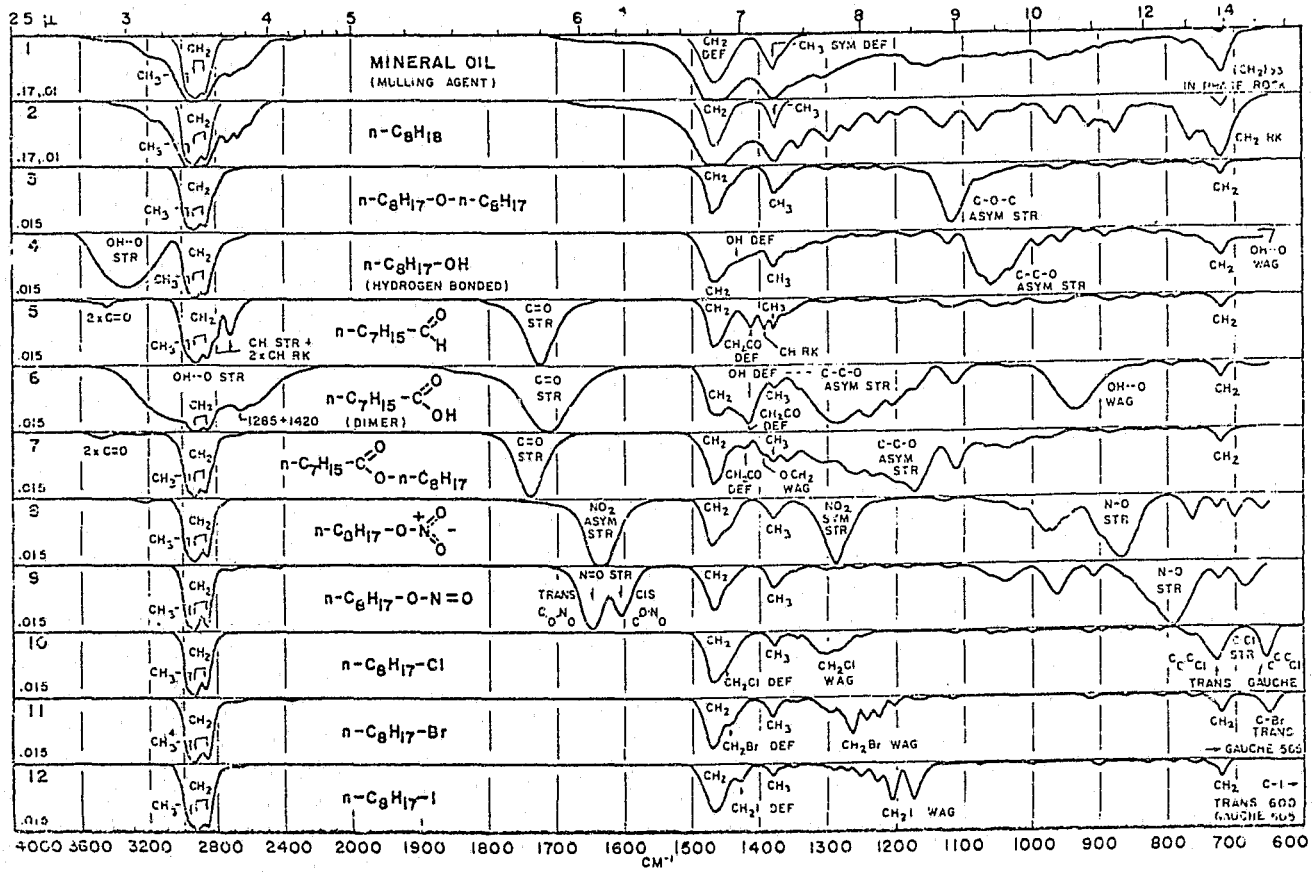
The amount of data present in an IR spectrum is enormous. However, there are only a limited number of methods of using this data for identification purposes. Figure 3 is a schematic diagram of the various approaches open to the analyst for identifying an unknown using an IR curve.

One is to make a determination of what types of bands are present in the IR spectrum by the use of functional group frequency correlations. This is basically a manual method and requires an analyst with substantial experience in infrared interpretation. Certain chemical groups such as the benzene ring, carbonyl, OH, N-H and methoxy have bands which are very common and easily recognized by the experienced chemist. Figure 4 is an example of the types of charts used in group frequency correlation. This technique provides the analyst with information about the substructure of the molecule. This information then has to be assembled by an experienced analyst to arrive at the molecular structure and hence the identity of the compound.



UNKNOWN COMPOUND ID PROCESS USING INFRARED DATA

Figure 3



FUNCTIONAL GROUP CORRELATION CHART [2]

Figure 4

[2] Reproduced from Introduction to Infrared and Raman Spectroscopy, Colthup, Daly, and Wiberly Academic Press, New York, 1964, p. 362-363.

Another method of identification is to manually compare the unknown spectrum with a known spectrum chosen from a "hard copy" file. This procedure is manual from selection of the spectrum to final verification. This is an almost impossible task considering there are hundreds of thousands of possible IR curves open to comparison.

The foregoing implies that a computerized data file can potentially aid forensic science laboratories in the solution of some of their IR data handling problems. There are several reasons for this.

-- A data file can increase the efficiency of an individual IR analysis by eliminating the need for laborious manual correlation interpretative techniques.

-- The reliance on experience, manual selection of standards from files, and searches of reference books can be diminished.

-- The ability of a computer file to store and rapidly retrieve data from thousands of compounds will increase the probability of identifications.

Section V discusses the data generally present in computerized IR search systems and possible ways of implementing such systems. Additionally, the criteria for choosing a system for implementation during the pilot program are presented.

V. SYSTEM CHARACTERISTICS

A. Possible Systems

As mentioned previously, a typical IR curve is "rich" in information. Band location, relative intensity and shape are three parameters that can be used by the chemist to arrive at a definitive identification.

Unfortunately, not all of this information can be conveniently represented for use in a computerized search. Use of relative band intensity leads to a complicated and unwieldy data input requirement; band shape is a non-quantitative parameter.

Therefore, recently developed IR search systems have tended to utilize band location data and functional group information for classification and search purposes. Table 2 is a list of systems that have been implemented to search IR data. Not all of these systems are commercially available and several of them are oriented toward specific computer systems.

Nearly all commercially available systems utilize the American Society for Testing and Materials (ASTM) data base of 100,000 coded spectra. Some of the systems are oriented to off-line searching based on keypunched data input cards while others are oriented to terminal operation.

TABLE 2

LIST OF COMPUTERIZED INFRARED DATA SYSTEMS[1]

Storage and Retrieval of Wyandotte-ASTM Infrared Spectra Data Using a Honeywell-400 Computer, T. A. Entzminger and E. A. Diephaus, Public Health Service, Robert Taft Sanitary Engineering Center, Cincinnati, Ohio 1964.

Fast Searching System for the Wyandotte-ASTM Infrared Data File, Duncan S. Erley, Chemical Physics Research Laboratory, The Dow Chemical Company, Midland, Mich. 1967.

Storage and Retrieval of Wyandotte-ASTM Infrared Spectral Data Using a 7090 Computer, L. D. Smithson, L. B. Fall, F. D. Pitts, and F. W. Bauer, Technical Documentary Report No. RTD-TDR-63-4265, Research and Technology Division, Wright-Patterson, AFB, Ohio, 1964.

Storage and Retrieval of Wyandotte-ASTM Infrared Spectral Data Using an IBM 1401, R. A. Sparks, American Society for Testing and Materials, Philadelphia, Pa., 1964.

IRIS (Infra Red Information System), University Computing Company, Palo Alto, Calif.

IRGO (Infrared Spectral Search Service), Singer Technical Services, Inc., New York, N.Y.

ISIS (Infrared Spectral Information System) User's Manual, Document No. LSR-98, Triangle Universities Computation Center, Research Triangle Park, N.C.

SIRCH (Infrared Spectral Data Retrieval System), R. W. Sherwood, ASTM Headquarters, Philadelphia, Pa.

Kodak Infrared Search Service, Kodak Park, Rochester, N.Y.

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[1]Taken in part from "New Computerized Infrared Substance Identification System," Sebesta, Robert W. and Johnson, Gerald G. Jr., Analytical Chemistry, Vol. 44, No. 2, February, 1972, p. 260.

In view of the number of commercial systems available, we developed a list of criteria for selecting the system to be tested in the pilot project.

B. Criteria for Selection

1. The data file must be large and contain compounds of potential interest to the user laboratories.

2. The system must be chemist oriented, not computer expert oriented.

3. The system must allow terminal input.

4. The search program must be compatible or easily adapted to the Burrough's 6500 computer system.

5. System cost must be within constraints of the LEAA grant and the CRB annual research and development budget.

6. An administrative mechanism must exist for obtaining the system.

After evaluating available systems, we chose to implement a system that was being operated by the Dow Chemical Company for its installation in Midland, Michigan. This system was developed by Duncan Erley, a research chemist with considerable experience in infrared analysis and interpretation.

The system characteristics had been reported in the literature.[2] Doctor Erley indicated that the system was available for implementation by other users upon the negotiation of a fee.

This system fulfilled all of the criteria for selection in that the file used for searching is the American Society for Testing and Materials (ASTM) file of infrared data which contains more than 100,000 chemical compounds collected from commercial suppliers and the chemical literature; the search program was written for the B5500 computer system and was designed for terminal operation by a chemist in his own laboratory environment; the negotiated price for obtaining the file and program was within the budget constraints imposed by the CRB and grant budget allocations for the program. We were able to execute a non-exclusive lease arrangement whereby Dow received compensation for program development and ASTM received a royalty fee for use of the data file.

C. System Implemented

1. Initial Test and Debugging

For initial testing the CRB obtained a Model 33 teletypewriter for on-line operation to the B5500 computer system.

[2] "Fast Searching System for the ASTM Infrared Data File," Duncan S. Erley, Analytical Chemistry, Vol. 40, No. 6, May 1968, pp. 894-898.

Only minimal control card type changes were necessary to make the program operate exactly as it does in the Dow installation. To conform with the DCJS operating system, and to allow more timely responses, we modified the program to operate using random disk access rather than tape.

The initial period of operation was directed toward evaluating the possibility that data could be transmitted to the central file over the telephone or through the mail for central searching by CRB staff. Subsequent to searching, we would transmit a "hit" list to the agency requesting the search. This approximates the operation of systems that are available on a per search fee basis with no "hands on" operation by the requesting chemist.

It was found that this type of system would not be satisfactory in the current or projected operating environment of the forensic labs of New York State.

First of all, this type of system does not allow convenient altering of the search argument by the chemist with subsequent rapid re-searches of the file. It was determined that an iterative search procedure is most beneficial and the "middle man" arrangement with mail or telephone response prevented iterative searching on a timely basis. A related problem is the fact that the chemist would not see the hit list until it arrived by mail.

This meant he had to evaluate initial search results over the telephone or at a later date. Immediate visual evaluation of the initial "hit" list is a much more desirable way to operate this type of program.

The foregoing conclusion is not meant to negate the possibility of a small laboratory, whose caseload could not support the cost of a terminal system, from receiving some benefits of a computer search of the data. It merely points to a clearly more desirable method of operation. That is, a full terminal capability at the local level.

2. File Characteristics

As stated previously, the file utilized is the ASTM file of data from more than 100,000 organic compounds. This major file is subdivided into various subfiles according to the origin of the spectra.

Table 3 gives the origin of each of the subfiles with their letter designators. The disk allocation for the base file plus expansion area is 132,000 records of eleven words each. Figure 5 is a graphic representation of the record layout of the file.

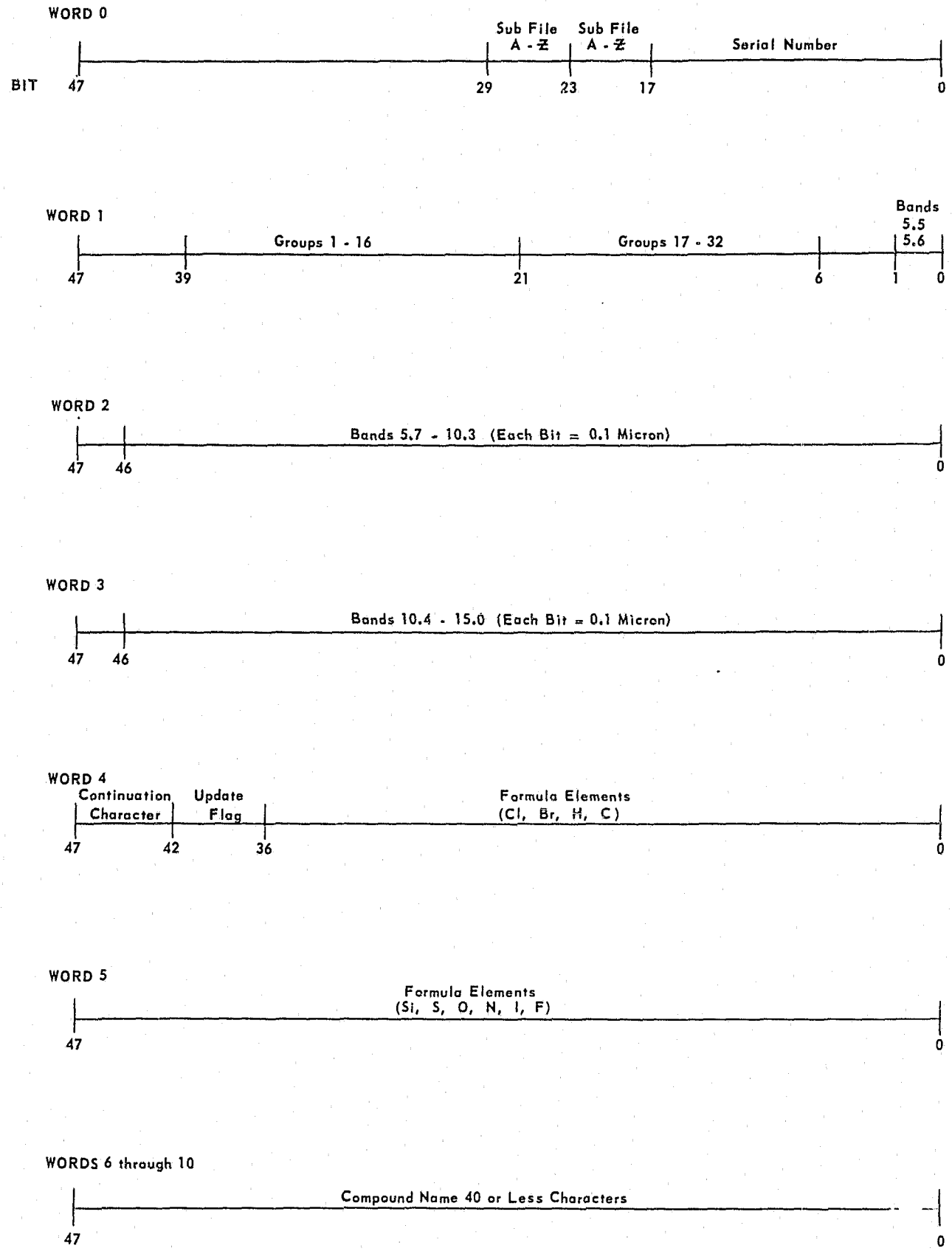
The original tape received from the Dow Chemical Company did not have the capability for printing out the chemical names of the standards matching the search argument.

TABLE 3

ORIGIN OF SUBFILES IN ASTM IR DATA FILE

Class. Symbol		Source/Type of Data
A		American Petroleum Instit. Proj. 44
C		Sadtler Catalogue of Spectrograms
SADTLER SUBFILES:		
	CA	Agricultural Chemicals
	CB	Polyols
	CC	Surface Active Agents
	CD	Monomers, Polymers, Resins, Gums, Pyrolyzates
	CE	Plasticizers
	CF	Perfumes, Flavors
	CG	Fats, Waxes, Derivatives
	CH	Lubricants
	CJ	Rubber Chemicals
	CK	Fibers
	CL	Solvents
	CM	Intermediates
	CP	Petroleum Chemicals
	CR	Pharmaceuticals
	C	Sadtler Standard Spectrograms
	CS	Steroids
	CT	Textile Chemicals
	CW	Attenuated Total Reflectance
	CX	Dyes, Pigments, Stains
	CY	Inorganics
D		NRC-NBS File of Spectrograms
E		Spectrograms Abstracted by ASTM-Sponsored Groups
FA		Inorganics
F		Documentation of Molecular Spectroscopy
G		Coblentz Society Spectrograms
H		MFG Chemists Assoc.
J		Infrared Data Com. of Japan
SP*		State Police Forensic File
ME*		Med. Examiner's Forensic File

*Added during this project by DCJS Criminalistics Research Bureau.



RECORD LAYOUT OF IR DATA FILE

Figure 5

Our current file contains the full chemical name and molecular formula of the compound as it appears in ASTM document AMD 32.[3]

3. Program Characteristics

A detailed description of the operation of the search program is presented in the previously referenced article by Dr. Duncan Erley. Additionally, Appendix A of this report is a preliminary operator's manual which describes the program functions in detail.

The controlling philosophy in the design of this program appeared to be a desire to provide a system that could be easily used by the spectroscopist and that would provide rapid turnaround at a reasonable cost.

> "The program described here, while not as flexible as those written for larger computers, has the singular advantage that the spectroscopist himself may use it on a low cost computer...The number of hits and their names (which can be looked up quickly) often suggest modifications of the initial search data which are easily done with this program. This is perhaps the greatest advantage of this system over others now in use."[4]

---

[3] Serial Number List of Compound Names and References to Published Infrared Spectra, American Society for Testing and Materials.

[4] "Fast Searching System for the ASTM Infrared Data File," Duncan S. Erley, Analytical Chemistry, Vol. 40, No. 6, May 1968, pp. 894-898.

Figure 6 illustrates a typical input-output page resulting from a search of the system. All operator entries have been underlined for illustrative purposes. Notice that the computer cues the operator for information necessary to proceed to the next step. Notice also that the operator has a number of options and is presented with certain diagnostic information.

In addition to the instructor's manual, a feature was added to the program which provides the operator with instructions during the program's operation. Using this feature, the operator can obtain a detailed explanation of the purpose of any option in the program. A portion of the output appears in Appendix B.

4. Terminals Utilized

As mentioned previously, the search program as operated by the Dow Chemical Company used a Model 33 Teletypewriter. Our initial testing was also accomplished with the Model 33. During this testing we identified several problems with the use of this terminal.

a. Reliability of the equipment was not high. We experienced frequent incidences of incorrect character transmission. This resulted in a high proportion of re-transmissions.

```
00000

INFRARED FILE SEARCH PROGRAM                11/21/72
DO YOU WANT PROGRAMMATIC INSTRUCTIONS--YES OR OCK



SAMPLE...
DEMONSTRATION SEARCH
GROUPS AND BANDS PRESENT
6.2 6.5 6.9 7.3 7.4 7.7 7.9 8.0 8.2 8.5 9.2
GROUPS ABSENT. NO BAND REGIONS



INPUT DATA
GROUPS
**** NO DATA ****
BANDS
 6.2  6.5  6.9  7.3- 7.4  7.7  7.9- 8.0  8.2  8.5  9.2
NO GROUPS
**** NO DATA ****
NO BANDS
**** NO DATA ****
OPTION...
1                                           SEARCH OPTION
SUBFILES...
CR,                                         SUBFILE SEARCH
TOTAL MATCHING 11-WORD RECORDS =      17
NUMBER OF UNIQUE SERIAL NUMBERS SAVED FOR REPRINT =      10     NO. OF HITS
OPTION...
2                                           PRINT HIT LIST OPTION
WHAT STARTING POINT - 3 DIGITS
001
00088CR        METHYLENE-BIS-/4-HYDROXYCOUMARINE/,3,3PR

00101CR        CARBAMATE, 2-HYDROXY-3-O-METHOXY-  PHENOXY-PROPYL

00163CR        CODEINE ALKALOID

00270CR        ESTRATRIEN-3-OL-17-ONE, 1,3,5/10/-

00277CR        PHENOTHIAZINE, 10-/2-DIETHYLAMINO- PROPYL/-, HCL

00311CR    1,2-PROPANEDIOL, 3-/O-METHOXYPHENOXY/-
```

INPUT – OUTPUT PAGE RESULTING FROM A SEARCH OF THE IR FILE

Figure 6

```
00324CR        PHTHALAZINE, 1-HYDRAZINO-, HCL

00555CR        PHENOTHIAZINE, 2-CHLORO-10-/3-/1- METHYL-4-PIPERAZINYL/PROPYL/

00578CR        PHENOTHIAZINE, 10-/2-/1-PYRROLIDYL/ ETHYL/-, HCL

00724CR        ETHANOL, 1-/P-BETA-DIETHYLAMINO-    ETHOXYPHENYL/-1-/P-TOLYL/-2-

OPTION...
4                          ALTER DATA OPTION
GROUPS AND BANDS PRESENT
6.2 7.6 10.3               NEW DATA
GROUPS ABSENT, NO BAND REGIONS
8.8 9.0                    NEW DATA

INPUT DATA
GROUPS
**** NO DATA ****
BANDS
 6.5  6.9  7.3- 7.4  7.6- 7.7  7.9- 8.0  8.2  8.5  9.2 10.3
NO GROUPS
**** NO DATA ****
NO BANDS
 8.8  9.0
OPTION...
1
SUBFILES...
SP,                        DIFFERENT SUBFILE SEARCHED
TOTAL MATCHING 11-WORD RECORDS =       4
NUMBER OF UNIQUE SERIAL NUMBERS SAVED FOR REPRINT =       2
OPTION...
2
WHAT STARTING POINT - 3 DIGITS
001
00128SP  D.B.-AMOBARBITAL(FREE ACID)

00128SP   NAME PENDING

00193SP  D.B.-PSILOCYBIN

OPTION...
3                          PRINT STANDARD DATA OPTION
ENTER SERIAL NO. -SPACE AFTER ALPHAS
00193SP
SERIAL NUMBER STARTS AT   119197
GROUPS
 1-SOLID   6-OXYGEN  7-N      23-AROM   24-HETCY
BANDS
 5.8  6.2- 6.3  6.5  6.7- 6.8  7.0  7.4  7.7  8.0  8.2  8.5  8.7  9.1  9.4  9.6
C   H   BR CL F   I   N   O   S   SI      COMPOUND  NAME
                                        D.B.-PSILOCYBIN

OPTION...
7                          PRINT PROCESSOR TIME OPTION
TIME FOR SAMPLE:
DEMONSTRATION SEARCH
005 MIN 35 SEC ELAPSED.  000 MIN 02 SEC PROCESS.  000 MIN 06 SEC I-O.

OPTION...
8                          EXIT PROGRAM OPTION

END OF PROGRAM..
```

INPUT – OUTPUT PAGE RESULTING FROM A SEARCH OF THE IR FILE (Cont'd)

Figure 6

b. The maximum line length of the Model 33 is 60 characters. The print speed of the Model 33 is 10 characters per second.

Although these limitations were not serious in terms of our initial operation, we anticipated that the future addition of chemical names to the printout would lead to a requirement of longer line length and greater print speed.

c. The Model 33 terminal is inflexible concerning programming capabilities and possible future file applications requiring specially formatted printouts.

d. Because only one character at a time is transmitted by the Model 33, a burden would be placed on the central computer for input-output handling.

It must be emphasized that none of these difficulties is insurmountable. Indeed, there are infrared data search systems currently operating successfully with Model 33 teletypes. However, due to a change in the DCJS operating system we had the opportunity to test a different type of terminal during this pilot project.

At about the time we planned to implement the "live system," the Burrough's Corporation under the terms of its contract with DCJS, replaced all Model 33 Teletype units then operating on the main DCJS system with Burroughs Model TC-500 terminal computers.

This terminal has a number of features which make it useful in the IR system and tend to minimize some of the problems found with operation of the Model 33 TTY.

a. Print speed is 20 characters per second.

b. Maximum line length is 150 characters.

c. Input-output message buffers are available.

d. The TC-500 is programmable for both local use and input-output formatting.

e. The TC-500 has fewer mechanical parts than the Model 33 TTY.

f. The TC-500 has a ball printer.

g. The TC-500 accepts many types of papers including pin feed.

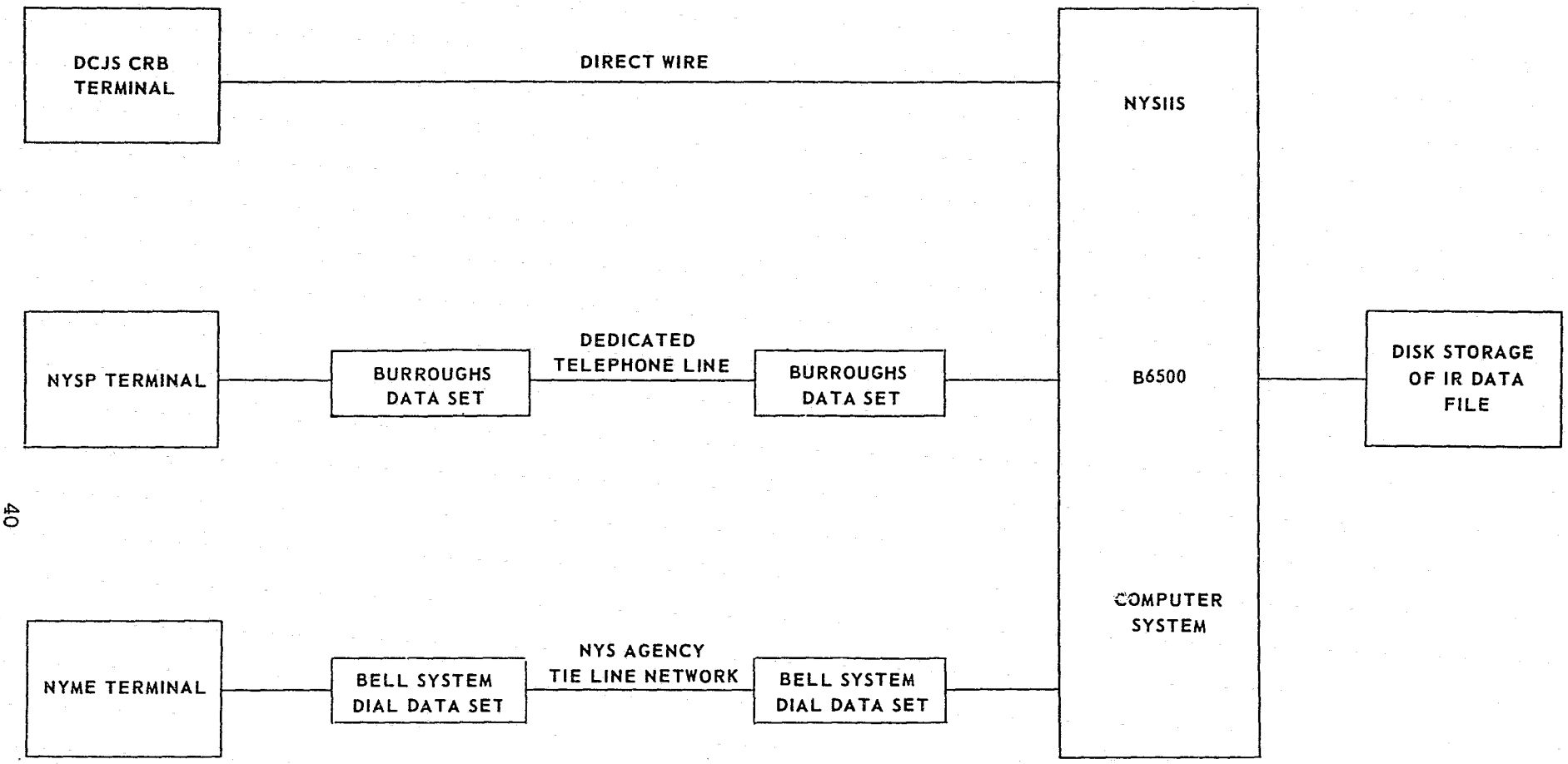
D. System Configuration

Figure 7 illustrates the system as it is currently configured.

Arrangements for the telephone connections to the terminals were made through the New York State Office of General Services which coordinates the operation of a New York State Agency tie-line network for telephone communications.

The New York State Police terminal is connected to the computer through Burrough's data sets direct wired on a dedicated line. This appears to be the most economical mode of connection of this terminal due to the short distance between the two agencies and the availability of non-Bell system data sets which were obtained at a considerable savings over Bell equipment. After initial testing and debugging we have experienced no problem with the communications line for this terminal.

The Medical Examiner's terminal is connected to the computer through Bell Data Phone utilizing the tie-line network. The technician dials a code to gain access to the tie-line between New York City and Albany and then dials a number which results in the computer automatically answering the data set in Albany.



CURRENT SYSTEM CONFIGURATION

Figure 7

Under current operating restraints, only one terminal can use the file search program at a time. A "PROGRAM IN USE" message is received by a requesting terminal if another terminal is already on the air. With current search frequency, this has not caused great problems. However, with the added traffic of file update procedures now being phased into the operation, and the prospect of adding additional terminals, we believe that a method will soon have to be devised to allow multiple users access to the file simultaneously.

The CRB terminal is used quite extensively for testing of program modifications and more significantly for file update procedures. One of the major modifications has been to incorporate file update and error correction routines that can be utilized by CRB staff at its own terminal. These routines are highly interactive and provide numerous checking steps so that file integrity is maintained. At the present time, all forensic subfile standards are added to the file using the terminal for input. There is no card or tape input except for updates of the commercial parts of the file obtained from the commercial supplier.

A vital part of the system is not shown on Figure 7. As alluded to in a previous section, the search of the computer file offers an assist to the chemist in identifying an unknown compound.

The chemist must still verify a potential identification by comparing the unknown spectrum with either a printed reproduction or an in-house prepared copy of a standard retrieved from the file. Although the design of a system for supplying the chemist with copies of the standards indexed in the computer file was not a goal of this project, we cannot ignore commenting on some of the needs in this area.

Basically, all standards indexed in the file are available in printed form. Each commercial contributor to the file can provide copies of the standards for a fee. Additionally, standards extracted from the literature are available in the original literature article.

However, the mere existence of the spectra reproductions does not mean that they are readily available to the forensic community. First of all, commercially supplied spectra are expensive. For instance, a complete set of all Sadtler spectra indexed in the file would cost an individual laboratory approximately $15,000. It would be impractical to extract and produce copies of the 16,847 literature spectra referenced.

This raises the obvious question of how to provide each laboratory with the maximum number of standards at minimum cost. The cost for each laboratory to purchase a complete set of commercially available spectra appears to be prohibitive.

It makes more sense to provide the standards from a central location with transmission to the laboratories at their request. The system to provide this service cannot be specified at this time.

Another difficulty with providing reproduced standards is the legal problem of obtaining permission from commercial suppliers for unlimited duplication for distribution from the central level. These suppliers have an interest in selling as many copies as possible and are reluctant to enter into an agreement to allow unlimited duplication upon payment by the user of a per copy or monthly royalty fee.

A more fundamental question, however, is whether all the printed standards are necessary. Unfortunately, this study did not generate enough data to provide definitive answers to the above questions.

The tentative conclusion reached during this study is that it may be practical to provide the laboratories with selected commercially available standard spectra and supplement the basic data file with forensic laboratory standards.

Within the budget constraints of the grant, we were able to purchase selected "hard copy" spectra for the cooperating laboratories. This was a stop-gap measure to increase the usefulness of the file until a study is done to specify the best system for providing this data.

E. System Cost

Table 4 summarizes both the one time and on-going costs to operate the system in its current configuration.

It must be emphasized that the costs indicated in Table 4 are only illustrative of the typical elements of cost incurred in operation of this system. Actual costs for any specific implementation of the system would depend on the type of terminal used, the particular communications network utilized, and the specific mechanism used for obtaining the file.

Table 4 ignores the cost of operating personnel required at the central level. Our experience to date indicates that the system, as it is currently operated, would require a full time analyst. The analyst would be responsible for maintaining liaison with user laboratories, developing procedures for coding forensic standards, trouble shooting problems occurring in day-to-day operations, and implementing improved versions of the basic search programs. A programmer would be required to devote approximately 50% of his time to file and program maintenance tasks. A clerk would be required to devote between 50% and 75% of his time to file update tasks using the CRB terminal as input and preparing reproductions of forensic standards contributed by user laboratories for distribution to the laboratories.

TABLE 4

SYSTEM COST

ONE TIME COSTS		
Data File and Program Fee		$2,500*
Compound Names Molecular Formula Tape		1,100
ONGOING COSTS		
Ongoing Update Tapes (Yearly if Created by Commercial Suppliers)		200
Communications		
State Police Terminal	**Cost/Mo.**	
Burroughs Data Sets (2)	$32.00	
Telephone Line	8.00	
Adaptor for B6500	45.00	
	85	
TC 500 Computer Terminal (Monthly Rental and Maintenance)	160**	
	Total Cost/Mo.	245
New York City Medical Examiner's Terminal	**Cost/Mo.**	
Bell System Dial up Data Sets (2)	$96.00	
Telephone Line (NYS Tie Line)	44.00	
Adaptor for B6500	45.00	
	185	
TC 500 Computer Terminal (Monthly Rental and Maintenance)	160**	
	Total Cost/Mo.	340

*Fee was negotiated.
**Under current terms of DCJS-Burroughs Corp. Contract.

This level of staffing would allow a limited amount of development effort directed toward supplementing the basic IR file with files of data from techniques such as ultraviolet spectroscopy and thin layer chromatography.

Of equal importance with the individual cost of the components of the system is the distribution of the costs among the users and the central agency. During the grant period, DCJS has paid the full cost of operating the system. However, it is our policy that a portion of the costs will be borne by the user agency after the grant period. For instance, we have worked out an arrangement with the Medical Examiner's Office whereby DCJS will be reimbursed for the cost of the terminal and the telephone line. DCJS will continue to pay the cost of the file maintenance, file search and update procedures.

It would also be possible to calculate an overall per search cost and distribute costs on a fee or time shared basis. The specific type of shared cost arrangement utilized by other implementations of this system would depend on the type of central computer utilized, the number of terminals on the line and the distribution of usage.

VI. EVALUATION OF PILOT OPERATION OF FILE

A. Observations Based on Operational Data

1. Training of Operators

Training required to operate the terminal and program is minimal and can be accomplished in approximately two days. There are several aids in accomplishing this mechanical training. Both the operator's manual (see Appendix A) which gives step-by-step directions for the operation of the program and the programmatically invoked explanations (see Appendix B) aid in training operators.

It is beneficial for the person operating the program to have some experience in interpreting IR data. This experience will be helpful in preparation of a search strategy. However, relatively unskilled laboratory technicians can also obtain usable "hit" lists for later scrutiny by more experienced personnel.

Professional short training courses such as those presented by instrument manufacturers or the American Chemical Society would be helpful in giving the inexperienced chemist confidence in applying the IR technique and would impart an appreciation of the value of IR data in identification problems.

An important aspect of operator training that should not be ignored is an introduction to computer technology. This does not have to be lengthy or overly technical. For instance, a tour of the central computer center given by an experienced systems analyst or computer operator will impart an appreciation of the operation of the system.

The necessity for this training is demonstrated by DCJS operational experience. The IR system was implemented at the time DCJS was installing a new B-6500 computer system. During the "shakedown" of the computer system, the chemists from the operating laboratories experienced many instances when the computer would "go down" in the middle of a search requiring a re-entry of all data. This led to much frustration and noticeable pessimism in the ability of the system to provide timely results on a routine basis. An in-depth tour of the DCJS computer center conducted by senior operating personnel increased the chemist's understanding of the complexity of the system, the need for periodic maintenance, and the reasons why a search might be aborted at the central level.

As a result of the tour of the computer center, operational experience in the use of the system, and increased reliability of the DCJS computer, the satisfaction level of the user agencies has increased drastically during the period of the study.

2. Program and File

The major questions to be answered in evaluating the program and file were:

a. Could a chemist make "hits" using the search argument?

b. Is the file responsive to forensic needs?

Based on more than six months operational experience we have come to the conclusion that the program in its present operating status is capable of making identifications of forensic samples. Tables 5 and 6 illustrate identifications made by each laboratory. Each of these "hits" is a unique compound identified by the file during the study period. They are categorized by investigation type to illustrate the file and search program's responsiveness to samples across the full range of forensic cases.

These "hits" represent both routine and specialized cases. Of course, the laboratories may place differing values on "hits" depending on the category. Some of the "hits" for the so-called routine cases provided unambiguous confirmation of a potential identification made by another technique. In these cases, the identification was made very rapidly with a minimum number of retrievals from the file. This is important because the forensic chemist requires the most complete information possible when preparing a case for court.

TABLE 5

NEW YORK STATE POLICE LABORATORY IDENTIFICATIONS*

Nature of Case	Chemical Compound Identified
Toxicology	Phthalic acid ester**
	Chloral Alcoholate**
	Methyl Silicone**
	Doriden
	Nitroglycerine
Narcotic	Barbiturate and Talwin
	Dehydrocortisone**
	Napain**
	Hydrocodinone
	Methyl silicone
	Mephobarbital
	Amphetamine Hydrochloride
	Quinoxaline, 2,3, Diphenyl**
	LBJ**
	Methadone
	Ephedrine
	Sodium Pyrophosphite**
	m-Sulfobenzoic acid**
	Hydroxylamine
	Pentobarbital
	Phenobarbital
	STP**
	Reaction intermediate**
	Methamphetamine
	Glycerol
	Atropine**
	Phentermine**
Explosives	Nitromethane
	Nitrocellulose
	Trinitro toluene
	Nitroglycerine
Hit and Run**	Pain pigment - dye
	Red 27 pigment
	Vat orange 3
	Lucite
Miscellaneous Unknown**	Toluidine Toner, pigment red 3
	Polymethyl silicone
	Tetrachloroethylene
	Lithium Hydroxide
	Manganese II sulfate hydrate
	Freon
	Tear Gas
	CS
	Calcium carbonate
	Surfonic M-300
	Tweed 30

* Not an exhaustive list of identifications made during the study period.

** Indicates Non-Routine Identification.

TABLE 6

NEW YORK CITY MEDICAL EXAMINER'S LABORATORY IDENTIFICATIONS*

Noludar

Simethicone (Polymethyl Silicone)

Formalin

Isopropyl Alcohol

Meprobamate

Acetophenetidene

Abrus Seeds (Jequirity)

Alstonine

* All Toxicology Cases.

The non-routine identifications represent cases that might not have been solved were it not for the availability of the computerized file. Indeed, the IR technique may not have been utilized were it not for the file.

The computerized IR file has increased the chemist's efficiency in using the IR technique. Experience to date indicates that the chemist will know if he can identify an unknown IR spectrum within 10-15 minutes after the spectrum is produced. Formerly, the process of identification could take hours, days, or weeks depending on the complexity of the problem.

The rapid answer provided by the computerized system will also guide the chemist's course of action concerning a particular case. Based on a rapidly obtained negative result, he may decide that a different analytical technique should be attempted.

The increased use of the IR will also lead to a further correlation of the data from the many techniques used by forensic chemists.

The data to date, therefore, indicates that the forensic chemist <u>can</u> make hits with the system as it currently exists.

Additionally, we have concluded that the file can lead to routine identifications (providing backup data for court purposes) and non-routine identifications.

It is impossible to describe in detail each of the different identifications. However, following is background information for some of the more important identifications.

Case 1: A 50 year old chemistry professor was found dead in his car. Found with him was a glass containing what appeared to be an alcoholic beverage. An acid extraction and IR analysis were performed on the liquid. A computer search on the IR spectrum identified the unknown as chloral alcoholate. Extraction of stomach contents of the deceased and subsequent computer search of data from an IR spectrum identified the unknown to be chloral. A visual comparison of the unknown curves with curves of chloral alcoholate and chloral confirmed the computer identification. These identifications led to the conclusion that the deceased had died from ingesting an adulterated alcoholic beverage.

Case 2: An unknown white colored substance suspected of being an explosive was submitted to the State Police for analysis. An IR analysis and computer search were performed. The substance was identified by the program as trinitrotoluene (TNT). Subsequent visual comparison with a spectrum of TNT confirmed the identification.

Case 3: A suspected clandestine drug laboratory was raided by a municipal police department. The program helped identify eight chemicals used in the synthesis of illicit drugs.

Case 4: During an investigation of a duck kill, the presence of large concentrations of several detergents in the water explained the cause of death as drowning due to the loss of natural feather oils. The identification of the detergents was affected through the use of IR analysis and the computer search.

Case 5: An example of the use of the forensic subfile occurred when the State Police identified an asphalt stain on a piece of clothing through a search of their subfile. This may not have been a significant identification from the standpoint of solving the case. However, the analyst doesn't know the significance of a stain when he begins his analysis.

In addition to the direct "hits" mentioned above, the program has assisted many times by giving an indication that the unknown is a particular type or class of compound. While there is no positive identification, the type or class of the compound often provides investigative leads in the solution of a case.

Although the above indicates that the file and program were judged to be extremely valuable tools in forensic work, two drawbacks were noted by the operating chemists. First of all, the version of the program currently used does not rank the "hits" in a probability order of match with the input argument. This makes it difficult for the chemist to evaluate the "hit" list.

Secondly, the program is not "forgiving" of erroneous input data. That is, if a band is said to be present in the input data, that band must be present in the standard data for a "hit" to result. This places a burden on the judgment of the chemist with respect to choosing the initial input data. Both of these problems can potentially be solved by updating our current search program to a new version created and marketed by Dr. Duncan Erley.

Another problem with the current program is that it has only limited utility in analytical problems dealing with mixtures of several chemical compounds. This problem is being addressed by Sebesta and Johnson in the development of the Multicomponent Infrared Retrieval (MIRET) System.[1]

The second question addressed by our evaluation of the file and program concerned the file's ability to be responsive to forensic needs.

Prior to the study we believed that forensic subfiles would be valuable additions to the basic data file. Their value would be in compensating for some of the inherent problems with IR data such as differences in spectra of the same compound caused by machine differences, solvent effects and impurities.

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[1] Sebesta, Robert W. and Johnson, Gerald G., "New Computerized Infrared Substance Identification System," Analytical Chemistry, Vol. 44, No. 2, February, 1972, pp. 260-265.

This opinion was confirmed by discussion during the study period with industrial and research chemists experienced in IR work. They generally stated that the IR file is one type of data file where it isn't necessarily inefficient to create multiple standards for a compound. The chances of overcoming the problems mentioned above increase as more versions of the same compound are contained in the file.

Therefore, we took steps early in the project to include standards submitted by the laboratories in a forensic subfile. To date, more than 250 standards from each laboratory have been added to the basic data file. A number of identifications have been made through use of this file which contains abused drugs, explosives and other compounds of forensic interest.

3. Overall System

As mentioned previously, the file and search program are only two components of the total identification system used for IR. The system starts with the chemist deciding which data to input to the search program and ends with a visual verification of an identification.

One of the most important outcomes of the pilot project has been the development of a systematic approach for performing a search on an unknown spectrum.

It has been found that if an analyst starts with a minimum of IR data and adds additional data gradually, he can accurately narrow down to a positive identification. The success of this approach confirms the suggestions proposed by Erley in his original literature article describing the fast searching system.

Following are the steps to be followed in the systematic approach:

a. Use case background to develop an idea of what the compound might be.

b. Choose seven (7) major bands.

c. Search relevant subfiles first.

d. Add a minimum amount of group data.

e. Add other significant bands.

f. Add no band data.

The use of this approach will result in manageable "hit" lists in the shortest period of time.

During this study we have developed draft procedures for updating the forensic subfiles. As the system matures, these procedures will be formalized. DCJS personnel must work very closely with the operating laboratories to develop standard coding methods, formats for the subfiles, and methods for distribution of reproduced standards.

Both laboratories had the opportunity to evaluate whether the IR system is responsive to forensic needs from the standpoints of ability to provide identifications and the ability of the central operating personnel to perform the necessary systems improvement tasks in an effective manner.

Appendices C and D contain complete evaluation reports prepared by the technical and administrative personnel of both the New York State Police and New York City Medical Examiner's Laboratories.

Concerning the question of effective liaison between the central and user agencies, the State Police have stated (Appendix C):

"We are most optimistic about the program and are looking forward to its continuance and the scientifically productive relationship with the Criminalistics Research Bureau of NYSIIS.

"The development areas delineated in the preceding paragraphs indicate that future development of this file concept will require a combination of systems studies, design of file update procedures, computer programming modifications and laboratory production of reference standards. In our opinion, these types of tasks could be most efficiently accomplished through a cooperative effort between the NYSIIS CRB and the forensic science laboratories that utilize the central files."[2]

The New York City Medical Examiner's Office agrees that the ability of a central agency to design the system around forensic needs was demonstrated during this project.

In fact, the following statements from Appendix D indicate that the Medical Examiner's Office doubts the ability of forensic laboratories to perform the systems development and maintenance tasks necessary in operating a scientific information system.

[2]Ferriss, S., Ellis, R., New York State Police Scientific Evaluation Report.

"...The present system for file maintenance works very efficiently. In my opinion, laboratory programming is a highly specialized science and could not be justified as a function for our laboratory. Nor do I see the need for other than a centrally operated location available to a number of laboratories.

"...Our laboratory doesn't have time nor the personnel to maintain even a rudimentary cabinet filing system. The problems of work overload and limited personnel is universal in all technical organizations that I know of. Our staff, which is the largest, nor the staffs of any of the others in this field, has the time for programming even if they had the expertise."[3]

4. Potential System Usage

The operation of the State Police terminal gave us the opportunity to determine the likely volume of requests that the program would handle from a busy forensic laboratory. Table 7 summarizes operational experience relative to samples (cases) searched and total number of searches likely to occur per month. The low figure in August resulted from decreased staff time available for IR analysis due to vacations and court commitments.

TABLE 7

	JUNE	JULY	AUGUST	SEPTEMBER	OCTOBER
Samples	40	55	20	62	42
Total Searches	166	201	75	206	141

[3]Umberger, Dr. C., Bungaro, Dr. E., New York City Medical Examiner's Laboratory Evaluation Report.

The figures in Table 7 suggest that during any week we can expect that the State Police Laboratory will require the search program for about 50 searches requiring about ten minutes elapsed time per search. This indicates that approximately eight hours of elapsed computer time will be required per week. There will be a random distribution of this time depending on caseload, sample preparation required and priorities concerning the type of case worked on in any one day. Computer usage will tend to level off at about this amount for this laboratory unless there is an increase in personnel.

Actual central processor and input/output time used by a laboratory during a given time period is important from the perspective of their impact on the overall DCJS operating system. The current program requires approximately 1 min 44 central processor and 3 min 45 input/output time for a search of the entire file. Of course, the laboratories frequently search only a small portion of the file requiring far less actual processing time.

During the study period, we have received numerous inquiries from forensic laboratories of the state concerning the IR search system. We are currently conducting preliminary studies which could result in the addition of five (5) laboratories to the network.

The specific timetable for these additions depends on the ability of DCJS to supply equipment and the ability of the laboratories to share in the cost. We anticipate that the volume of searches generated by the addition of these laboratories will not hinder the operation of on-going DCJS information systems.

B. Conclusions

Based on the preceding observations of the operating IR system, we have formulated the following project conclusions:

1. The central data file concept for forensic science laboratories is not only feasible, but is a highly desirable addition to the laboratories' analytical capabilities.

2. The Infrared Data File search system in its present state of development is of definite assistance in infrared data interpretation connected with cases across the full range of forensic problems. The degree of assistance can be increased by the addition of forensic subfiles.

3. The existence of the IR data file search system has resulted in a definite increase in the utility of the IR spectrophotometer in the forensic laboratory.

4. To dervice maximum benefits from the system, the chemist should be on-line to the computer system.

5. File and system update maintenance, and improvement should be performed by the central agency staff subject to the advice and counsel of the user agencies.

6. A system for providing standard "hard copy" spectra for final verification will increase the utility of the computer system.

7. The current communication system is capable of handling the current amount of traffic generated by the two laboratories and the maintenance functions performed at the central level. However, as additional laboratories are added, a method for allowing searches by all laboratories simultaneously will be required.

C. Recommendations

1. The IR system should continue to be operated for all laboratories who can share in the cost.

2. The data file should be expanded to include forensic subfiles containing standards contributed by as many forensic laboratories as possible.

3. The search program should be modified to a version (already commercially available) which would make it more "forgiving" when erroneous search data is entered. This should increase the utility of the system by raising the identification rate.

4. A study should be made of the alternative ways of providing "hard copy" standard spectra to each laboratory.

5. Based on the conclusion that scientific data storage and retrieval is a valuable asset to forensic work, additional files should be created to store the following data from the following techniques:

   a. Ultraviolet spectrophotometry.

   b. Gas-liquid and thin layer chromatography.

   c. Mass spectrometry.

   d. Color and crystal tests.

   A correlated cross referenced type search procedure could then be developed using all the data in the file.

APPENDIX A

PRELIMINARY OPERATOR'S MANUAL

INFRARED DATA FILE SEARCH NETWORK*

INSTRUCTION MANUAL

The Infrared Data File Search Network brings to the forensic chemist a fast, interactive means for retrieving possible identifications of unknown infrared spectra from a centrally stored file of data on standard spectra.

To use the system effectively, the spectroscopist must recognize that a comprehensive data file plus a good searching program are only two parts of the system. His own role, selecting the data to use as input, is the vital third part. This selection is often a trial-and-error process. The search program used is designed to make that process more efficient.

The spectroscopist must know not only what data from his sample to use as input, but also how the data were coded that went into the standard file.

The following pages describe the technical characteristics of the data file, search program, and terminal equipment used in the searching system. Also included are operating instructions for the terminal and suggested search strategies.

*Taken in part from SIRCH™ Instruction Manual by ASTM.

TABLE OF CONTENTS

I. FILE CHARACTERISTICS

The standard data file currently utilized in the infrared search system was obtained from the American Society for Testing and Materials. The file consists of standard data coded for approximately 102,000 organic compounds.

These data are coded into a sub-file designation depending on their origin. Each standard has a zero to five digit numerical designation followed by a one or two letter sub-file designation. Table 1 enumerates the sub-file designations. Note that the Sadtler sub-file is additionally divided into several sub-sub-files.

Data stored for each standard consists of Group and Band data.

The Group data can be elemental, functional group or physical state in nature. Each Group has a unique numerical representation as described in Table 2.

Band data was coded in the range 5.5 to 15.0μ. There currently is no specific code for the relative intensity of the bands coded.

An important factor in using the file is knowing the criteria that were used to determine which bands to code for storage on individual spectra.

The following information is taken in part from Codes and Instructions for Wyandotte - ASTM Punched Cards, published by ASTM and describes generally the criteria used for building the data file. This should provide the spectroscopist with guidelines for strategic entry of search data.

CRITERIA FOR THE SELECTION OF BANDS TO BE CODED

Experience has shown that it is not desirable to code all of the bands of most spectrograms. Actual search operations usually can isolate the possible identifications in searches on approximately seven bands. However, negative searching for the identification of components in a mixture requires that all moderately strong bands be coded. Therefore, the selection of which bands to code and which to omit requires some judgment, and because of the nature of published spectrograms the judging can be guided only by a rather flexible rule. Several factors enter into the determination of the strength of an absorption band, and what may be a good set of factors for the production of an excellent spectrogram from one material is not necessarily a good set to provide a similar spectrogram from another material. Moreover, the quality of published spectra varies

TABLE I

ORIGIN OF SUBFILES IN ASTM IR DATA FILE

Class. Symbol	Source/Type of Data
A	American Petroleum Instit. Proj. 44
C	Sadtler Catalogue of Spectrograms
SADTLER SUBFILES:	
CA	Agricultural Chemicals
CB	Polyols
CC	Surface Active Agents
CD	Monomers, Polymers, Resins, Gums, Pyrolyzates
CE	Plasticizers
CF	Perfumes, Flavors
CG	Fats, Waxes, Derivatives
CH	Lubricants
CJ	Rubber Chemicals
CK	Fibers
CL	Solvents
CM	Intermediates
CP	Petroleum Chemicals
CR	Pharmaceuticals
C	Sadtler Standard Spectrograms
CS	Steroids
CT	Textile Chemicals
CW	Attenuated Total Reflectance
CX	Dyes, Pigments, Stains
CY	Inorganics
D	NRC-NBS File of Spectrograms
E	Spectrograms Abstracted by ASTM-Sponsored Groups
FA	Inorganics
F	Documentation of Molecular Spectroscopy
G	Coblentz Society Spectrograms
H	MFG Chemists Assoc.
J	Infrared Data Com. of Japan
SP	State Police Forensic File
ME	Medical Examiner's Forensic File

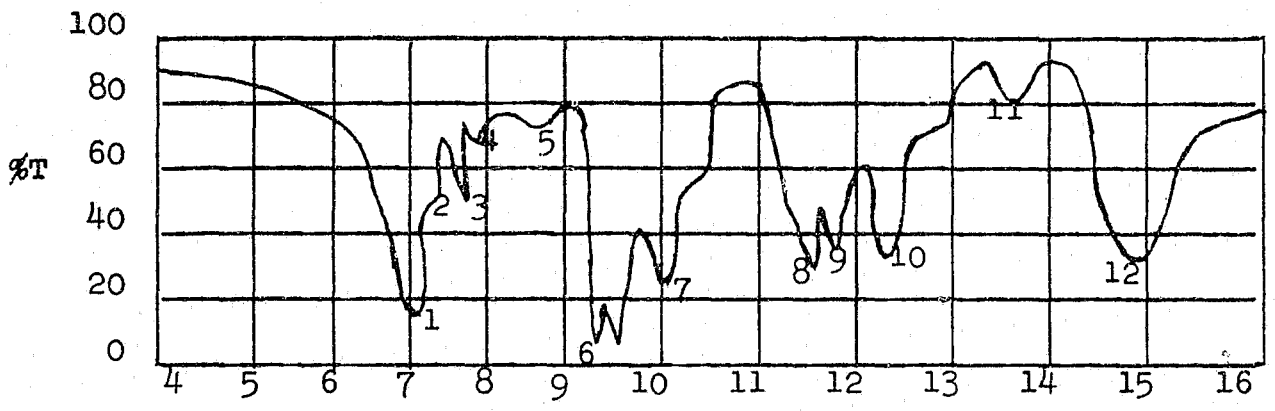
TABLE II

GROUP DATA

Numeric Code	Identification
1	Solid
2	Liquid
3	Solution
4	Polymer
5	Inorganic
6	Oxygen
7	Nitrogen
8	Sulfur
9	Fluorine
10	Chlorine
11	Bromine/Iodine
12	Phosphorus/Bismuth
13	Arsenic/Antimony
14	Silicon/Germanium
15	Tin/Lead
16	Boron/Aluminum
17	Metals
18	Salt
19	C=C
20	C=C
21	Acyclic
22	Alicyclic
23	Aromatic
24	Heterocyclic
25	Fused
26	C=O
27	OH
28	NH
29	C-O-C
30	C=N
31	NO_2
32	S=O

widely and any system of coding absorption bands must allow for making the best possible use of all such data.

As a general rule, all bands should be coded that have an absorbance ratio with the absorbance of the strongest band in the spectrogram of 1:10 or more. This means that when the strongest band in the spectrum has between 1 and 5 per cent transmittance, all bands having 70 per cent or less transmittance as measured from a reasonable adjacent background (not necessarily at 100 per cent transmittance) should be coded. Thus, to be coded, a band must stand out from its adjacent background, at least on one side, by a distance corresponding to at least 20 to 30 per cent transmittance on the chart. Therefore, "shoulders" and weak bands on the sides of strong bands are not coded. Likewise, bands whose percentage transmittance may be as strong as 60 to 50 as read from the chart, but extending from backgrounds having transmittance values of 80 to 70 per cent, should not be coded. Actually, the process is not as difficult as it may appear and minimal searching risks are introduced since one seldom, if ever, is called upon to make positive sorts on any of the relatively weak bands which lie in the "to code or not to code" region of intensity. Figure 1 provides an example of the coding of a hypothetical IR spectrum giving the rationale for coding or not coding a band.



WAVELENGTH IN MICRONS

FIG. 1 - EXAMPLE OF INFRARED CURVE

The above hypothetical spectrogram is included to assist in describing the application of rules prescribing which bands were coded and which were omitted from the data file. Band No. 9 is the strongest and has a transmittance value between 1 and 5 per cent; therefore all bands having a transmittance of 70 per cent or less as measured against a reasonably adjacent background should be coded. The dotted lines indicate what is meant by such an adjacent background. The distance by which coded bands must project from such a background is equal to one and a half units of the vertical scale. Applying this rule, one can code without question the following bands: Nos. 1, 3, 6, 7, 8, 9, 10, 12.

Band No. 2 was not included. This is a case of a rather weak band on the side of a strong one which has no value in searching and need not clutter up the stored data. Therefore, it was omitted. On the other hand, band No. 7 was included since it is prominent enough to be used in searching operations. Also, No. 9 which does not fit the coding criteria when measured from its immediately adjacent background is coded because it obviously is one of three rather strong bands which are close enough together to overlap appreciably. An ill-defined shoulder on the side of band No. 7 is ignored as is the fine structure in the band No. 6. Band No. 11 represents a possible borderline case that should not be coded.

A good rule is, "When in doubt, leave it out." The spectrogram is typical of many that appear published in the literature and serves to illustrate why a coding resolution of 0.1μ is entirely adequate.

Searching spectra on the absorption band codes is much the same as coding the bands. First, the spectrogram of the unknown material should have its strongest bands between 1 and 20 per cent transmittance since it is to be compared with coded data obtained from such spectra. Searching can then proceed on the basis of bands or groups coded and regions where there are no bands or groups. The step-by-step procedure is outlined in another section of this manual.

II. OPERATING PROCEDURE

CRB/SIRCH

As mentioned in the introduction, the search program used with the infrared data file is highly interactive. That is, the operator communicates with the file through the program and vice versa. The purpose of this section is to describe the search procedure by detailing operator entries, computer responses and options available to the operator during a search.

Specific operating procedures for the Burrough's TC-500 terminal equipment are presented when applicable.

PROGRAM INITIATION

TC-500 INITIALIZATION PROCEDURES

NOTE: General control button identification and operating functions for the TC-500 are explained in the Burrough's publication, "Operator Manual Series TC Terminal Computer."

OPERATOR ACTION	TC-500 RESPONSE
1. Press ON button	All keyboard indicator lights turn on.
2. Wait 30 seconds	Bell rings; printer ball travels to right and returns to left. "Ready," "Start," "Load," "Utility" lights are on.
3. Press "Start"	Carriage line spaces; "Load," "Utility" lights go off; "Num" light on.
4. If program has just been entered through memory loader (see page 1-10 Burroughs manual), enter [terminal identification number and maximum line length] on numeric (lavender) keyboard followed by OCK. If program is already stored in machine, go to instruction 5.	Terminal prints terminal identification number and maximum line length and line spaces.

OPERATOR ACTION	TC-500 RESPONSE
5. Press OCK	System listening lights will blink.
6. Press OCK	Initiates infrared program; prints message: INFRARED SEARCH PROGRAM; lines spaces several times and prints SAMPLE.

PROGRAM OPERATION

NOTE: All operator entries must terminate with OCK to allow transmission to computer.

COMPUTER REQUEST	OPERATOR ACTION
SAMPLE	Enter a SAMPLE IDENTIFIER: Information may be 0-48 characters and may be ALPHA, NUMERIC or a combination of both.
GROUPS AND BANDS PRESENT	Enter data about the presence of functional groups or elements (see Table 2 in File Characteristics Section for numeric codes). Enter data about the positions of observed absorption bands.

Data Entry Rules:

1. Group and band data are entered at the same time.
2. Group data codes must be within the range 1-32.
3. Absorption Bands:
   a. Enter by wavelength to the nearest 0.1 micron.
   b. Wavelength must be in range 5.5 to 15.0 microns.
   c. Consecutive entries can be generated by using a dash (10.1-10.4).
   d. Maximum line length is 140 characters. Entries of more than 140 characters must use another line. To send the first line, add a + sign

after the final data for the line and transmit an OCK. This will send one line and bring the program back to GROUPS AND BANDS PRESENT.

GROUPS AND BANDS ABSENT — Enter the absence of groups or elements, and position of "no band" regions of the spectrum. This is done in the same manner as for GROUPS AND BANDS PRESENT.

Figure 2 shows how data would be entered for a typical sample. Operator entries have been underlined. After the final data entry, the program retypes the data for operator verification.

After entry of data and verification of the retyped data, the computer will print "OPTION." The subsequent course of the search is dependent on which of the available options are chosen by the operator. Section III presents a discussion of each option together with specific operator instructions.

FIGURE 2

INFRARED FILE SEARCH PROGRAM

SAMPLE
BRUCINE ALKALOID
GROUPS AND BANDS PRESENT
6.0 6.7 6.9 6 7.2 7.9 26 8.2 8.4 9.0 11.8 11.9 12.7 13.2
GROUPS ABSENT. NO BAND REGIONS
13.5-14.8 17 10.4 9

INPUT DATA
GROUPS
    6-OXYGEN 26-C=O
BANDS
    6.0 6.7 6.9 7.2 7.9 8.2 8.4 9.0 11.8-11.9 12.7 13.2
NO GROUPS
    9-F 17-METALS
NO BANDS
    10.4 13.5-14.8
OPTION...

III. SEARCH OPTIONS

OPTION NUMBER	FUNCTION	COMPUTER AND/OR OPERATOR ACTION
1 SEARCH FILE	Part or all of the infrared data file is searched for matches corresponding to the data entered by the operator. Following the search, the computer prints NUMBER OF HITS followed by the number of compounds matching the search argument.	After operator enters [OCK] the computer prints, "SUBFILES." Operator chooses one of the following search arguments: a. <u>Search entire file</u> Operator enters ALL[OCK]. b. <u>Search Individual or group of subfiles</u> The program has the capability of searching any combination of subfiles. Consult Table I in the <u>File Characteristics Section</u> for specific subfile codes. The subfile search is initiated by entering the letter or letters designating the particular subfile desired, followed by a period. Multiple subfile entries are separated by a space. e.g., A. CA. [OCK] would cause a search of the API Project 44 and Sadtler Agricultural Chemicals subfiles. Entry of C followed by a period would cause a search of the entire Sadtler file. Individual subfiles may be eliminated from a search by entering NOT followed by the subfile letter and a period.

OPTION NUMBER	FUNCTION	COMPUTER AND/OR OPERATOR ACTION
2 PRINT SERIAL NUMBER/CHEMICAL NAME/FORMULA	Prints serial numbers and subfile designator for each standard matching the search argument. A maximum of the first 500 hits are stored for printing.	After operator enters 2[OCK], computer prints serial numbers. In the future, chemical names will also be printed by this option. At present, the operator retrieves the chemical name in the ASTM index.
3 PRINT STANDARD DATA	Group and bands coded for a particular serial number are printed for operator information. This option enables an operator to determine why a standard was missed.	After operator enters 3[OCK], computer prints ENTER SERIAL NUMBER. Operator then enters the desired serial number. Numbers must contain sufficient leading zeroes to make a five digit number (e.g., 00032). Single letter subfile designators must be followed by a space (e.g., C).
4 ALTER DATA	Alters data in search argument.	After entry of 4[OCK], computer prints GROUPS AND BANDS PRESENT. Operator then alters data. Data entered by the operator that matches data already entered in search argument is deleted. New data will be added to the search argument. Data is entered in the same manner as previously described.

OPTION NUMBER	FUNCTION	COMPUTER AND/OR OPERATOR ACTION
5 REVERSE WIGGLE	Enables operator to request a search with or without a search tolerance. The tolerance (searches plus or minus 0.1 micron around each band) is called a "wiggle" and is not utilized until after the "no band" comparisons have been made; thereby having no effect on them. "Wiggle" is a variable in the search program having a true or false value. This option reverses the value and prints the new status. Wiggle starts as true upon initiation of the program.	After entry of 5[OCK] the program prints one of the following two messages. WIGGLE IS NOW FALSE. WIGGLE IS NOW TRUE. The computer then prints OPTION.
6 NEW SAMPLE	Returns the program to initiation point.	After entry of 6[OCK] computer prints SAMPLE. Operator then begins new search as described above.
7 TIME FOR SAMPLE	Prints clock time since last option 6 or 7 was invoked.	After entry of 7[OCK], computer prints the elapsed, central processor and input-out clock times and the name of the current sample.
8	Prints summary time information, and terminates program.	After entry of 8[OCK], computer prints END OF PROGRAM and the program is terminated.

NOTE: The word OPTION entered at any point in the program requiring an operator entry will return the operator to OPTION at which time he can determine the course of the search.

IV. OPERATOR ERROR MESSAGE LIST

OPERATOR ERROR MESSAGE LIST

Operator entries can cause the computer to print several error messages. The following is a list of these messages together with action required by the operator to remove the error condition.

ERROR MESSAGE	CAUSE	COMPUTER AND/OR OPERATOR ACTION
BAD ENTRY	During OPTIONS 1, 2, or 3 the operator does not follow rules for entry of serial numbers or subfile designators. E.g., Omission of the period after subfile designator; omission of leading zeroes on serial number; illegal subfile designator.	After printing error messages, computer will print OPTION. Operator then chooses the appropriate option and re-enters the required data.
	During data entry, this message indicates that the operator has entered group and/or wavelength data outside the allowable ranges or did not enter spaces between entries.	After printing error message, computer will continue with data entry procedure. When data is printed back for verification, data that was not correct will cause all data of that type to be eliminated. This means that this data must be re-entered. The operator should verify which data was received correctly (Scan INPUT DATA) then request Option 4 which will return him to GROUPS AND BANDS PRESENT at which time he can re-enter the data correctly.
BAND/NO BAND DATA OVERLAP. RE-ENTER ALL DATA	Operator has entered the same groups and/or bands in the GROUPS AND BANDS PRESENT/GROUPS AND BANDS ABSENT sections.	After printing error message, computer prints GROUPS AND BANDS PRESENT to allow operator to re-enter data.

V. INFRARED DATA FILE SEARCH NETWORK DATA COMMUNICATIONS DIAGNOSTIC MESSAGE LIST

The following messages can be used by the TC-500 operator as diagnostic aids in determining the nature of problem conditions likely to occur in the operation of the IR search system. Each of the messages are sent to the computer by pressing the operator control key (OCK) after entering the messages into the TC-500 transmit memory. The message syntax is presented together with expected responses by the computer and suggested operator action.

MESSAGE: ?W(OCK)

RESPONSE: YOU ARE: CRB___(__). SYSTEM STA NO. ___.

This message can be used as a diagnostic aid to determine if the Data Communications Processor (DCP) and the Message Control System (MCS) are currently operating.

If the operator gets no response or if the TC-500 fails to transmit the message, there is a good chance that either the DCP or MCS are not operating.

The operator should wait for approximately 5 minutes and then call the computer room to determine the extent of the problem.

If the computer is processing normally, and the search program cannot be initiated, ask the computer operator to "PD CRB/IRDISK and CRB/SIRCH" to determine if the file and search programs are currently in storage.

If the file and program are not on disk storage, the computer operator will require several minutes to load them into memory.

MESSAGE: ?TO[STATION NAME]: [MESSAGE] (OCK)

This is the general syntax used to send a message to another station on the network.

RESPONSE: *OK*

This response indicates that the message has been sent by the TC-500 and received by the MCS for routing to the proper terminal. The operator should then wait for a response from the terminal he called. This can require a varying length of time depending on machine load, typing ability of the sender, etc.

NETWORK ALLOWABLE STATION NUMBERS

The operator at one station may want to send a message to another station to tell the operator that he wishes to use the program.

To maintain the integrity of our data communications network, we must limit the number of stations callable by an operator on the IR search network.

Currently, stations in the following locations can be called:

	Station Name
NYSIIS Criminalistics Research Bureau	CRB006
NYS Police Scientific Laboratory	CRB012
NYC Medical Examiner's Off. Lab. (can only be called if telephone line is open to New York City)	CRB003

Use of any other station name will result in an error message.

MESSAGE: PROGRAM IN USE BY _____.

This message will be written by the computer if the IR program is being used by another terminal on the network.

Find out which station is using program by sending a message using the ?TO syntax.

RESPONSE: On-line to B-6500 you are CRB___(__). System Station No. _____.

This response by the computer is automatic and will occur anytime the entire system has been restarted after a "down" condition. The response indicates that the IR program has probably been terminated, while the computer was down. Therefore, the operator should restart the program in the normal manner.

VI. SUGGESTED SEARCH STRATEGIES

The spectroscopist will, in all probability, develop an individualized search strategy based on his personal infrared data interpretation knowledge and the particular case at hand. However, the following information should be helpful as a guidelines search strategy for searches until experience with the file is gained. This information was taken in part from an instruction manual published by ASTM for use with their version of the data file.

The CRITERIA FOR THE SELECTION OF BAND TO BE CODED section of this manual should be read carefully before entering search data. These criteria have been applied with considerable latitude, and the spectroscopist must use some care in selecting the data he enters for a search. For example, differences in concentration, thickness, spectrometer performance, etc., cause variations in band positions and intensities. The search program allows for position errors of $\pm$ 0.1μ (wiggle feature), but the spectroscopist must judge which bands are strong enough to have been coded. Chemical and physical data (accessed by the codes 1-32 in Table 2, File Characteristics Section) are subject to even more variation; in fact, data not known by the coder at the time the spectrum was processed may have been omitted entirely, for example when a spectrum indicated only the commercial name of the compound.

Experience has shown that the most reliable data are, in order:

1. Position of bands stronger than 0.5 absorbance.
2. "No-Band" regions where absorbances are less than 0.01.
3. Elemental Data.
4. Functional Group Data.
5. Physical State Data.

It is suggested that the initial search use only band/no-band data, and that "no-band" regions stay at least 0.2μ away from observed absorption bands. If too many hits are obtained, data may then be added to improve selectivity. When a reasonable number of hits is obtained, the serial numbers should be printed. Mixtures will also require iterative searching with several combinations of bands being ruled. As much "no-band" information as possible should be used as this data is common to all the components.

Finally, it should be recognized that some spectra simply do not contain enough useful information to permit their identification no matter how good the search system is. The user is encouraged to select several spectra at random from his own standard file, enter the data, and, if the correct answer is not obtained, use option Number 3 to determine why.

VII. GENERAL LOGIC FOR INFRARED SEARCH PROGRAM

1. The program REJECTS as hits all standards which have data coded corresponding to data entered by the operator as "NO BAND" or "NO GROUP" data.

2. The data is "wiggled" (depending on value of Option 5, Reverse Wiggle) so that for each wavelength entered, the wavelengths on either side are treated as though they also have been entered. (E.g., 8.0 entered; search takes place on 7.9, 8.0, 8.1) The "wiggled" data is compared with each standard.

3. The program REJECTS as hits all standards not containing the same elements of data as input by the operator.

All standards <u>not</u> REJECTED by above are considered HITS.

APPENDIX B

PROGRAMMATIC OPERATOR'S INSTRUCTIONS

```
INFRARED FILE SEARCH PROGRAM          11/13/72
DO YOU WANT PROGRAMMATIC INSTRUCTIONS--YES OR OCK
YES
THE OPTIONS ARE 0 = DISPLAY OR CHANGE DATA ON FORMULA FILE
                1 = SEARCH FOR MATCHING STANDARDS
                2 = PRINT DATA OF STANDARDS MATCHING THE UNKNOWN
                3 = PRINT DATA OF A SPECIFIC SERIAL NUMBER
                4 = ALTER INPUT DATA IN MIDSTREAM
                5 = REVERSE STATUS OF WIGGLE-THE TOLERANCE BOOLEAN
                6 = RE-INITIALIZE FOR A NEW SAMPLE
                7 = GIVE TIME TOTALS FOR THIS SAMPLE
                8 = TERMINATE THE PROGRAM
                9 = ADD STATE POLICE STANDARDS TO ADD./FORMULAE
               10 = ADD MED. EXAMINER STANDARDS TO ADD./FORMULAE
               11 = DISPLAY OR CHANGE DATA ON ADD./FORMULAE FILE
               12 = EXPLANATION OPTION
N.B. AT ANY POINT (OPTION) MAY BE KEYED IN TO GET BACK TO THE
     POINT WHERE YOU MAY SELECT 1 OF 13 OPTIONS.  (OPTION...)
     WILL APPEAR, IN RESPONSE TO WHICH YOU KEY IN DESIRED OPTION
     NUMBER AND AN OCK.  ALL OPERATOR ENTRIES MUST TERMINATE
     WITH OCK TO ALLOW TRANSMISSION TO THE COMPUTER.
     SHOULD YOU LEAVE THE TERMINAL, OR NOT INPUT ANYTHING, FOR
     APPROXIMATELY 8 MINUTES THE PROGRAM WILL TIMEOUT AUTOMATICALLY
     SAYING (TIME LIMIT EXCEEDED).  TO END THE PROGRAM MORE QUICKLY
     SELECT OPTION 8
     FOR A MORE DETAILED EXPLANATION OF THE OPTIONS CONTROLLING
     THIS PROGRAM SELECT OPTION 12.

SAMPLE...

*** TIME LIMIT EXCEEDED ***


END OF PROGRAM..
```

APPENDIX C

NEW YORK STATE POLICE SCIENTIFIC LABORATORY

EVALUATION REPORT

STATE OF NEW YORK

NEW YORK STATE POLICE
STATE CAMPUS
ALBANY, N. Y., 12226

SCIENTIFIC LABORATORY

March 23, 1972

Frank G. Madrazo, Associate Research Criminalist
Criminalistics Research Bureau
New York State Identification & Intelligence System
Executive Park Tower, Stuyvesant Plaza
Albany, New York

Dear Frank:

Enclosed herewith is our report of progress, to date, using the infrared data file. In it, we have set forth some conclusions and suggested system improvements - both for the purpose of providing you with a solid basis on which to determine the future direction of the program.

We are most optimistic about the program and are looking forward to its continuance and the continuance of the scientifically productive relationship with the Criminalistics Research Bureau of NYSIIS.

Sincerely yours,

S. Ferriss
Captain
Director

SF:r
Enc.

The New York State Police Scientific Laboratory has been cooperating, since October, 1971, with the NYSIIS Criminalistics Research Bureau (CRB) in a Federally funded program of NYSIIS, a program designed to demonstrate the feasibility of a remote access infrared data file. The project's major goal has been to determine if such a file can aid forensic science laboratories in identifying unknown evidentiary materials.

Under the terms of the grant, NYSIIS provided the State Police Laboratory with a Burroughs TC-500 computer terminal together with its associated telephone communications lines, a search program, access to the infrared data file and computing time on the Burroughs B-6500 computer system. Training in the use of the equipment and other technical services were also provided by the CRB and NYSIIS programming staff.

The State Police Laboratory provided technical personnel to perform file searches in both test and production modes. These personnel were asked to evaluate systems from the viewpoint of the operating forensic science lab and to provide input to NYSIIS Criminalistics Research Bureau personnel so that appropriate systems modifications could be designed.

The search system became operational in mid-October, 1971, and consists of a TC-500 computer terminal connected from the State Police Laboratory by direct telephone wire to the B-6500 at NYSIIS headquarters. The infrared data file stored at NYSIIS consists of data collected by the American Society for Testing and Materials from more than 88,000 organic chemical compounds.

An initial test series of 100 tests, conducted by two Senior Chemists with considerable infrared experience, soon established that the search program could, in fact, make "hits" on samples commonly encountered by forensic laboratories. This test series also served to furnish a genuine sense of confidence to all of the program participants.

Since the initial test period, the file has been used on about 50 actual forensic cases, representing approximately 150 searches. Nineteen unknown samples were identified which would not have been identifiable without the aid of the program.

The types of compounds that have been identified have varied greatly. It has been successful in identifying many narcotics and dangerous drugs, and has been used in toxicology for the identification of poisons. Success has also been achieved in the area of paints, dyes, pigments and polymers. It also has been useful in the identification of components of bombs and various high explosives. The system has, in fact, been used in practically every area of the Laboratory.

Based on the results of approximately five months of operation, the following conclusions have been reached:

1. The system, as it presently exists, is of definite assistance in forensic infrared data interpretation. Its real value has not been to speed up routine cases, but rather to provide an extended capability in those cases which involve new or unfamiliar problems.

2. The program is easy to use and usually leads to a meaningful answer within ten minutes after the unknown data is obtained from an infrared spectrophotometer.
3. The nature of forensic laboratory work requires ready access to the infrared file, thus the central computer system must be constantly available for searching. If the computer is "down", valuable time is lost, and the operator easily becomes frustrated with the system. After an initial shakedown period during which much "downtime" and frustration was experienced, the overall reliability of the system improved significantly and now appears to be well within the desirable limits of availability.
4. Based on experiences to date, the estimated normal use of the infrared search system is expected to be from 30 to 40 cases per month, requiring from 100 to 120 actual searches of the file per month.

Our operational experience with the file leads us to recommend the following system improvements:

1. Samples run at our Laboratory and the same samples coded in the file vary, apparently caused by differences in both the quality of the spectrums and the differences in sample preparation. Therefore, the addition of a forensic science subfile of data obtained at our Laboratory is suggested. Such

a file would increase the effectiveness of the file in meeting our data interpretation needs.

2. Modifications should be made in the search program to make it more "forgiving" when erroneous search data is entered. As the program is constructed now, fifteen correct items and one incorrect piece of data will result in a miss. If the program were more flexible, our "hit" rate would be increased.

3. To confirm an identification, the examiner should have available a "hard copy" of the standard infrared curve for use in a visual comparison with the unknown curve.

   There is no access to such a hard copy with the present system. Although our Laboratory maintains some hard copies of selected infrared spectrums, the retrieval operation for those curves is cumbersome and represents the greatest time lost in the system.

   Thus, a major improvement in the system would be for our Laboratory to have access to hard copies of all the standards in the file through an automatic or semi-automatic retrieval system. With such a system, the actual copy of the known infrared spectrum could be rapidly compared with the unknown spectrum - making confirmation of identification a simple matter.

4. Based on our experience to date with infrared file, we believe that the concept of storing scientific data in a computer and retrieving it when needed is certainly feasible. File effectiveness would be greatly enhanced if additional files could be created to store additional data such as: ultraviolet data, gas-liquid and thin-layer chromatography data, color and crystal test data. We could then correlate all of these different types of data into a complete cross-referenced master search and retrieval program.
5. Potentially, the TC-500 type computer terminal, because it has its own memory capability, could be utilized for various off-line applications.

The development areas delineated in the preceding paragraphs indicate that future development of this file concept will require a combination of systems studies, design of file update procedures, computer programming modifications and laboratory production of reference standards. In our opinion, these types of tasks could be most efficiently accomplished through a cooperative effort between the NYSIIS CRB and the forensic science laboratories that utilize the central files.

APPENDIX D

NEW YORK CITY MEDICAL EXAMINER'S LABORATORY

EVALUATION REPORT

The City of New York

OFFICE OF CHIEF MEDICAL EXAMINER
520 FIRST AVENUE, NEW YORK, N. Y. 10016
Telephone: 212-684-1600

MILTON HELPERN, M.D., *Chief Medical Examiner*

March 22, 1972

Mr. Frank G. Madrazo
Associate Research Criminalist
State of New York
Executive Department
Identification & Intelligence
System
Executive Park Tower
Stuyvesant Plaza
Albany, New York 12203

Dear Mr. Madrazo:

In answer to your request for an evaluation of the NYSIIS Pilot Infrared Data File program, my only criticism is that it does not go far enough. Otherwise, from my limited knowledge of the various programs sponsored and supported by the State in its effort to combat crime, yours is the most constructive and potentially useful that I know of.

The New York City Medical Examiner's Laboratory has tried for years to collect the necessary data for carrying out medico-legal work without any provision for personnel other than the routine and with no financial support. Additionally, there has been no time allotted for experimentation. In fact, some years ago when I attempted to incorporate research into the operational part of the table of organization, I was told that research is a dirty word in City Hall.

Unfortunately, few people in government other than the lower level scientific personnel have any concept or appreciation of the necessity of collecting, filing, and retrieving basic data. I will be very happy to appear before or to write to any body or committee to discuss the need for computerized data storage and retrieval services for the toxicology or medico-legal fields. The type of program you have initiated can only be maintained by the State or Federal governments. If your experience is anything like mine, your major problem is to convince those that control the finances of the necessity of the work being done.

You included seven questions for comment in your letter to me. Following are my comments:

1. The concept of central files is not only invaluable in toxicology, but also in all scientific work involving criminal investigations. In the limited time the tie line between our laboratories has been in operation, we have had positive computer findings on many samples of material whose identity was unknown to us at the time. Computer data provided confirmation of suspected identity and, of equal importance, ruled out substances which our previous testing had indicated. Information that a chemical substance is not what is suspected can sometimes be just as important as positive identifications.

2. With regard to IR in combination with gas chromatography, I would estimate that the overall effectiveness of IR would be increased by a factor of three to four. The major problem in identifying chemicals isolated from tissue and body fluids with IR is purity of the sample. With IR following gas chromatography, much better specimens would be analyzed. The limits would depend on the limiting sensitivity of the microtechnique employed.

3. In view of the success of the pilot program and the potential for further development of the central file concept, I incorporated $3,000 into the laboratory budget which becomes available in July 1972 for maintaining the TC-500 terminal and associated telephone lines.

4. The present system for file maintenance works very efficiently. In my opinion, laboratory programming is a highly specialized science and could not be justified as a function for our laboratory. Nor do I see the need for other than a centrally operated location available to a number of laboratories.

5. Our laboratory doesn't have time nor the personnel to maintain even a rudimentary cabinet filing system. The problems of work overload and limited personnel is universal in all technical organizations that I know of. Our staff, which is the largest, nor the staffs of any of the others in this field, has the time for programming even if they had the expertise.

6. As previously discussed, computerized data for toxicology should be expanded to include ultraviolet spectrophotometry, gas chromatography, thin layer chromatography and micro-color reactions.

Attached is a partial list of laboratory cases requiring an IR search since inception of the program. This list is by no means complete, but is representative of the types of samples worked on by the laboratory and the results achieved through use of the file.

Within this list there are some very important cases that would not have been finalized without the aid of the computer. Also, I would like to point out that in some of these cases in which normal tissue is indicated the IR provided invaluable information to us in that they show that the samples submitted did not contain drugs as we had suspected, or that they were too impure for accurate chemical evaluation.

Sincerely yours,

Charles J. Umberger
Chief Toxicologist

Attach.
CJU:cki

REPRESENTATIVE CASES REQUIRING IR DATA SEARCH

	CASE	IDENTIFICATION
1.	5528/71 stomach - acid extraction (sublimated)	Noludar
2.	5228/71 evidence-white tablet-acid-ether extraction	Simethicone
3.	5228/71 evidence-white capsule-acid-ether extraction	Hits 0
4.	Sample from the City of NY-Inspection Division-Purchasing Department-Product of distillation	Formalin
5.	1619/71 stomach-routine acid extraction	Hits 0
6.	1619/71 stomach-routine basic extraction	Hits 0
7.	2221/71 stomach-routine acid extraction	Fatty tissue-normal
8.	2243/71 stomach-routine acid extraction	Fatty tissue-normal
9.	2247/71 stomach-routine acid extraction	Fatty tissue-normal
10.	2258/71 stomach-routine acid extraction	Fatty tissue-normal
11.	2258/71 stomach-routine basic extraction	Fatty tissue-normal
12.	2258/71 stomach-basic extraction-paper chromatogramed	Polyethylene Glycol
13.	2258/71 Urine basic extraction	Hits 0
14.	2547/71 Stomach-acid extraction	Fatty tissue-normal
15.	2830/71 Stomach-neutrals	Fatty tissue-normal
16.	2838/71 Stomach-neutrals	Fatty tissue-normal
17.	3018/71 Stomach acid extraction	Fatty tissue-normal
18.	3688/71 Brain-acid extraction	Fatty tissue-normal

	CASE	IDENTIFICATION
19.	3709/71 Evidence	Isopropyl alcohol
20.	3777/71 Stomach acid-phenols extraction	Secobarbital Amobarbital
21.	3803/71 Stomach acid-phenols extraction	Secobarbital Amobarbital
22.	3825/71 Stomach acid-phenols extraction (sublimated)	Secobarbital Amobarbital
23.	3838/71 Stomach acid-phenols extraction	Pentobarbital
24.	3869/71 Stomach acid-phenols extraction	Pentobarbital
25.	4067/71 Liver-acid extraction-sublimated	Pentobarbital
26.	4127/71 Stomach-acid extraction	Meprobamate
27.	4130/71 Stomach-acid extraction	Acetophenetidine
28.	4199/71 Stomach-acid extraction (sublimated)	Pentobarbital
29.	4512.71 Stomach-acid (sublimated)	Acetophenetidine
30.	5321/71 Stomach-acid (sublimated)	Noludar
31.	Red material found in instant coffee submitted to analysis for possible toxic agent - special case	Abrus seeds
32.	Water sample from CIA (TLC purified)	Alstonine
33.	529/72 Liver-acid (sublimated)	Tissue Absorption (normal)

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