

U.S. DEPARTMENT OF COMMERCE
Office of Inspector General



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*NATIONAL INSTITUTE OF
STANDARDS AND TECHNOLOGY*

*CRADA with the Coblenz Society
Should Receive Greater Scrutiny*

Final Inspection Report No. IPE-13200/February 2001

Office of Inspections and Program Evaluations





UNITED STATES DEPARTMENT OF COMMERCE
The Inspector General
Washington, D.C. 20230

February 23, 2001

MEMORANDUM FOR: Dr. Karen H. Brown
Acting Director
National Institute of Standards and Technology

FROM: Johnnie E. Frazier

SUBJECT: Final Inspection Report: *CRADA with the Coblenz Society Should Receive Greater Scrutiny* (IPE-13200)

As a follow up to our January 5, 2001 draft report, attached is our final report examining the cooperative research and development agreement (CRADA) between the National Institute of Standards and Technology and the Coblenz Society. The report includes comments from your written response, which is included in its entirety as an appendix to the report. We are pleased that you and your staff have agreed with most of our recommendations. However, we are concerned that NIST has not made a commitment to develop policies and procedures for evaluating whether it should undertake a project that may compete with the private sector or for submitting proposed database projects to a peer review. Please provide your action plan addressing the recommendations in our report within 60 calendar days.

We thank your staff for the assistance and courtesies extended to us during our evaluation. If you have any questions about our report or the requested action plan, please contact me at (202) 482-4661, or Jill Gross, Assistant Inspector General for Inspections and Program Evaluations, at (202) 482-2754.

Attachment

cc: Dr. Hratch G. Semerjian, Director, Chemical Science and Technology Laboratory
Dr. Richard F. Kayser, Director, Technology Services
Michael R. Rubin, Deputy Chief Counsel
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EXECUTIVE SUMMARY

In November 1994, the National Institute of Standards and Technology entered into a cooperative research and development agreement (CRADA) with the Coblenz Society, a nonprofit professional organization. The purpose of the CRADA, which is to run for a period of 10 years, was to establish a joint NIST/Coblenz Society infrared spectral database. Infrared spectra are often regarded as the "fingerprint" of a specific chemical substance and are used in a wide range of applications, including the identification of chemical substances and the determination of their amounts.

To develop the database, approximately 10,000 spectra in paper format owned by the Coblenz Society were provided to NIST for scanning and conversion into an electronic format. These spectra are to be combined with approximately 10,000 infrared spectra in NIST's possession to form the database that will be sold by NIST to the public. NIST plans to make the database available in early spring 2001. Over time, NIST and the Coblenz Society intend to increase the size of the collection by soliciting contributions of spectra from the many laboratories—private, government, and academic—where infrared spectra are measured.

The House Committee on Science received a complaint from a private sector firm in February 2000 alleging that the infrared spectral database to be created under NIST's CRADA with the Coblenz Society would unfairly compete with one sold by the firm. After some correspondence between the Committee and NIST regarding the complaint, in May 2000, the Committee's Subcommittee on Technology referred the matter to our office.

After reviewing the complaint, our office decided to perform an inspection of NIST's CRADA with the Coblenz Society. The objectives of our inspection were to determine whether (1) NIST is unfairly competing with the private sector by entering into a CRADA for the purpose of producing and publishing a spectral database, and (2) the CRADA is consistent with the law (15 U.S.C. § 3710a) and an appropriate instrument for this project. A summary of our specific findings follows:

Competition with Private Sector Firms Is Not Prohibited, but the Project Must Be Scrutinized.

Two legislative mandates, the Standard Reference Data Act and NIST's organic legislation, authorize NIST to provide high-quality standard reference data to the scientific community. While neither mandate specifically prohibits the creation of databases that might compete with the private sector, both contain terms that could be interpreted as discouraging NIST from duplicating reference data available elsewhere.

Our review concluded that the NIST/Coblentz Society database will compete with the databases of private sector vendors because both NIST, in its capacity as a database vendor, and the private sector database firms meet most of the same customer needs for infrared spectral databases. In addition, NIST did not perform a sufficient analysis of the merits or drawbacks of the project before proceeding. Specifically, we are concerned that NIST did not adequately assess the need for the database, given other NIST priorities, and whether it would duplicate or compete with data that was already available from other sources. Thus, before any decision is made to make the NIST/Coblentz Society database available to the public, we recommend that NIST perform the planning and analysis that it should have done prior to entering into the CRADA. In addition, because it is NIST and the Coblentz Society's intention to add spectra to the database in the future, we believe that NIST should develop policies and procedures to ensure that any substantial additions are sufficiently publicized and analyzed before proceeding. NIST should also submit such a project expansion, as well as any future database projects of this nature, to a peer review (see page 6).

A CRADA Was Not the Appropriate Instrument for the NIST/Coblentz Society Project. The key criterion for entering into a CRADA was not met in the case of the CRADA between NIST and the Coblentz Society. CRADAs are generally designed to allow federal laboratories to work with nonfederal entities to transfer technologies for future commercial application. However, under this CRADA, no technology transfer is taking place. We believe that for this specific project another type of legal agreement would have been preferable. It is a good management practice to use the most appropriate instrument for any particular project in order to adequately protect all parties and avoid unnecessary complexities. For future database collaborations between NIST and outside entities, NIST should carefully assess its options to ensure that it selects the most appropriate legal instrument for the project (see page 18).

On page 19, we offer recommendations to the NIST Director to address the concerns raised in this report.



In responding to our draft report, the Acting NIST Director stated that the agency is in agreement with our findings and recommendations. We generally agree with NIST's proposed corrective actions. However, as discussed on page 16, we are concerned that NIST has not agreed to put in place the necessary policies and procedures to ensure that future additions to the NIST/Coblentz Society database, as well as any future database projects of this nature, are sufficiently evaluated before proceeding. In particular, we want to ensure that before it decides to proceed with a database project, NIST will, (1) solicit comments from interested parties, such as cognizant scientists and database vendors, and consider those comments when deciding whether to proceed, (2) analyze the need for the

additions and/or a new database in the scientific community, (3) assess the impact of the proposed project on the private sector firms, particularly with regard to competition, and (4) submit proposed projects to a peer review. We are requesting that NIST address this issue in its action plan.

INTRODUCTION

Pursuant to the authority of the Inspector General Act of 1978, as amended, the Office of Inspector General conducted an inspection of the cooperative research and development agreement (CRADA) between the National Institute of Standards and Technology and the Coblenz Society. The inspection was conducted in accordance with the *Quality Standards for Inspections* issued by the President's Council on Integrity and Efficiency. Fieldwork was performed during the period from May through October 2000.

Inspections are special reviews that the OIG undertakes to provide agency managers with timely information about operations, including current and foreseeable problems. Inspections are also done to detect and prevent fraud, waste, and abuse, and to encourage effective, efficient, and economical operations. By asking questions, identifying problems, and suggesting solutions, the OIG hopes to help managers move quickly to address problems identified during the inspection and avoid their recurrence in the future. Inspections may also highlight effective programs or operations, particularly if they may be useful or adaptable for agency managers or program operations elsewhere.

OBJECTIVES, SCOPE, AND METHODOLOGY

The objectives of this inspection were to determine whether (1) NIST is unfairly competing with the private sector by entering into a CRADA with the Coblenz Society for the purpose of producing and publishing a spectral database, and (2) the CRADA is consistent with the law (15 U.S.C. § 3710a) and an appropriate instrument for this project. The scope of this inspection was limited to this specific CRADA, although, for comparison purposes, we also reviewed how NIST creates, markets, and sells other spectral databases.

Our review methodology included interviews with NIST personnel in the Chemical Science and Technology Laboratory, the Standards Reference Data Program, the Office of Technology Partnerships, and the Office of the Deputy Chief Counsel. We also conducted interviews with Coblenz Society personnel, representatives of private sector companies that sell spectral databases, and a number of infrared spectroscopists who are familiar with or work with spectral databases. Technical assistance was provided by staff from the National Science Foundation's Office of Inspector General. Finally, we observed the process NIST is using to digitize the Coblenz Society's paper spectra. At the conclusion of the review, we discussed our findings with the Director, Chemical Science and Technology Laboratory; the Deputy Chief Counsel; the Director, Technology Services; and the Chief, Standard Reference Data Program.

BACKGROUND

In February 2000, the House Committee on Science received a complaint from a private sector firm alleging that the infrared spectral database to be created under NIST's CRADA with the Coblenz Society would unfairly compete with one sold by the firm. After some correspondence between the Committee and NIST regarding the complaint, in May 2000, the Committee's Subcommittee on Technology referred the matter to our office. OIG officials reviewed the complaint and, in late May, decided to perform a review of the allegations.

CRADAs were authorized in 1986 under the Federal Technology Transfer Act (15 U.S.C. §§ 3710a-3710d) to promote technology transfer and the commercialization of federally developed technology by providing the private sector with access to the research and development being done by federal laboratories. CRADAs allow a federal laboratory to agree to grant, in advance, patent licenses, assignments, or options to the CRADA partner for any invention made under the CRADA. In addition, CRADAs provide for the protection of proprietary information and the sharing of any royalties generated.

Infrared spectroscopy is the study of the interaction of light and matter in the infrared region of light. Infrared light, which occurs at lower frequencies than visible light, cannot be observed with the naked eye, and its measurement requires the use of an instrument called an infrared spectrometer. The infrared spectrometer uses infrared light to produce an infrared spectrum, which expresses the degree of interaction between matter and light, in terms of intensity, at a specific frequency over a range of frequencies. Infrared spectra are often regarded as the "fingerprint" of a specific chemical substance. Infrared spectroscopy has applications ranging from fundamental scientific studies of molecular structure to quality control of commercial materials. It has been applied to a range of problems dealing with both the identification and measurement or composition of chemical substances, such as in forensic or crime laboratories. Infrared spectroscopy is also used in education to demonstrate fundamental properties of matter.

The Coblenz Society is a nonprofit organization founded in 1954 to foster the understanding and application of infrared spectroscopy. The idea of NIST working with the Coblenz Society to make the Society's infrared spectra more usable in the digital age was first discussed at a 1982 NIST workshop on standard reference data. However, it was not until November 1994 that a CRADA between NIST and the Society was signed. The CRADA is to run for a period of 10 years. The project to be completed under the CRADA is to establish a joint NIST/Coblenz Society infrared spectral database. The intention of the project is to combine approximately 10,000 gas phase spectra in NIST's

possession¹ with 10,000 condensed phase spectra owned by the Coblenz Society. The joint database would administratively be controlled by NIST.

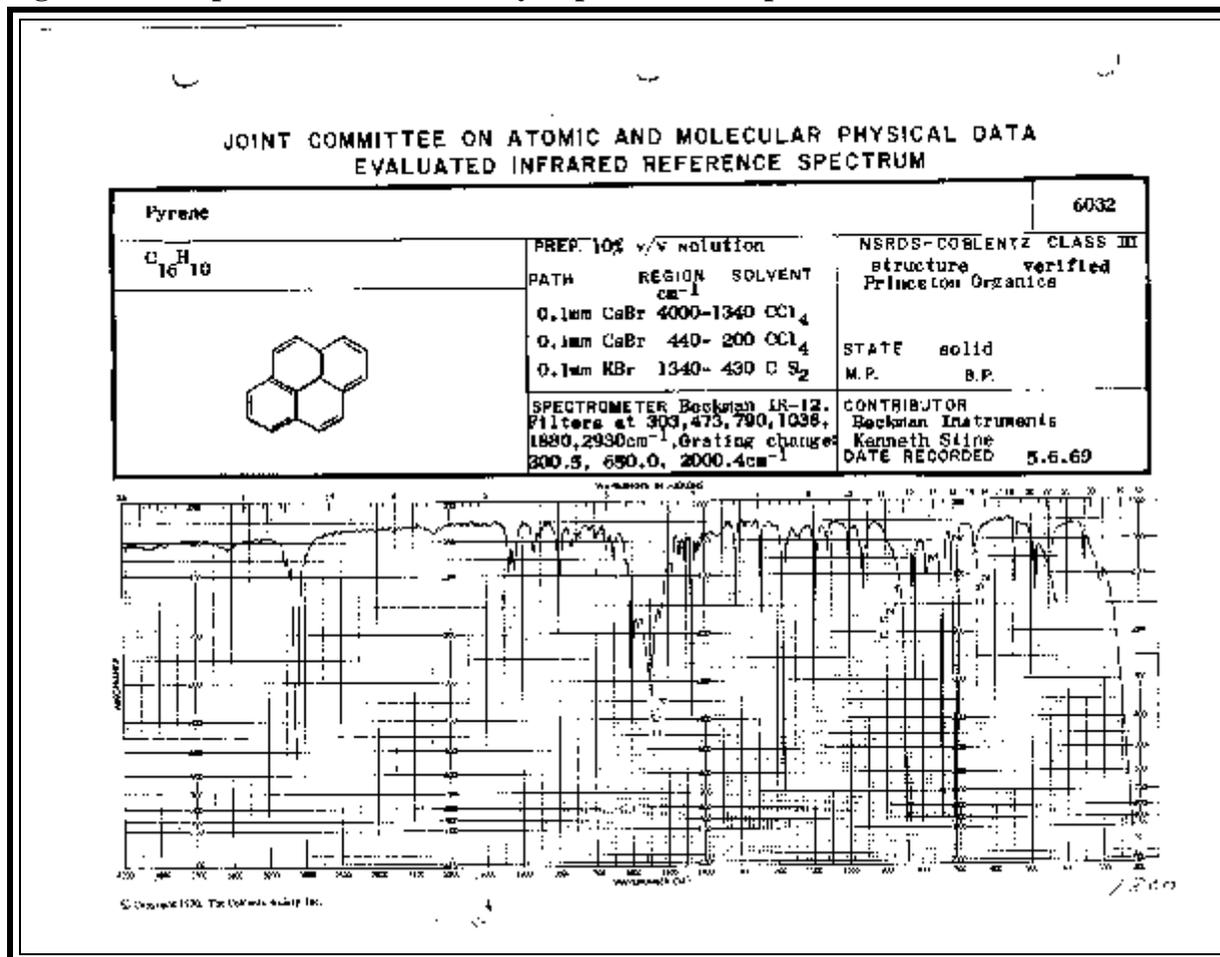
The original intent was that, over time, the two parties would increase the number of spectra in the collection and retain the high quality of the database. To that end, the Coblenz Society was to solicit contributions of spectra from the many laboratories—private, government, and academic—where infrared spectra are measured. Together, NIST and the Society would arrange for the evaluation of all contributed spectra and approve, for inclusion in the database, those which were of high quality and for which there was adequate identifying information.

The 10,000 condensed phase infrared spectra to be contributed to the project by the Coblenz Society are in paper format (see Figure 1) and were all measured using older infrared spectrometers during the 1950s and early 1960s.² The spectra were mostly donated to the Coblenz Society by chemical laboratories and instrument companies for the purpose of fostering the application of infrared spectroscopy and making good reference spectra available for public use. The Coblenz Society's collection of infrared spectra is widely recognized for its quality, particularly in terms of the authenticity and purity of the samples used to generate the spectra and the evaluation of the spectra by experienced infrared spectroscopists to ensure their accuracy.

¹ 5,228 of these spectra are currently sold by NIST as the "NIST/EPA Gas-Phase Infrared Database."

² The older instruments were prism spectrometers and grating spectrometers. The standard and preferred instrument for measuring infrared spectra today is a Fourier transform infrared spectrometer, also called an FT-IR spectrometer.

Figure 2: Example of a Coblenz Society Paper Infrared Spectra



The Coblenz Society has been selling its collection of paper spectra for many years. At least four private sector firms also sell infrared spectral databases, but in a digital format. The databases offered by these firms almost exclusively contain FT-IR spectra. The FT-IR spectra are in electronic format and are of higher resolution and clarity than spectra measured on the older instruments. The databases sold by the private sector firms are used mostly for spectral searching, which involves identifying an unknown compound by comparing it against the numerous spectra contained in the database. Because the Coblenz Society spectra are in paper format, they are being used less frequently since the development of FT-IR spectrometers and spectral searching capabilities. Therefore, a large part of the

effort under the CRADA would be to digitize the paper spectra, using an optical scanner, to make the Coblenz Society's spectra usable for spectral searching.

Even though the CRADA was signed in 1994, little activity occurred on this project until 1997. In August 1997, NIST contracted with a research scientist to evaluate some infrared spectra already in NIST's possession, as well as to digitize the approximately 10,000 paper spectra contributed to the project by the Coblenz Society. The contract runs for four years and has a maximum value of \$396,085. Through October 2000, the contractor had been paid \$257,956 for his work on this project.

All of the Coblenz Society spectra have been digitized. The contractor, NIST staff, and Coblenz Society staff are currently evaluating the spectra for accuracy and adding textual attributes to the electronic files. NIST anticipates that this technical work will take about four more months and should be completed by late winter 2001. During this time, NIST will discuss with Coblenz Society representatives the possibilities for disseminating the database. Any dissemination arrangement will be covered by a written agreement reviewed and approved by all appropriate NIST and departmental authorities. Current plans call for NIST to begin selling the database in early spring 2001.

OBSERVATIONS AND CONCLUSIONS

I. Competition with Private Sector Firms Is Not Prohibited, but the Project Must Be Scrutinized

The primary issue that our office was asked to review was whether NIST was unfairly competing with the private sector by creating an infrared spectral database under a CRADA with the Coblenz Society. Two legislative mandates provide NIST with direction in its efforts to provide high-quality standard reference data to the scientific community—the Standard Reference Data Act and NIST’s organic legislation. While neither mandate specifically prohibits the creation of databases that might compete with the private sector, both contain terms that are open to interpretation. Given the lack of clarity and multiple purposes of the legislative mandates, there are wide differences of opinion among the supporters and opponents of the project, particularly with regard to the pros and cons of digitizing the Coblenz Society spectra, the level of overlap between the NIST/Coblenz Society database and commercial databases, and the format of the database.

Based on our review, we conclude that the NIST/Coblenz Society database will compete with the databases of the private sector vendors. As a result, we believe that before any decision is made to make the NIST/Coblenz Society database available to the public, NIST should perform the planning and analysis that it should have done before it entered into the CRADA. Moreover, NIST’s and the Coblenz Society’s intention is to add spectra, over time, to their database. However, as the database grows, competition between NIST and the private sector database firms will also increase. Therefore, NIST should scrutinize and seek public comment on any planned additions to the database before proceeding. In addition, expansions to this project, as well as any future database projects of this nature, should be subjected to a peer review to ensure that the projects are both needed by the scientific community and will not unfairly compete with private sector databases already on the market.

A. NIST’s legislative mandate does not specifically prohibit the creation of databases that might compete with the private sector

Representatives of four private sector firms that compete in the infrared spectral database market complained to either the House Committee on Science or our office about the unfair competition that would be created by the NIST/Coblenz Society CRADA. In many discussions and in correspondence with our office, representatives of all four firms registered strong opposition to the database being created under the NIST/Coblenz Society CRADA. The firms’ key complaint was that it is inappropriate for NIST to duplicate what is already commercially available.

The Standard Reference Data Act states that NIST should, to the maximum extent practical, avoid duplication in its efforts to collect, evaluate, publish, and disseminate standard reference data. In addition, NIST's organic legislation states that the agency should only compile and disseminate data that is not available with sufficient accuracy elsewhere. Thus, while neither mandate specifically prohibits the creation of databases that might compete with the private sector, they discourage NIST from duplicating reference data that is available elsewhere.

NIST is authorized under the Standard Reference Data Act (15 U.S.C. § 290b) to "provide or arrange for the collection, critical evaluation, publication, and dissemination of standard reference data." However, in carrying out this mandate, NIST should, to the maximum extent practical, "utilize the reference data services and facilities of other agencies and instrumentalities of the Federal Government and of State and local governments, persons, firms, institutions and associations, with their consent and in such a manner as to avoid duplication of those services and facilities."

NIST is also authorized under its organic legislation (15 U.S.C. § 272) to take all actions necessary and appropriate to "determine, compile, evaluate, and disseminate physical constants and the properties and performance of conventional and advanced materials when they are important to science, engineering, manufacturing, education, commerce, and industry and are not available with sufficient accuracy elsewhere." Finally, under the same legislation, NIST may "compile, evaluate, publish, and otherwise disseminate general, specific and technical data resulting from the performance of the functions specified in this section or from other sources when such data are important to science, engineering, or industry, or to the general public, and are not available elsewhere."

Neither of these mandates governing NIST's operations expressly prohibits the agency from creating databases that might compete with the private sector. However, the mandates do imply that NIST should make sufficient efforts not to collect data that is already available with sufficient accuracy elsewhere. In addition, despite the fact that competition with private sector firms is not expressly prohibited by NIST's legislative mandate, competing with the private sector is not something that the U.S. government generally condones. For example, OMB Circular A-76, *Performance of Commercial Activities*, states that "in the process of governing, the government should not compete with its citizens" and that "the Federal Government shall rely on commercially available sources to provide commercial products and services." However, as discussed in detail in the next section, there is a significant difference of opinion among the various parties with an interest in the NIST/Coblentz Society database as to whether NIST is in compliance with its mandate and whether it is unfairly competing against the private sector.

B. Because the NIST/Coblentz Society database will compete with private sector databases, the project should be thoroughly scrutinized before proceeding

We spoke with numerous individuals, on both sides of the debate, who felt strongly that NIST either was in clear violation of its legislative mandate or, conversely, was in full compliance with it. The difference of opinion centered on the two key terms contained in NIST's legislative mandate: "avoid duplication" and "not available with sufficient accuracy elsewhere." These terms are highly subjective and open to interpretation, resulting in the wide differences of opinion that we encountered during our review.

In weighing both sides of the debate, we concluded that the NIST/Coblentz Society database will compete with the database offerings of the private sector database vendors. While it is impossible to quantify by how much the sale of the NIST/Coblentz database will negatively affect the sales of the private sector databases, it is clear that there will be an impact. For this reason, we believe that NIST should scrutinize the propriety of making the database available to the public before taking any action toward that end. We emphasize that such planning and analysis should have been done before NIST ever entered into the CRADA.

The Standard Reference Data Act states that NIST should "avoid duplication" with the reference data services and facilities of other federal agencies, state and local governments, persons, firms, institutions, and associations. Generally, the four private sector database vendors interpret this mandate to mean that NIST should not create databases that contain any of the same spectra that their databases do. Conversely, the parties in favor of the NIST/Coblentz Society database, including NIST officials, interpret the mandate more broadly to mean that NIST should not exactly duplicate other databases. They recognize, however, that when NIST creates a new database, similarities in content are unavoidable.

Similarly, NIST's organic legislation states that the agency should only determine, compile, evaluate, and disseminate scientific data that is "not available with sufficient accuracy elsewhere." Private database vendors contend that they are meeting the needs of the users of infrared spectral databases with high quality products and that there is no need for NIST to add its database to the marketplace. Conversely, NIST and other potential users of the NIST/Coblentz Society database that we spoke to during our review assert that there is a need for high quality, highly evaluated infrared spectra and that private sector database vendors are not adequately meeting that need.

Given the subjective nature of the wording in NIST's legislative mandate, it is not surprising that there are wide differences of opinion about whether the NIST/Coblentz Society database was an appropriate project for NIST to engage in. The debate over NIST's mandate, and the propriety of the creation of the NIST/Coblentz Society database in general, really centers on three primary issues—(1) the pros

and cons of digitizing the Coblenz Society spectra, (2) the level of overlap between the NIST/Coblenz Society database and commercial databases, and (3) the format of the database. In the following sections we discuss these three issues, in considering whether the NIST/Coblenz Society database is needed by the users of infrared spectral databases.

Pros and cons of digitizing the Coblenz Society spectra

As mentioned previously, the Coblenz Society spectra being digitized under the CRADA are from the 1950s and 1960s, and they were measured with prism and grating spectrometers, rather than the current industry standard, the FT-IR spectrometer. There is general agreement that the original spectra are of high quality due to the authenticity and purity of the samples used to obtain the spectra and the expert evaluation performed by Coblenz Society members to ensure their accuracy. However, there is disagreement about whether digitizing the spectra degrades their quality and, as a result, makes them unusable for spectral searching.

NIST and Coblenz Society officials contend that digitizing the older spectra does not degrade their quality. They say that the computer program used to digitize the spectra is extremely accurate. Further, while they admit that there may be some minor issues involved in using the digitized spectra for spectral searching, they intend to disclose those issues in the text file that will be incorporated into the database package. NIST officials also told us that they did not undertake the digitization effort solely to aid in spectral searching. They point out that there are other significant applications that the spectra can be used for such as a wide variety of methods for identifying and studying compounds, addition and subtraction of spectra to reveal additional information about a compound, and spectral simulation to predict spectral features from a chemical structure. Therefore, NIST officials believe that it is worthwhile to provide data from the Coblenz Society collection in digital form for those applications.

Several of the private sector database vendors expressed concern that by digitizing old data, NIST would be misleading the users of the data. They contend that spectra measured with an FT-IR spectrometer are vastly superior in resolution to the digitized Coblenz spectra, but that purchasers of the NIST/Coblenz database may not be aware that they are purchasing digitized prism and grating spectra, although they agree that NIST's plan to notify users of the digitization will help.

The underlying concern here is that because the NIST/Coblenz Society database will likely be sold for a far lower price than that of comparable private sector database vendors, buyers will choose the NIST/Coblenz database over other offerings. The database vendors contend that their experience shows that purchasers of infrared spectral databases tend to purchase based on price, not quality. Thus, the vendors are concerned that they will lose sales. While the extent of this potential problem is

impossible to quantify, NIST does sell other databases, most notably its mass spectral database,³ for less than similar private sector offerings. In the case of the mass spectral database, sales of the private sector firm's offering have reportedly declined over time. The firm told us that since the release of NIST's largest and most recent version of its mass spectral database, sales of its mass spectral database have declined considerably. Therefore, we believe that the private sector database vendors have a valid reason to be concerned.

Another point brought to our attention by one of the database vendors is that approximately 50 percent of the Coblenz Society collection is made up of spectra measured on a prism spectrometer (the other half were measured on a grating spectrometer). The resolution of reference spectra measured on a prism spectrometer is insufficient to define all bands in the short wavelength region of the infrared spectrum. The private sector database vendor contends that this problem means that once the spectra are digitized and used for spectral searching, the user may have difficulty making matches during searching. Several manufacturers of spectrometers also expressed concern that a user having problems searching the NIST/Coblenz Society database may tend to blame the instrument, not the NIST database, because the NIST name implies high quality. They worried that they would be faced with dealing with a number of unhappy customers who were having difficulty searching using the NIST/Coblenz Society database.

NIST officials to whom we spoke about this problem believe that the prism spectra can be effectively used for searching despite the resolution problem in the short wavelength region. However, they stated that because they did not undertake the digitization effort solely to aid in spectral searching, they had no reason to test searching methods to ensure that they would work with the digitized Coblenz Society spectra. Due to the technical complexity of this particular issue, we were unable to ascertain whether spectra measured on a prism spectrometer can effectively be used in spectral searching. Regardless, we are concerned that NIST did not do any research to determine whether this issue may be a problem before proceeding with the project. While the database can be used for purposes other than spectral searching, the searching function is the most widely used. Thus, we believe that NIST should have ensured that the entire database, both the prism and grating spectra, would be usable for spectral searching before proceeding with the project.

³ Mass spectrometry is concerned with the separation of matter according to atomic and molecular mass. It is also used to identify chemical compounds, but is not considered to be as precise as infrared spectroscopy.

Overlap between the NIST/Coblentz Society database and commercial databases

NIST's legislative mandate states that the agency should not "duplicate" standard reference data that is available from other sources. Both NIST and the private sector database vendors agreed, in discussions with our office, that if there was a significant overlap between the Coblentz Society collection and the databases offered by the vendors, NIST would not be in compliance with its mandate. At our request, NIST and one of the private sector database vendors performed separate assessments of how large the overlap might be by taking samples from their respective databases and comparing them to the spectra contained in the other's database. NIST concluded that there was likely a 17-percent overlap, whereas the private sector database vendor found at least a 60-percent overlap.

There is such a wide disparity between the overlap calculations because there are different ways to measure it. For example, a particular compound can be measured in several different solutions or solvents, which may produce some differences in the spectra that may be of interest to a scientist. Under its calculation method, NIST would count the same compound measured in three different solutions as being three distinct spectra. Only if the other database contained the compound measured in the same solution would NIST count the spectra as overlapping. NIST's rationale for its approach is that each spectra, regardless of the solution it is measured in, is unique and as such, has value as a reference spectra. Conversely, the private sector firm would count any of the three spectra, regardless of the solution they are measured in, as overlapping if the same spectrum was found in the other database. The private sector firm's rationale for its approach is that, regardless of the solution they are measured in, the spectra are nearly identical.⁴ Thus, in spectral searching, a compound measured in one solution would be accurately matched with the same compound measured in another solution.

There are also other reasons for the disparity in the overlap, including the fact that NIST only used a portion of the private sector database (approximately 75,000 out of 200,000 spectra) to compare against the NIST/Coblentz Society database. The private sector firm was unwilling to provide NIST with the remainder of the database because the firm's policy is not to give its databases to a competitor, which is what it now considers NIST to be.

Regardless of the actual level of overlap between the NIST/Coblentz Society database and private sector infrared spectral databases, we are troubled by the fact that NIST made no attempt to assess the extent of overlap before proceeding with the project. This should have been an important item to

⁴ There are some compounds that should not be measured in some solutions because the solutions radically alter the spectra. We are presuming that the Coblentz Society collection and the private sector databases do not contain any spectra that were measured in solutions that would dramatically change them.

check to ensure that the project was in compliance with the two key terms in NIST's mandate—to “avoid duplication” and to ensure that the spectra were “not available with sufficient accuracy elsewhere.”

Format of the database

Private sector database vendors currently sell their databases along with proprietary software packages to search and view the spectra contained in the database. Users are able to search and match spectra, as well as view those spectra on the screen, but they are unable to access the underlying computer file containing the data that makes up the spectra. The vendors do not want to release their underlying data files, primarily because they would be very easy to copy and, thus, steal. However, private sector database vendors told us that on the few occasions a user has requested the underlying data files, they have obliged and have provided it for a small fee under a contract that stipulates that the user may not copy or transfer the files to another party.

NIST officials and several other researchers and users of infrared spectral databases that we spoke with contend that it is very important to provide unrestricted access to the underlying data. As a result, NIST intends to release the NIST/Coblentz Society database in the JCAMP-DX format,⁵ which allows a user to view and manipulate the underlying information contained in an infrared spectrum. According to NIST officials, the benefits of having the database in the JCAMP-DX format are that (1) the raw spectral data can be fully utilized by software and data systems developed by any party, thus not tying the user to the proprietary system of the database vendor, and (2) users can freely decide for themselves exactly how they wish to process and examine the data. NIST contends that full availability of the basic data is a key to the development of science and technology in many fields and that enhancing the availability of such data is at the core of its mission and the Standard Reference Data Act.

We agree with NIST's position that, if the agency is going to produce and make standard reference data available, it should be in a format that can be most widely used. However, before proceeding with the project, NIST did not determine whether the databases currently available from private sector firms are or could be made available in the JCAMP-DX or other open format. In fact, the smallest of the private sector database firms does release its data in the JCAMP-DX format. And, as stated previously, at least one of the database firms has made the underlying data files available for a nominal fee under a contract.

⁵ Joint Committee on Atomic and Molecular Physical Data Exchange Standards.

Conclusions

Based on our assessment of the above issues, including extensive discussions with all interested parties, we believe that if NIST decides to release the NIST/Coblentz Society database to the public, it will compete with the database offerings of the private sector database vendors. It is important to note that we define competition strictly as the actual and potential rival offerings and substitutes that buyers of infrared spectral databases might consider. Or, put another way, competitors are entities that can satisfy the same customer need. Clearly both NIST, in its capacity as a database vendor, and the private sector database firms meet most of the same customer needs for infrared spectral databases.

In our discussions with buyers and users of infrared spectral databases, we were told that they would likely purchase the NIST/Coblentz Society database for two primary reasons—the database’s high quality in terms of critical evaluation and its low price. However, most users stated that they would also continue to purchase one of the databases offered by the private sector database vendors. Because the NIST/Coblentz Society database will initially contain only 10,000 condensed phase spectra,⁶ the database will need to be supplemented with one or more of the private sector database offerings, some of which contain well over 100,000 spectra. It is impossible to quantify how much sales of the private sector databases will be affected by the sale of the NIST/Coblentz Society database. It is clear, however, that there will be an impact, and it will likely be more of an impact on the smaller vendors than the larger ones. While NIST officials recognize that there may be some impact on the database vendors’ sales, they stated that the database vendors are eligible to become licensed distributors for all of NIST’s databases, including the NIST/Coblentz Society database. As licensed distributors, the vendors would be able to sell NIST’s databases at a profit.

Given the fact that the NIST/Coblentz Society database will compete with the database offerings of the private sector database vendors, we believe that it is prudent for NIST to proceed cautiously. While recognizing that NIST’s mandate does not specifically preclude competition with the private sector, it is important to emphasize that OMB Circular A-76 states “the government should not compete with its citizens,” and if NIST chooses to publish and sell the NIST/Coblentz Society database, it could well be in violation of this directive. Therefore, we believe that NIST should thoroughly scrutinize the propriety of making the NIST/Coblentz Society database available to the public before taking any action toward that end. Specifically, NIST should perform the analysis that it should have performed before entering

⁶ There will also be 10,000 gas phase spectra in the NIST/Coblentz Society database. However, according to database users and sellers alike, condensed phase spectra are much more widely used, and their presence in the database would be the primary reason to purchase it.

into the CRADA. This would first include reviewing whether the prism spectra in the database are suitable for spectral searching. If the prism spectra cannot be used for spectral searching, NIST should notify potential users of this fact before they purchase the database. Second, NIST should determine what the level of overlap is between the NIST/Coblentz Society database and commercial databases and whether the level of overlap is sufficiently low to justify making the NIST/Coblentz Society database available in the marketplace. We recognize that NIST will require the cooperation of the private sector database vendors to meet this recommendation. We urge NIST to work with the database vendors to obtain copies of their databases or otherwise determine the most accurate level of overlap before proceeding any further with this project.

The Acting NIST Director's written response to our draft report stated that NIST accepts this recommendation and, based on currently available information, believes that the NIST/Coblentz Society database should be made available to the public. Specifically, the agency has determined that prism data are quite suitable for searching, but will prepare a technical note providing detailed instructions on the use of the database for spectral searching. In addition, as stated above, NIST's analysis shows that 17-percent of the compounds (in the same physical state) in the NIST/Coblentz Society database are found in the largest commercially available database. NIST will request access to other commercial databases to carry out similar analyses. We urge NIST to ensure that it has sufficiently addressed these issues before proceeding.

C. Substantial future additions to the database, and future database projects, should be well publicized and analyzed

NIST and the Coblentz Society's intention is to add spectra, over time, to the their database. As discussed previously, because of the current size of the NIST/Coblentz Society database, users may still purchase one or more of the private sector databases to supplement the spectra found in the NIST/Coblentz Society database. However, if the NIST/Coblentz Society database grows, competition between NIST and the private sector database firms will become more pronounced. Users may eventually be able to just purchase an expanded NIST/Coblentz Society database, thus seriously reducing the market or sales for the private firms' databases. Therefore, if NIST does determine it is appropriate to proceed with the initial offering of 20,000 spectra in the NIST/Coblentz Society database, it must also be judicious in how and when it makes additions to the database. To that end, additions to the database should be well publicized and scrutinized by NIST before proceeding. In addition, NIST should submit such a project expansion, as well as any future database projects of this nature, to a peer review.

As discussed in the previous section, NIST performed no analysis before entering into the CRADA. For example, no peer review of the scientific and commercial merits and/or drawbacks of the project

was done, and NIST's intention to enter into the CRADA was not publicly announced, thus denying interested parties an opportunity to comment. Because no analysis was done, several issues, such as the overlap issue, have not been adequately addressed. Yet, the project is nearly complete, and NIST and the Coblenz Society have both invested a great deal of time and, in NIST's case, funding in the project. While this lack of analysis is unsatisfactory from a management perspective, such analysis is not currently required by NIST. NIST has no policies and procedures for evaluating whether it should undertake such a project that may compete with the private sector. At a minimum, it should have an internal review process that considers that issue as well as the relative merits of different potential uses of NIST's resources.

While NIST may not have been in violation of its own policies and procedures when it entered into the CRADA with the Coblenz Society without doing sufficient analysis, it was in violation of OMB Circular A-130, *Management of Federal Information Resources*, which states that "agencies shall plan in an integrated manner for managing information throughout its life cycle." It further states that agencies shall "consider the effects of their actions on members of the public and ensure consultation with the public as appropriate" and "seek to satisfy new information needs through interagency or intergovernmental sharing of information, or through commercial sources, where appropriate, before creating or collecting new information." In addition, the circular states that "...improvements to existing information systems and the development of planned information systems" should not "duplicate information systems available within the same agency, from other agencies, or from the private sector."

Finally, OMB Circular A-130 requires that agencies develop internal agency information policies to conform to the circular. The Department of Commerce's information technology policies are contained in the *Commerce Information Technology Management Handbook*. The handbook requires that Commerce's operating units seeking to acquire information technology resources conduct a requirements analysis, which is to include an analysis of the available alternatives. The handbook encourages operating units to rely on the private sector, where appropriate, to provide information technology resources.

According to the Department's Office of the Chief Information Officer, the policies of Circular A-130 and the Information Technology Management Handbook clearly apply to NIST's requirement for an infrared spectral database. A requirements analysis should have been prepared addressing all the available alternatives, including whether the need could have been met through the use of existing databases from the private sector database firms. The threshold for departmental review and approval of NIST's information technology requirements is \$500,000. Below this threshold, NIST is not required to get departmental approval, but the agency is still required to document the requirement. NIST did not meet this requirement.

NIST's lack of planning and analysis should not continue with any future additions to the NIST/Coblentz Society database, nor with any future database projects of this nature. More specifically, NIST should not proceed with any expansion of the database without carefully evaluating the merits and consequences of any future additions to the database. It is even more important that this evaluation be done on future additions because, as the database grows, it represents greater competition with the databases offered by the private sector database firms. Therefore, we believe that for any substantial future additions to the NIST/Coblentz Society database, as well as any future database projects of this nature, NIST should develop policies and procedures to ensure that it will (1) publicize the proposed project in the Federal Register, (2) solicit comments from interested parties, such as cognizant scientists and database vendors, and consider those comments when deciding whether to proceed, (3) analyze the need for the additions and/or a new database in the scientific community and the impact of the proposed project on the private sector firms, particularly with regard to competition, and (4) submit proposed projects to a peer review, and (5) conduct a requirements analysis, as required by the *Commerce Information Technology Management Handbook*.



In responding to our draft report, the Acting NIST Director stated that the agency accepts our recommendation. We are encouraged that NIST has agreed to place a notice of its proposed projects in the Federal Register. However, we are concerned by the agency's comment that items (2) and (3) are part of NIST's normal procedure for project evaluation and selection. While NIST officials told us during our review that they had discussed the proposed database with experts in the field of infrared spectroscopy, such consultations were not held with the database vendors. In addition, NIST did not perform any sort of analysis to assess the impact of the NIST/Coblentz Society database on private sector firms, particularly with regard to competition. As stated on page 15, NIST does not have any policies and procedures for evaluating whether it should undertake such a project that may compete with the private sector. Therefore, we question whether items (2) and (3) are always part of NIST's normal procedures for evaluating and selecting database projects. We request that NIST, in its action plan, clearly set forth what policies and procedures it intends to put in place to fully meet the intent of our recommendation.

In its response, the agency also stated that it views peer review as expert peers participating in workshops and other meetings organized to develop technical plans. However, in our recommendation, we use the term to mean that proposed projects are evaluated by a team of qualified independent reviewers, using established criteria, to determine the merits and drawbacks of projects. After its review, the peer review team would make recommendations to NIST management as to whether the projects should proceed. In its action plan, we request that NIST further explain what

specific policies and procedures it intends to put in place to ensure that its peer review of proposed additions to the NIST/Coblentz Society database and future proposed database projects meets the intent of our recommendation.

Finally, we ask that NIST clarify its comment that by responding to our recommendations, it “will also fulfill the policy objectives of the Department of Commerce set out by the *Commerce Information Technology Management Handbook*.” We are reaffirming our recommendation that NIST’s policies and procedures for assessing any additions to the NIST/Coblentz Society database, as well as similar database projects, stipulate that a requirements analysis be performed, not just that the policy objectives of the Department are met. Therefore, we request that NIST clarify, in its action plan, whether or not it intends to perform the requirements analysis as is required by the handbook.

II. A CRADA Was Not the Appropriate Instrument for the NIST/Coblentz Society Project

For the CRADA between NIST and the Coblentz Society, we found that the key criterion for entering into a CRADA was not met. Specifically, CRADAs are designed to allow federal laboratories to work with nonfederal entities to transfer technologies for future commercial application. However, no technology transfer is taking place on this project. The Coblentz Society provided its paper spectra to NIST, and NIST contracted with a research scientist to digitize those spectra. Representatives of the Coblentz Society are not learning how to use the spectra scanning and conversion program, nor is NIST transferring the program to the Coblentz Society for its use in commercial applications.

Also, the use of a contractor to digitize the Coblentz Society spectra does not conform to NIST policy. According to NIST's Administrative Manual, specifically the section covering CRADAs, non-NIST employees are not to participate in CRADAs unless an exception is authorized in writing by the appropriate official. This policy is in place mainly to protect NIST and the CRADA partner from problems in invention rights and protection of proprietary information. For this CRADA, no exception was authorized in writing. In addition, the CRADA did not contain the required "Disclosure of Proprietary Information" clause giving NIST consent to release the Coblentz Society's spectra to the contractor for the purposes of carrying out the CRADA. However, because the appropriate "rights and data clause"⁷ was contained in the contract with the research scientist, there was no negative impact resulting from the violation of the policy.

Instead of using a CRADA, a more appropriate instrument for this project would have been an agreement similar to those used for other database projects under the Standard Reference Data Program. Both the Director of that program and NIST's Deputy Chief Counsel agreed that a CRADA was not the right instrument for this project. These NIST officials stated that using another type of legal agreement would have permitted the use of a contractor without having to obtain written authorization from the CRADA partner. We believe that it is a good management practice to use the most appropriate instrument for a particular project. Therefore, we believe that for its future database collaborations with outside entities, NIST should carefully assess its options to ensure that it selects the most appropriate instrument for the project.

The Acting NIST Director's written response to our draft report stated that NIST accepts our recommendation and that although a CRADA was legally permissible, in hindsight it was not the most appropriate instrument for the project.

⁷ Federal Acquisition Regulation (48 CFR Chapter 1) clause 52.227-14 "Rights in Data-General" (June 1987.) This clause allocates to the government unlimited rights to all data created under the contract.

RECOMMENDATIONS

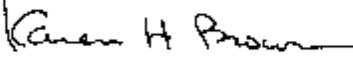
We recommend that the Director, National Institute of Standards and Technology, direct appropriate officials to take the following actions:

1. Determine whether the NIST/Coblentz Society database should be made available to the public. The decision-making process should, at a minimum, include an analysis to determine:
 - C whether the prism spectra in the database are suitable for spectral searching. If the prism spectra cannot be used for searching, NIST should notify potential users of this fact before they purchase the database; and
 - C what the level of overlap is between the NIST/Coblentz Society database and commercial databases, and whether the level of overlap is sufficiently low to justify making the NIST/Coblentz Society database available in the marketplace. NIST should work closely with the database vendors to obtain copies of their databases or otherwise determine the most accurate level of overlap (see page 13).

2. For any substantial future additions to the NIST/Coblentz Society database, as well as any future database projects of this nature, develop policies and procedures to ensure that:
 - C proposed projects are publicized in the Federal Register,
 - C comments are solicited from interested parties, such as cognizant scientists and database vendors, and those comments are considered when deciding whether to proceed,
 - C the need for the additions and/or a new database in the scientific community is analyzed and the impact of the additions on private sector firms is considered, particularly with regard to competition,
 - C proposed projects are submitted to a peer review, and
 - C a requirements analysis is conducted, as required by *the Commerce Information Technology Management Handbook* (see page 16, 17).

3. For future database collaborations between NIST and outside entities, carefully assess available options to ensure that the most appropriate legal instrument is selected for the project (see page 18).

APPENDIX
NIST Response to Draft Report

		<p>UNITED STATES DEPARTMENT OF COMMERCE National Institute of Standards and Technology Gaithersburg, Maryland 20899- OFFICE OF THE DIRECTOR</p>
<p>FEB - 5 2001</p>		
<p>MEMORANDUM FOR Jill Gross Assistant Inspector General for Inspections and Program Evaluations</p>		
From:	Karen H. Brown Acting Director	
Subject:	Draft Inspection Report No. IPE 13200 CRADA with the Coblenz Society Should Receive Greater Scrutiny	
<p>Thank you for the opportunity to review the subject draft inspection report examining the cooperative research and development agreement (CRADA) between the National Institute of Standards and Technology (NIST) and the Coblenz Society. Following are the draft report's three recommendations and our responses to those, as well as comments on some other statements made in the report.</p>		
<p>A. Recommendations and NIST Responses</p>		
<p>We recommend that the Director, National Institute of Standards and Technology, direct appropriate officials to take the following actions:</p>		
<p>1. Determine whether the NIST/Coblenz Society database should be made available to the public. The decision-making process should, at a minimum, include an analysis to determine:</p>		
<ul style="list-style-type: none">▪ whether the prism spectra in the database are suitable for spectral searching. If the prism spectra cannot be used for searching, NIST should notify potential users of this fact before they purchase the database; and▪ what the level of overlap is between the NIST/Coblenz Society database and commercial databases, and whether the level of overlap is sufficiently low to justify making the NIST/Coblenz Society database available in the marketplace. NIST should work closely with the database vendors to obtain copies of their databases or otherwise determine the most accurate level of overlap (see page 13).		
		

NIST Response

NIST accepts this recommendation. NIST has determined, based on currently available information, that the NIST/Coblentz Society database should be made available to the public. We have analyzed the suitability of prism data for searching, and the level of overlap between the NIST/Coblentz and commercial databases, and:

- We have determined that prism data are quite suitable for spectral searching. NIST will prepare a technical note providing detailed instructions on the use of these data for spectral searching; and
 - Our analysis indicates (as pointed out on page 11, paragraph 1, of the report) that approximately 17 percent of the compounds (in the same physical state) in the NIST/Coblentz database are found in the largest commercially available database, a very low level of overlap. NIST will request access to other commercial databases to carry out similar analyses.
2. For any substantial future additions to the NIST/Coblentz Society database, and any future database projects of this nature, develop policies and procedures to ensure that:
- proposed projects are publicized in the *Federal Register*;
 - comments are solicited from interested parties, such as cognizant scientists and database vendors, and are considered when deciding whether to proceed;
 - the need for the additions and/or a new database in the scientific community is analyzed and the impact of the additions on private sector firms is considered, particularly with regard to competition;
 - proposed projects are submitted to a peer review; and
 - a requirements analysis is conducted, as required by the *Commerce Information Technology Management Handbook* (see page 15).

NIST Response

NIST accepts this recommendation. The second and third items are, in fact, part of our normal procedure for project evaluation and selection, and we will place a notice of proposed projects in the *Federal Register*. Peer review is generally an integral part of the second and third items; that is, expert peers participate in the workshops and other meetings organized to develop technical plans.

By responding to the above recommendations, we feel that NIST will also fulfill the policy objectives of the Department of Commerce set out by the *Commerce Information Technology Management Handbook*.

3. For future database collaborations between NIST and outside entities, carefully assess available options to ensure that the most appropriate legal instrument is selected for the project (see page 17).

NIST Response

NIST accepts this recommendation.

B. Other Comments

We also would like to address some other statements made in the report.

On page ii, paragraph 1, the report states that "the NIST/Coblentz Society database will compete with the databases of private sector vendors because both NIST, in its capacity as a database vendor, and the private sector database firms meet most of the same customer needs for infrared spectral databases." On page 11, paragraph 4, the report states that "NIST made no attempt to assess the extent of overlap before proceeding with the project." However, on page 8, paragraph 4, the reviewers point out that "NIST and other potential users of the NIST/Coblentz Society database that we spoke to during our review assert that there is a need for high quality, highly evaluated infrared spectra and that private sector database vendors are not adequately meeting that need."

Indeed, the need for high quality digital data was brought to the attention of NIST by the Coblentz Society, which represents a significant fraction of the infrared spectroscopists in the United States. The NIST Workshop on National Needs for Molecular Spectroscopy, held in December 1996, reaffirmed the community's need for such data to provide them with the ability to analyze and manipulate spectral information. Interactions at subsequent scientific meetings and conferences continued to convince us of the need for such data. Therefore, we feel that NIST performed sufficient research on the need for additional high quality, digital infrared data.

NIST agrees that although a CRADA was legally permissible, in hindsight a CRADA may not have been the most appropriate instrument for this project. The decision to use a CRADA was based upon the information available to NIST and procedures followed by NIST in 1994, and appeared at that time to be completely appropriate. After 1994, however, numerous changes were made to the work of the CRADA, many the result of the untimely death of the NIST principal investigator. Moreover, as pointed out on page 17, paragraph 2, "there was no negative impact resulting" from the use of a CRADA. Since the signing of the Coblentz CRADA in 1994, NIST has significantly improved its internal review processes to lessen the likelihood of such occurrences in the future.