Abstract

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Equation (3)

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3.2.1 Fluorescence Correction of Absorbance Measured Inside the IS

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Table 1 Properties of 2.0 μm microspheres at 266 nm obtained from the fit of the L-M apparent cross section to the absorbance measurements

4. Conclusion

5. References

[1]
[2]
[3]
[4]
[5]
[6]
Footnote

1 Authors

OMNIDATA and the Computerization of Scientific Data

NBS pioneers computerized scientific data management

OMNIDATA established

Use by outside organizations

Chemical Information System (CIS)

The Standard Reference Data program

Computerized materials data

Materials Property Data Network (MPDN)

Microsoft Windows operating system and the Internet explosion

The forefront of computerizing scientific data

Joseph Hilsenrath

Bettijoyce Breen

John Rumble, Jr

Bibliography

[1]

[2]

[3]

[4]

[5]

[6]

NEXT

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Story

**NIST Scientific Data for Data Science**

The recent NIST Data Science Symposium identified the need for NIST to publish their scientific data for data science to support their Big Data at NIST Workgroup use cases.

In the broader context, NIST and other agencies need to support the following Federal Government Initiatives:

- Big Data
- Digital Government Strategy
- Public access mandated for "scientific results" supported by the U.S. government
- Federal agencies have submitted their "initial plans" for public access to scientific data to OSTP
• Digital Object Architecture: One result will be to make the scientific record into a first class scientific object

The author has suggested that all of these can be addressed with agency digital content by following the Data Mining Standard (see below).

Figure 2-2.png

NIST Supports its employees and others with the following Information Services:

• Research Library
• Publishing Services
• NIST Museum and Archives

The NIST Digital Archives (NDA) present images of NIST Museum artifacts and full-text NIST publications:

• NBS Bulletins
• Journal of Research of NIST
• NBS-NIST Directors
• NBS-NIST Histories
• NBS Circulars and Reports

My current Data Science for VIVO IVMOOC Part II work is to pilot NIST Scientific Data for Data Science and present it at the Federal Big Data Working Group Meetup using the Data Mining Standard. I examined the IVMOOC Federal Library Collection Analysis and its data from the Federal Library Bibliographic Records Analysis 2013, and concluded that the NIST Digital Archives would be a better source of data.

Applying the Data Mining Standard here:

• Business Understanding:
  ◦ NIST Mission (standardize measurement)
• Data Understanding:
There are three modeling approaches the Federal Big Data Working Group Meetup semantic data science teams are using:

- **Semantic Medline**
  - Semantic MEDLINE Query: mesothelioma and Data Science for VIVO
    - http://semanticommunity.info/@api/deki/files/28559/TomRindflesch02272014.doc
    - http://semanticommunity.info/Data_Science/Data_Science_for_VIVO#Semantic_MEDLINE_Query:_mesothelioma

- **Data Papers**:
  - Sepublica 2014: The Semantics for e-science in an intelligent Big Data Context
    - http://sepublica.mywikipaper.org/

- **Nanopublications**:
  - The smallest unit of publishable information: an assertion about anything that can be uniquely identified and attributed to its author.
    - http://nanopub.org/wordpress/?page_id=65

The Evaluation and Deployment examples of each is as follows:

- **Knowledge Base (this Wiki)**
  - Spreadsheet

- **Selected Data Papers**:
  - Measurement of Scattering and Absorption Cross Sections of Microspheres for Wavelengths between 240 nm and 800 nm
  - OMNIDATA and the Computerization of Scientific Data

- **Nanopublication: Extracts from the Data Papers**

The NIST Information Services Office says it will help NIST scientists disseminate their research results, manage references, and navigate the NIST editorial policies and review process using the NIST Virtual Library Publishing Tools, but this is on the NIST internal internet and not available to the public.

MORE TO FOLLOW
NIST Scientific Data for Data Science

http://semanticommunity.info/Data_Science/NIST_Scientific_Data_for_Data_Science

IVMOOC Federal Library Collection Analysis

http://ivmooc.cns.iu.edu/forums/node/385

Federal Library Bibliographic Records Analysis 2013-CoverPage

http://calhoun.nps.edu/public/bitstr...pdf?sequence=1 (PDF)
Fed OCLC Access Data Set Explanation

https://docs.google.com/file/d/0BzGL...ExWWI3NFk/edit (Access)

Federal Library Bibliographic Records Analysis:
Initial Findings, Use Cases, and Recommendations

May 2013
Fed OCLC Access Data Set Summary

IVMOOC Data Science for the Federal Big Data Initiative

http://ivmooc.cns.iu.edu/forums/node/408

NIST Home Page

http://www.nist.gov
NIST Virtual Library

http://www.nist.gov/nvl

NIST Virtual Museum

http://museum.nist.gov
NIST Library Catalog

https://library.nist.gov/uhtbin/cgis...70034/60/502/X

NIST Journal of Research

http://nistdigitalarchives.contentdm...on/p13011coll6
Measurement of Scattering and Absorption Cross Sections of Microspheres for Wavelengths between 240 nm and 800 nm

A. K. Goljanek; L.H. Wong; and Steven Charters
National Institute of Standards and Technology, Gaithersburg, MD 20899

A commercial instrument with a 150 mm integrating sphere 1, designed to measure the scattering and absorption cross sections of microspheres prepared reproducibly, was developed for use in the manufacturing and quality control of microspheres. The instrument has been developed at the National Institute of Standards and Technology (NIST) and is based on the design of an integrating spectrometer created at the Lawrence Livermore National Laboratory (LLNL) 2, 3. The instrument is currently being used at NIST to measure the scattering and absorption cross sections of microspheres, which are in the wavelength range of 240-800 nm.

1. Introduction

In a previous paper [1] referred to in a paper [2], we determined that the Lorenz-Mie (L-M) model applied to a wide range of microspheres. The new data have been evaluated in terms of the L-M model. The results were obtained using a computer program to calculate the L-M model parameters. The L-M model was used to calculate the efficiency of scattering and absorption of light by the microspheres. The results were analyzed using the L-M model, which is a mathematical model that describes the scattering and absorption of light by particles of different sizes and shapes.
Fig. 8. The solid circles show the measured absorbance (denoted by the parameter $a$) at 525 nm for the red and 435 nm for the blue. The solid line shows the expected absorbance for the blue according to Eq. (1). The solid line shows the expected absorbance for the red according to Eq. (2). The dashed line shows the expected absorbance for the red according to Eq. (3). The dashed line shows the expected absorbance for the red according to Eq. (4). The dashed line shows the expected absorbance for the red according to Eq. (5).

Table 1. Properties of 15% microcapsules at 200 nm absorption from the fit of the 525 nm apparent cross section to the absorbance measurement.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Diameter (um)</th>
<th>Red</th>
<th>Blue</th>
<th>Red Scattering Area (nm²)</th>
<th>Blue Scattering Area (nm²)</th>
<th>Red Scattering Volume (nm³)</th>
<th>Blue Scattering Volume (nm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.50</td>
<td>1.76</td>
<td>1.50</td>
<td>1.50</td>
<td>1.76</td>
<td>1.50</td>
<td>1.76</td>
</tr>
<tr>
<td>2</td>
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<td>1.75</td>
<td>1.50</td>
<td>1.50</td>
<td>1.75</td>
<td>1.50</td>
<td>1.75</td>
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<tr>
<td>3</td>
<td>1.50</td>
<td>1.75</td>
<td>1.50</td>
<td>1.50</td>
<td>1.75</td>
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<tr>
<td>4</td>
<td>1.50</td>
<td>1.75</td>
<td>1.50</td>
<td>1.50</td>
<td>1.75</td>
<td>1.50</td>
<td>1.75</td>
</tr>
</tbody>
</table>

The value of the diameter uncertainty with the value of 0.001595 is provided by the manufacturer of the microcapsules. The reproducibility of the diameters is measured as a mean by the values of the standard deviation (SD) in the last row of Table 1. However, the values of the scale of the standard deviation contain systematic uncertainty due to the uncertainty in the estimation of the collection efficiency of the scattered light. This uncertainty leads to uncertainty in the $x$ parameter which scales the measured absorbance to the inferred absorption cross section. The systematic uncertainty becomes apparent if a comparison is made between the imaginary component of the fill of collection shown in Table 1 and the average value of the imaginary part of the values of absorption obtained from measurements on microcapsules with diameters 1.3 mm, 2.4 mm, and 3.8 mm, which is 0.07965 ± 0.02. Thus the uncertainty in the estimate of the fill of the microcapsules is uncertain due to random variation in independent measurements on microcapsules with the same diameter.
Knowledge Base in Excel Spreadsheet

http://semanticommunity.info/@api/deki/files/28860/NISTDataScience.xlsx

NIST Data Science Spotfire Cover Page

Web Player
NIST Digital Archives Century of Excellence

Web Player
Federal Library Bibliographic Records Analysis 2013

Web Player

NIST Library Catalog Search for Data

Web Player

http://semanticommunity.info/Data_Science/NIST_Scientific_Data_for_Data_Science

Updated: Sat, 19 Sep 2015 07:29:15 GMT
Spotfire Dashboard

For Internet Explorer Users and Those Wanting Full Screen Display Use: Web Player Get Spotfire for iPad App

Media, iframe, embed and object tags are not supported inside of a PDF.

Research Notes

NIST Virtual Library

Source: http://www.nist.gov/nvl/

Welcome

Welcome to the public home page of the NIST Virtual Library (NVL), the portal to the services of the NIST Information Services Office (ISO). The links on this page provide access to publications and information services available to the public.

About ISO

The Information Services Office (ISO) is responsible for creating, maintaining, and disseminating a NIST knowledge base which supports the research and administrative needs required to fulfill the scientific, engineering, and technical mission of NIST. Learn more about the work and best practices of ISO by reading papers and viewing presentations by ISO staff. More about ISO...
NIST Publications

Source: http://www.nist.gov/nvl/nist_publications.cfm

NIST series publications, can be identified via the NIST Research Library's online catalog. Some NIST publications, including Special Publications, Technical Notes, etc., are freely available electronically, or some copies can be digitized upon request.

For more information about types of NIST series publications: Types of NIST Publications

The NIST Publications Portal is another way to locate NIST publications. There you will find links to publication databases specific to the NIST laboratories which represent broad areas of research such as chemistry, physics, information technology, and materials science.

The Journal of Research of the National Institute of Standards and Technology, is freely available to the public. Full text articles back to 1934 are currently available. Articles from the former title Bureau of Standards Journal of Research are available from 1928-1934, as well as the earlier publications from the Bulletin of the Bureau of Standards, 1904-1919.

Also, search the NIST Digital Archives (NDA) for the full-text publications, including the Journal of Research and selected series publications.

Some popular collections of NIST publications:

- Special Publication 800 Series (Computer Security)
- FIPS (Federal Information Processing Standards)

Standards

Source: http://www.nist.gov/nvl/standards.cfm

National Center for Standards and Certification Information (NCSCI)

The National Center for Standards and Certification Information (NCSCI) answers questions regarding standards from ASTM, ANSI, ISO, and most other standards organizations. For help, contact NCSCI, x4040.

Popular standards databases available from NIST

Federal Information Processing Standards (FIPS)

Standards and guidelines issued by NIST for Federal computer systems. See also NIST Special Publication 800 series on computer security.

Global Standards Information (GSI)

Gateway to a wealth of standards and conformity assessment information. Contact the Standards Information Center (NCSCI; x4040) for access to standards.
NIST Standard Reference Materials (SRMs)

SRM catalog and archived certificates.

More Information

For more information or assistance searching these databases, contact the Information Desk, x3052.

Library Collections

Source: http://www.nist.gov/nvl/library_collections.cfm

The goal and purpose of the NIST Research Library collections is to support the research needs of the NIST community and laboratories. The Library is not open to the public and does not loan materials from its collections with the exception of NIST series publications, which include Special Publications, Interagency Reports, Technical Notes, etc.

For more information about visiting the NIST Research Library or using the collections: FAQs

For more information about the Library’s loan policies for non-NIST employees and other libraries: ILL for non-NIST

For more information about NIST publications: NIST Publications

Library Catalog

Source: https://library.nist.gov/uhtbin/cgi/70034/60/502/X

MY NOTE: Explore

FAQs

Source: http://www.nist.gov/nvl/library_faqs.cfm

Is the NIST Research Library open to the public?

The NIST campus is not open to the public. Access to the NIST campus to use the Research Library is granted on a case by case basis. Provide your name, address, phone number, citizenship, position, affiliation, detailed reason for access request, and desired access date and time to: library@nist.gov.

Can I borrow or obtain copies of materials from the NIST Research Library?

The NIST Research Library accepts requests for copies of NIST publications only. Email the request to: library@nist.gov and include the publication title, author(s), year, pages, and any other information about the NIST publication.
Documents are usually sent as an email attachment at no cost. Generally, we will fulfill your request within 24 hours of its receipt. However, lengthy documents or large volumes of requests may take several days to process. Alternatively, many NIST publications are available for purchase through the National Technical Information Service (NTIS).

The NIST Research Library does not honor interlibrary loan lending requests for copies of non-NIST publications, articles, or other materials.

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Information on how to identify and locate NIST publications can be found on the [NIST Publications](http://nist.gov) page.

**Are librarians available to assist me?**

The NIST Research Library's primary responsibility is to serve NIST researchers and staff, but we will provide limited reference assistance to the public on topics related to NIST or NIST research.

**How do I contact a librarian for help?**

You may contact a librarian for help via phone (301-975-3052) or by email ([library@nist.gov](mailto:library@nist.gov)). Librarians are on duty 8:30 to 5:00, Monday through Friday except Federal holidays.

**I have visited the NIST Virtual Museum Can I visit the physical museum?**


The NIST campus is not open to the public. Access to the NIST campus to use the Museum is granted on a case by case basis. Provide your name, address, phone number, citizenship, position, affiliation, detailed reason for access request, and desired access date and time to: [library@nist.gov](mailto:library@nist.gov).

Alternatively, we may be able to assist you with NIST Museum inquiries without the need to visit the Museum. Send your Museum questions to [library@nist.gov](mailto:library@nist.gov).
Can I visit the NIST Archives?

The NIST campus is not open to the public. Access to the NIST campus to use the Archives is granted on a case by case basis. Provide your name, address, phone number, citizenship, position, affiliation, detailed reason for access request, and desired access date and time to: library@nist.gov.

Alternatively, we may be able to assist you with NIST Archives inquiries without the need to visit the Archives. Send your Archives questions to library@nist.gov.

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NIST/NBS History

NIST Museum


Last update: July 13, 2009

MY NOTE: Old

NIST Digital Archives

Source: [http://nistdigitalarchives.contentdm.oclc.org/](http://nistdigitalarchives.contentdm.oclc.org/)

MY NOTE: This is it!

About the collections

*Note: You have been redirected to a library consortium site, which contains content managed and owned by the National Institute of Standards and Technology. For questions about this content, please contact nde@nist.gov.*

The NIST Digital Archives (NDA) present images of NIST Museum artifacts and full-text NIST publications. NIST (the National Institute of Standards and Technology) is a non-regulatory agency within the U.S. Department of Commerce.

The images showcase the scientific instruments on display in the NIST Museum located on the NIST campus in Gaithersburg, Maryland. The publications include the Journal of Research of the National Institute of Standards and Technology, which covers the broad range of research undertaken by NIST research staff, focusing on measurement methodology.

These collections continue to grow as more images and full-text publications are added to the NDA.

Browse these suggested topics

- [Browse NIST Journal of Research by Volume](http://semanticommunity.info/Data_Science/NIST_Scientific_Data_for_Data_Science) (9602)
About

Source: http://nistsdigitalarchives.contentdm...org/cdm/about

The NIST Digital Archives (NDA) provide access to full-text NIST publications and images from NIST’s archives and Museum. NIST (the National Institute of Standards and Technology) is a non-regulatory agency within the U.S. Department of Commerce.

The publications included in this site covers the broad range of research undertaken by NIST research staff, focusing on measurement methodology. Archival images showcase many aspects of NIST’s long and rich history.

These collections continue to grow as more images and full-text publications are added to the NDA.

Browse All

Source: http://nistsdigitalarchives.contentdm...org/cdm/search

My Note: 9602 in spreadsheet format (see first 200 in Excel)

Search Tips

Using the Simple Search

The simple search box (in the heading of the website) searches for items across all fields in all collections for any term that you put in the search box, in any order. For example, if you search for "westward migration", the search engine searches for items containing "westward" AND "migration". (Or click advanced search - See Below to use other types of searches.)

The simple search box supports the use of a wildcard operator that enables you to search for approximate terms. Using an asterisk (*) at the end of a search term will search for results with none, or any number of any characters appended to the root search term. For example, test* will find results with the words "test," "tests," "tested" and so on.

New Search

After using the simple search or advanced search, you can start a new simple search by typing the search term and selecting New Search instead of Within Results. To clear an Advanced Search, click the Clear All button.

Refining Your Search

After using the simple search or advanced search, you can make your initial results more specific by searching Within Results from the simple search box or by choosing from the keywords listed in the Narrow Your Search By box. You also can add or remove collections from the search.
If you have narrowed your search too far, you can step back and display previous results by removing the keywords you used in your search path (click the X next to the search term displayed at the top of your results).

**Using the Advanced Search**

The Advanced Search pane enables you to select specific collections and to build a more complex search query on selected fields.

**Building Your Search**

First determine which search to use (across all fields, by selected fields or by date). The default selection is to search across all fields.

Then build your query and specify the collections to search. Add more search fields by clicking Add Another Field. Reduce the number of search fields by clicking Remove. You can have as many as four search fields and as few as one field.

Advanced Search offers four search types (or operators):

- **All of the words** — searches for all of the words in any order. Using Boolean logic, this search is similar to using "AND". For instance, if you entered "President Theodore Roosevelt" in this search box, the search results would contain only those items containing all three terms. Do not include "AND" with your search terms. The Boolean operator "AND" is used automatically with the All of the words search and will be ignored if it is entered as a search term.

- **The exact phrase** — searches for all of the words in the exact order. This is similar to using quotation marks in other search engines. For instance, if you were searching for "President Theodore Roosevelt", search results would contain only those items that contain the phrase "President Theodore Roosevelt".

- **Any of the words** — searches for any of the words entered in the search box. Using Boolean logic, this search is similar to using "OR". For instance, if you entered "President Theodore Roosevelt" in this search box, the search results would contain all items containing any of the three terms, including results with only "President", only "Theodore", and only "Roosevelt". Do not include "OR" with your search terms. The Boolean operator "OR" is used automatically with the Any of the words search and will be ignored if it is entered as a search term.

- **None of the words** — use this option with any of the other search boxes to exclude a term. Using Boolean logic, this search is similar to using "NOT". For instance, if you entered "President Roosevelt" in the exact phase search box and "Franklin" in this search box, the search results would contain all items containing "President Roosevelt" that do not contain the word "Franklin". Do not include "NOT" with your search terms. The Boolean operator "NOT" is used automatically with the None of the words search and will be ignored if it is entered as a search term.

**Note**: If you build a search query of multiple search fields that uses more than one type of operator, the query is executed from left to right, regardless of the operator.

Advanced Search supports the use of a wildcard operator that enables you to search for approximate terms. Using an asterisk (*) at the end of a search term will search for results with none, or any number of any characters appended to the root search term. For example, test* will find results with the words "test," "tests," "tested" and so on.
Search By Date

If available, you may have the option to search by date within collections. The default mode searches across all fields. Use the drop-down list to specify a date range, or to search after, before, or on a particular date. Entering a year (yyyy) is required to perform a search. You also can search by year and month, or by month and day and year.

NIST Virtual Library


**MY NOTE:** See above

NIST Virtual Museum


**MY NOTE:** See above

NIST/NBS History 1901-1993


The NIST/NBS history volumes are a 3-volume set that traces the history of the National Institute of Standards and Technology (NIST), formerly the National Bureau of Standards (NBS), from its creation in 1901 through 1993. The volumes are available as searchable PDF files in entirety, and as individual chapters below.


**Measures for Progress: A History of the National Bureau of Standards (MP275)**
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Chapter Six: Metrology Makes Room for Industrial Productivity (February 1990--April 1993) p. 641 - 788
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Responding to National Needs: Supplement to the Appendices 1994-2009 (SP955 Suppl.)

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Century of Excellence

Source: http://nistdigitalarchives.contentdm...T=/p15421coll5

MY NOTE: Can scrape to Excel with links
About this collection

Published in 2001, *A Century of Excellence in Measurements, Standards, and Technology: A Chronicle of Selected NBS/NIST Publications, 1901-2000* (SP958) commemorates the centennial of the National Institute of Standards and Technology (NIST) by presenting brief accounts of selected classic NIST publications. These publications illustrate the rich history of the Institute’s scientific and technical accomplishments and the broad scope of its contributions to the U.S.

The Century of Excellence collection, based on the printed publication, consists of short accounts describing 102 representative publications that had a significant impact during the agency’s first century. Out of the tens of thousands of papers appearing in print, these 102 were chosen to illustrate the range of activities covered by the NIST publication program, which includes articles published in scholarly journals as well as papers in NIST’s own publication series. Many other deserving papers are listed in the bibliographies accompanying each account.

*A Century of Excellence* is edited by David R. Lide. Its 102 vignettes were written by NIST staff.

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Measurement of Scattering and Absorption Cross Sections of Microspheres for Wavelengths between 240 nm and 800 nm

Source: [http://dx.doi.org/10.6028/jres.118.001](http://dx.doi.org/10.6028/jres.118.001) (PDF)

Volume 118 (2013) [http://dx.doi.org/10.6028/jres.118.001](http://dx.doi.org/10.6028/jres.118.001)

Journal of Research of the National Institute of Standards and Technology

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National Institute of Standards and Technology, Gaithersburg, MD 20899

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**Abstract**

A commercial spectrometer with a 150 mm integrating sphere (IS) detector was used to estimate the scattering and absorption cross sections of monodisperse polystyrene microspheres suspended in water. Absorbance measurements were performed with the sample placed inside the IS detector. The styrene absorption was non zero for wavelengths less than 300 nm. Correction for fluorescence emission by styrene was carried out and the imaginary part of the index of refraction, ni, was obtained. Absorbance measurements with the sample placed outside the IS detector were sensitive to the loss of photons from the incident beam due to scattering. The absorbance data was fitted with Lorenz-Mie scattering cross section and a correction for the finite acceptance aperture of the spectrometer. The fit parameters were the diameter, the suspension concentration, and the real part of the index of refraction. The real part of the index was parameterized using an expansion in terms of powers of the inverse wavelength. The fits were excellent from 300 nm to 800 nm. By including the imaginary part obtained from the absorbance measurements below 300 nm, it was possible to
obtain a good fit to the observed absorbance data over the region 240 nm to 800 nm. The value of $n_i$ at 266 nm was about $0.0060\pm0.0016$ for microspheres with diameters of 1.5 μm, 2.0 μm, and 3.0 μm. The scattering cross section, absorption cross section, and the quantum yield at 266 nm of microsphere with a diameter of 2.0 μm was $5.65\pm0.01 \text{ μm}^2$, $1.54\pm0.03 \text{ μm}^2$, and $0.027\pm0.002$ respectively. The styrene absorption reduces the scattering cross section by 20% at 266 nm.

Key words: integrating sphere detector; Lorenz-Mie; microspheres; scattering.

Accepted: December 18, 2012
Published: January 10, 2013
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1. Introduction

In a previous paper [1] referred to as paper #1, it was demonstrated that the Lorenz-Mie (L-M) cross section for light scattering from monodisperse microspheres suspended in water gave a good description of absorbance measurements with a commercial spectrometer with an integrating sphere (IS) detector for wavelengths greater than 300 nm. The spectrometer configuration, shown in Fig. 1, allowed measurements with the suspension located outside the IS (holder 1 in Fig. 1) and measurements with the suspension located inside the IS (holder 3 in Fig. 1). In addition to the L-M cross section it was also necessary to include a description of the collection efficiency of forward scattered light which entered the IS detector and influenced the measurement of absorbance. With the suspension placed in the holder outside the IS, mainly transmitted light was collected by the IS detector, while in the case of the suspension placed inside the IS all of the light (transmitted and scattered) from the suspension was collected by the IS detector. In this paper we extend the analysis of the absorbance measurements to wavelengths below 300 nm and include the strong absorption band of styrene at 270 nm. Central to the analysis is the observation that when the cuvette containing the polystyrene (PS) microsphere suspension was placed inside the IS detector (holder 3), the entire measured absorbance was due to molecular absorption which was non-zero only for wavelengths below 300 nm. It was assumed that after a correction for fluorescence, the measured absorbance with the suspension placed inside the IS detector was equal to the molecular absorption. For wavelengths greater than 300 nm, the measured absorbance for the suspension placed inside the IS detector was within instrument uncertainty. In the present work, the absorbance measured in holder outside the IS in the wavelength range 240 nm to 300 nm was analyzed by including both absorption and scattering contributions. The analysis was divided into three parts. First, the analysis of the absorbance measured in the holder outside the IS above 300 nm was used to obtain the microsphere diameter, the real part of the index of refraction, and the concentration of the microsphere suspension. Second, the microsphere properties obtained for wavelengths above 300 nm were used for wavelengths below 300 nm to analyze the absorbance observed in the holder inside the IS. This latter analysis yielded an estimate of the imaginary part of the index of refraction. Finally, the results of the two steps were combined to analyze the absorbance measured in the holder outside the IS in the wavelength range 240 nm to 300 nm. In the following we describe a method to combine the measurements of absorbance for suspensions placed inside and outside the IS detector to obtain the complex index of refraction, the microsphere diameter, and the suspension concentration.

**Figure 1** A schematic of the Perkin Elmer dual beam Lambda 850 spectrophotometer

The rectangle next to the number 1 represents the normal cuvette holder outside the integrating sphere (IS) detector. The rectangle next to the number 3 represents the cuvette holder inside the IS detector. For both cuvette positions, the
The same reference beam enters the IS detector through a reference port and hits the wall of the IS detector. In practice, the same ‘auto zero’ spectrometer function is used for both cuvette holders. The reference beam also has a cuvette holder which is not shown in the diagram. In addition, there is a cuvette holder in front of the IS sample beam entrance aperture which is also not shown.

2. Interpretation of Integrating Sphere (IS) Measurements

The proposed method for measuring the scattering cross section of microspheres utilized a commercial spectrophotometer with an integrating sphere (IS) detector. The method was described previously [1] and here we provide only a short summary. The path of the light beam that probed the sample contained two mechanical cuvette holders labeled 1 and 3 in Fig. 1. The cuvette holder 1 was located outside of the IS detector in the normal sample compartment while the cuvette holder 3 was located inside the IS detector. The mirrors shaped the light beam so that it passes unobstructed through the cuvette holders. Measurements of absorbance were performed with the cuvette placed outside the IS (holder 1), and with the cuvette inside the IS (holder 3). The response in holder 3 was complicated by the detection of fluorescence, and possible biases due to settling of suspensions in holder 3 (no stirring).

The total extinction coefficient, $a = \sigma N$, was expressed as a product of the total extinction cross section, $\sigma$, in units of cm$^2$ and the concentration of microspheres, $N$, in units of cm$^{-3}$. The path length through the cuvette was 1 cm. The total extinction coefficient was written as $a = a_s + a_m$ where $a_s = \sigma_s N$ is the apparent absorption coefficient due to scattering, and $a_m = \sigma_m N$ is the molecular absorption coefficient. This description assumed that scattered photons were not detected and therefore appeared to have been absorbed. In most commercial spectrometers, the detector has a finite acceptance aperture and some of the forward scattered photons are detected. In order to correct for the detection of the forward scattered photons, the total extinction coefficient was modified as $a = a_s + a_m - a_{sp}$ with the definition $a_{sp} = \sigma_{sp} N$ where $\sigma_{sp}$ the integral of the differential scattering cross section over the angles subtended by the detector aperture at the location of the cuvette. In many cases, the measured total absorbance was less than 0.2 and the analysis could be simplified greatly by using a first order approximation $10^{-x} = 1 - x \ln(10)$, which is valid for $x \ll 1$, and obtain the following approximate relation shown in Eq. (1).
Equation (1)

$$2.303(A - A_{buf}) \approx \sigma_s + \sigma_n - \sigma_{sp}$$  \hspace{1cm} (1)

Equation (1) was used to relate the measured absorbance ($A$) in any of the holders. (It is assumed that the buffer absorbance, $A_{buf}$, was also measured in each holder) to the suspension properties embodied in the total extinction coefficient. To a good approximation, $\sigma_{sp} \approx 0$ for the sample placed outside the IS, and $\sigma_{sp} \approx \alpha_2$ for the sample placed inside the IS. In order to compare the calculated cross section with the data, the values of the cross sections were multiplied by a concentration, a unit conversion factor 0.01, and 1/2.303 to obtain the expected absorbance. Assuming the validity of Eq. (1) and a cuvette path length of 1 cm, the relation between the measured absorbance and the calculated cross section is given by Eq. (2).

Equation (2)

$$2.303(A - A_{buf}) = N \cdot 10^6 \text{cm}^{-3} \cdot \sigma \cdot 10^{-1} \text{m}^2 \cdot 10^6 \text{cm}^2 \cdot 1\text{cm}$$

$$= N \cdot \sigma \cdot 0.01$$  \hspace{1cm} (2)

As an example, if measurements were performed on a cuvette with a suspension of microspheres with a concentration of $2.0 \times 10^6 \text{ cm}^{-3}$, the calculated cross section was multiplied by a concentration 2.0 and 0.01/2.303 to give a predicted absorbance of about 0.13. In the following, the calculated cross sections will be presented in units of $\mu m^2$, and the microsphere concentrations in units of $10^6 \text{ cm}^{-3}$. In the following section, Eq. (1) is used to analyze the measured extinction in holder 3 with $\sigma_s - \sigma_{sp}$ set to zero.

3 Analysis of Absorbance Measurements from 240 nm to 800 nm

Measurements of absorbance of samples placed inside the IS showed that absorption occurred only for wavelengths below 300 nm. Therefore for wavelengths greater than 300 nm the measured absorbance for samples placed outside the IS was due to scattering and the analysis was performed using the L-M formalism with a real index of refraction. The fit to the data taken for samples outside the IS above 300 nm provided estimates of the microsphere diameter, real part of the index of refraction, suspension concentration, and the instrument acceptance angle. The next step involved the analysis of the absorbance measurement for samples placed inside the IS, which had only a contribution from molecular absorption. After correcting for fluorescence and residual background, the data acquired inside the IS was analyzed using the absorption cross section calculated according to the L-M formalism. The imaginary part of the index of refraction (below 300 nm) was assumed to possess a shape given by the function in Eq. (3).

Equation (3)

$$f(x) = \frac{1}{1 + \exp(330(x - 0.272))} \cdot \frac{1}{1 + \exp(-100(x - 0.235))}$$  \hspace{1cm} (3)

The variable $x$ stands for wavelength in units of $\mu m$ to be consistent with the units used in the calculation of the L-M cross section. The function $f(x)$ decreases for wavelengths greater than 272 nm and wavelengths less than 235 nm. In between these wavelengths the function has a plateau. The shape of the function reproduced the shape of the styrene
absorption band centered on 270 nm and only a scale factor was needed to fit the absorbance taken in the holder inside the IS. The product of the scale factor and the function \( f(x) \) gave the imaginary part of the index of refraction needed to calculate the scattering cross section between 240 nm and 800 nm. The three main steps of the analysis are summarized below.

1. The data taken for the sample outside the IS in the region 300 nm to 800 nm was fitted to the L-M scattering cross section with the parameters: microsphere diameter, real part of the index of refraction, microsphere concentration, and the instrument acceptance angle.

2. The data taken for the sample inside the IS in the region 240 nm to 320 nm was fitted to the L-M absorption cross section using Eq. (3) to model the imaginary part of the index of refraction. The values of microsphere diameter, the real part of the index of refraction, and concentration determined in step 1 were used in this analysis.

3. The data taken for the sample outside the IS in the region 240 nm to 800 nm was compared to the calculated L-M scattering cross section with the parameters obtained in steps 1 and 2. The parameters include the microsphere diameter, real part of the index of refraction, imaginary part of the index of refraction, the microsphere concentration, and the instrument acceptance angle. There was no fitting in this step.

In what follows, the three steps of the analysis described above are presented in greater detail. Measurements were performed on PS microspheres suspended in aqueous PBS buffer or deionized water (DI). The suspensions were sufficiently dilute so that the absorbance was less than 0.2, and the simplified analysis given by Eq. (1) and Eq. (2) was used to model the data.

### 3.1 Analysis of the Absorbance Due to Scattering

Figure 2 shows measurements and analysis for a suspension of 3.0 μm microspheres in distilled water. The suspension was prepared by pipetting 10 μL of stock suspension obtained from Polysciences, Inc, (catalog number 17134, lot 621930) into 10 mL of distilled water. The Lambda 850 spectrometer was scanned from 800 nm to 220 nm in increments of 1 nm with an integration time of 0.8 s, and a slit width of 2 nm. Four measurements were taken with a water sample and a suspension sample placed sequentially in holders outside and inside the IS. The solid circles in Fig. 2a show the measured absorbance due to scattering (trace A1-A3) and the absorbance due to molecular absorption (trace A3). The absorbance due to scattering was obtained by subtracting the measured absorbance of a sample placed inside the IS (A3) from the measured absorbance of the sample placed outside the IS (A1). In both cases, the measured absorbance of the cuvette filled with water was subtracted. The solid trace in Fig. 2b shows the best fit to the trace A1-A3 of a model based on the calculation of the L-M scattering cross section in the wavelength range from 300 nm to 800 nm. The Lorenz-Mie calculations were performed using MatLab with Maetzler code for Mie scattering. The fit resulted in a diameter of 3.011 μm which was consistent with the value, (3.004±0.065) μm, provided by the manufacturer. The best fit shown in Fig. 2b was obtained from the minimization of residuals defined in Eq. (4).

**Figures 2 (a) and (b)** Shows the measured absorbance due to scattering

The trace was obtained by subtracting the measured absorbance, A3, for a sample inside the IS from the measured absorbance, A1, for a sample outside the IS. In both cases, the buffer contribution was subtracted. The dotted trace
labeled $A_3$ shows the absorption due to styrene polymer. (b) The solid circles reproduce the trace labeled $A_1$-$A_3$ from part (a), and the solid trace is a best fit to the apparent L-M cross section for PS microspheres with a diameter of 3.0 μm.

$$\text{Equation (4)}$$

$$\text{Residuals} = \sum_i \frac{A_i - A_3}{c} - \frac{Mie(d, n)}{\pi} \int_0^{\Delta} \frac{dQ}{d\Omega}(d, n, \theta) d\theta$$

$$c = N \cdot 0.01 / 2.303$$

$$d = \text{diameter}$$

$$n = \text{index of refraction}$$

$$\Delta = \text{acceptance angle}$$

The quantities $A_1$ and $A_3$ stand for the measured absorbance outside and inside the IS detector respectively (with the buffer contribution subtracted). The quantity $\text{Mie}(d, n)$ is the calculated total scattering cross section. The integral of the differential L-M scattering cross section was performed over the angle subtended by the instrument entrance aperture at the location of the cuvette (symbol $\Delta$ in Eq. (4)). The integral models the effect of the finite acceptance aperture of the instrument. Because of the finite aperture some of the radiation scattered in the forward direction enters the instrument and reduces the measured absorbance. In what follows, the two calculated terms in Eq. (4) will be referred to as the apparent scattering cross section. The residuals in Eq. (4) were summed over a selected range of wavelengths with the lower bound set to a wavelength of about 300 nm. It was possible to obtain an excellent fit for wavelength region between 500 nm and 800 nm with a constant value of the index of refraction. For fitting below 500 nm, it was necessary to introduce a wavelength dependent index of refraction as described in paper #1. The fitting provided estimates of the diameter, real part of the index of refraction, concentration, and the acceptance angle. The imaginary part was set to zero for wavelengths greater than 300 nm. In order to obtain a good fit below 300 nm it was necessary to introduce an imaginary component to the index of refraction. The value of the imaginary component was obtained from analysis of $A_3$ as described in the next section.
3.2 Measurement of Molecular Absorption in Scattering Suspensions

The comparison of absorbance measurements of samples placed inside and outside the IS detector showed that the measurements inside the IS detector were not sensitive to scattering losses. There was a small background absorbance (of the order of 0.003) which was most likely due to the escape of backward scattered photons through the entrance aperture of the IS detector. The background observed for measurements inside the IS was relatively constant over the wavelength region 300 nm to 800 nm, and we assumed that the background below 300 nm could be estimated from the scattering background spectrum between 300 nm to 800 nm. The trace $A_3$ in Fig. 2a shows the result of measurements of absorbance inside the IS on a suspension of 3.0 μm microspheres. The trace labeled $A_3$ in Fig. 2a was obtained by subtracting the buffer absorbance and an additional absorbance of 0.003 from the measured absorbance for the sample inside the IS. The absorbance value of 0.003 is close to the uncertainty introduced by variability of cuvette position and instrument drifts. Following the buffer and background subtractions, the $A_3$ trace in Fig. 2a may still not represent the true absorbance because the emitted fluorescence from microspheres will reduce the observed absorbance.

3.2.1 Fluorescence Correction of Absorbance Measured Inside the IS

The effect of fluorescence on absorbance measurements for samples inside the IS is demonstrated in Fig. 3a. The solid and dashed traces in Fig. 3a show the absorbance measurements carried out for 10 mol/L aqueous solution of tryptophan placed outside and inside the IS respectively (the solution did not have measurable scattering). The reduction of the tryptophan absorbance measured inside the IS was attributed to the fluorescence emitted by the excited tryptophan molecules. Figure 3b shows the observed fluorescence emission when the same tryptophan solution was placed in a fluorimeter and excited with 266 nm light. Clearly the emitted tryptophan fluorescence will reduce the observed tryptophan absorbance measured inside the IS because the IS detector will not distinguish between photons transmitted through the cuvette and photons emitted by the solution inside the IS. Figure 4a shows the emitted fluorescence spectrum from a suspension of 1.5 μm microspheres placed in a fluorimeter and excited with 266 nm light. A comparison of the spectra in Fig. 4a and Fig. 3b shows that the fluorescence emission from the microspheres is similar to the fluorescence emission from the tryptophan solution. Therefore it was assumed that the measure absorbance of a suspension of 1.5 μm microspheres shown in Fig. 4b would include a reduction by the emitted fluorescence and that the actual absorbance of the microsphere suspension is larger. In order to quantify the reduction in the measured absorbance due to fluorescence, it was assumed that the relative reduction in absorbance is proportionate to the quantum yield as indicated in Eq. (5).

\[
\frac{A - A_3}{A} = m \Phi 
\]  

(5)

Here $A$ is the true absorbance, $A_3$ is the absorbance measured inside the IS, $\Phi$ is the quantum yield, and $m$ is the proportionality constant. In the ideal case where every photon is detected with the same probability, the value of $m$ should be 1 since if the quantum yield is 1, every absorption leads to an emitted photon and the measured absorbance, $A_3$, would be 0. In practice, the photon detection probability varies significantly in the UV region so that the value of $m$ will be different from 1 as discussed in a previous work [3]. Equation (5) was treated as a phenomenological relation.
The tryptophan measurements shown in Fig. 3a were used to estimate the proportionality constant $m$ because the true absorption of tryptophan could be obtained from measurements in holders outside the IS while the quantum yield of tryptophan has been determined to be 0.13 \cite{4, 5}. Explicitly, the proportionality constant was assumed to be given by Eq. (6).

Equation (6)

$$\frac{A_i - A_0}{A_i} = m \cdot 0.13$$

Figures 3 (a) and (b) The solid and dashed traces show the measured absorbance for 10 μmol/L aqueous tryptophan solution placed in holders outside (solid), and inside (dashed) the IS detector respectively. In both cases the buffer contribution was subtracted. There is a large difference in the measured absorbance in the two holders. The difference is due to fluorescence emission which is detected whenever the sample is inside the IS detector. The IS detector does not differentiate between the transmitted photons and the fluorescence photons thus recording a smaller absorbance for fluorescing samples. (b) The emitted fluorescence spectrum from a 10 μM tryptophan solution placed in a fluorimeter and excited with 266 nm light. The maximum emission is at 360 nm. The emitted fluorescence from either the microspheres or the tryptophan will reduce the recorded absorbance for samples placed inside the IS detector.
Figure 4 (a) and (b) The emitted fluorescence spectrum from a suspension of 1.5 μm microspheres
placed in a fluorimeter and excited with 266 nm light. The maximum emission is at 350 nm. (b) The measured absorbance from a suspension of polystyrene microspheres with diameter 1.5 μm. The trace was obtained by placing the sample in the holder inside the IS detector and subtracting the buffer contribution and a small background contribution (0.003).

![Fluorescence Spectrum](image)

![Absorbance](image)

Where $A_1$ and $A_3$ are the absorbance measurements obtained outside and inside the IS as shown in Fig. 3a. Figure 5 shows the result of applying Eq. (6) to the data in Fig. 3a. From the trace in Fig. 5 it is clear that the quantity $m$ in Eq. (6) is not a constant and varies from 2.5 to 2.0 over the tryptophan absorption band. We will use $m = 2.4$ in the estimate of the true absorbance of microspheres. This choice is motivated by the desire to minimize systematic errors in the vicinity of 266 nm. It was also assumed that the emission spectra of tryptophan and the microspheres were sufficiently similar so that spectral response corrections could be ignored in the first approximation. The quantum yield of microspheres was obtained relative to the quantum yield of tryptophan by using the relation given in Eq. (7) [6].

**Equation (7)**

$$\frac{I}{I_{\text{ref}}} = \frac{A}{A_{\text{ref}}} \frac{\Phi}{\Phi_{\text{ref}}} n^2$$

(7)
The data shown in Fig. 3a was used to form the ratio, \( m \), given by Eq. (6) in the text. The quantity 0.13 in Eq. (6) is the quantum yield of tryptophan in aqueous solution. The ratio, \( m \), characterizes the effect of fluorescence emission on the observed absorbance of tryptophan samples placed inside the IS detector. Ideally the ratio should be constant. The variation with wavelength reflects the difference in spectral response between the fluorescence and the incident light.

Here \( I \) and \( I_{\text{ref}} \) are the integrated fluorescence intensities obtained by summing the spectra shown in Fig. 4a (\( I \)) and 3b (\( I_{\text{ref}} \)). \( A \) and \( A_{\text{ref}} \) are the absorbance values at 266 nm of the microsphere suspension and tryptophan reference solution respectively. The indexes of refraction \( n \) and \( n_{\text{ref}} \) refer to the material in the sample cuvette and are both very close to the value for water, hence their ratio was set to 1 in Eq. (7). Equation (7) indicates that the value of \( A \) is needed to find the microsphere quantum yield \( \Phi \), while Eq. (5) states that \( \Phi \) is needed to determine the true microsphere absorption \( A \). Solving Eq. (7) for \( \Phi \) in terms of \( A \), and substituting into Eq. (5) lead to an estimate of the true absorbance of the microsphere suspension given by Eq. (8).

Equation (8)

\[
A = A_3 + m \frac{I}{I_{\text{ref}}} A_{\text{ref}} \Phi_{\text{ref}}
\]  

(8)

Inserting the various measured values into Eq. (8) resulted in an increase in \( A_3 \) of only several percent. Inserting the corrected absorbance of microspheres into Eq. (7) lead to a quantum yield of about 0.018 for microspheres with diameter of 1.5 \( \mu \)m. Repeated measurements for microspheres with a diameter of 2.0 \( \mu \)m gave a quantum yield of 0.026±0.004. If the uncertainty in the measurements for the 1.5 \( \mu \)m microspheres is assumed to be ±0.004 then the two measurements are consistent. Alternately it may be that the QY for the smaller microspheres is smaller due to the decrease in the density of final states. The quantum yield of styrene monomers in dilute solution is 0.24 [7]. However as the molecular weight of the styrene polymers increase, the quantum yield decreases, reaching a limit of 0.018 for very long strands [8]. Therefore there is a substantial quenching of fluorescence in the styrene polymer and the observed quantum yield for PS microspheres is reasonable. Since the correction of absorbance measurement due to fluorescence emission is so small, the values of \( A_3 \) in Fig. 4b were used to represent the “true” absorbance of the microsphere.
suspension. A second correction that was neglected was the increase in the measured absorbance $A_3$ due to the repeated passage of the light reflected inside the IS through the cuvette inside the IS. This correction was expected to be small because the suspension has a small absorption value (Fig. 1a). This was collaborated by measurements of absorbing, non-fluorescing solutions (e.g. myoglobin or fluorescein in pH 5 buffer) which gave indistinguishable responses outside and inside the IS detector [3].

3.2.2 Analysis of the Microsphere Absorbance Measurements

The microsphere absorbance recorded inside the IS (an example shown in Fig. 4b) was assumed to be the true molecular absorption and it was used to obtain the microsphere absorption cross section using the relation shown in Eq. (9).

\[ \text{Equation (9)} \]

\[ \text{Residuals} = \sum \left( \frac{A_i - \text{Absorbed}}{c} - \text{Mie}(d, n) \right)^2 \]

\[ c = N \cdot 0.01 / 2.303 \]

\[ d = \text{diameter} \]

\[ n = \text{index of refraction} \]

Where $\text{Mie}(d, n)$ calculates the total absorption cross section for a given set of parameters. The parameters $c$, $d$, and the real part of $n$ were taken from the fits to the measured absorbance outside the IS for wavelengths greater than 300 nm. The functional shape of the imaginary component of the index of refraction was taken as function $f(x)$ given in Eq. (3). The function $f(x)$ was multiplied by a scaling parameter in order to fit the measured absorbance. The solid and open circles in Fig. 6a show the estimated absorption cross section for 1.5 μm and 3.0 μm microspheres respectively obtained by dividing the measured absorbance by the parameter $c$ in Eq. (9). The solid traces in Fig. 6a show the best fits to the data using the imaginary index of refraction given by Eq. (3). Figure 6b shows the imaginary part of the index of refraction which best described the absorption cross section shown in Fig. 6a. The comparison of the absorption cross sections in Fig. 6a shows that for 266 nm the absorption cross section of the 3.0 μm microsphere is only four times larger than the absorption cross section of the 1.5 μm microsphere, whereas the volume is eight times larger. The greater absorption efficiency of the 1.5 μm microsphere accounts for the factor of two. The comparison of the imaginary components of the index of refraction in Fig. 6b shows that the values for the 1.5 μm microsphere are about 1.4 times larger than the values for the 3.0 μm microsphere. In principle the two values should be the same since the imaginary part of the index of refraction is a property of the polymer material which is presumably identical for the two microspheres. It is likely that the difference in the imaginary part of the index of refraction is due to systematic uncertainties inherent in the measurement and analysis. A central problem, which has been mentioned before, is the estimate of the efficiency of collection of forward scattered light by the detector with a finite aperture.

3.3 Estimate of the Scattering Cross Section between 240 nm and 800 nm

In the third and final part of the analysis, the fit to the scattering cross section above 300 nm and the fit to the absorption cross section below 300 nm were combined to obtain an estimate to the scattering cross section in the wavelength range 240 nm to 800 nm. There was no additional fitting, the parameters obtained for the fits above and below 300 nm were combined to obtain the response over the entire range. The solid circles in Fig. 7a show the scattering cross...
section obtained for 1.5 μm microspheres and the solid trace shows the best fit for wavelengths between 240 nm and 800 nm. Figure 7b gives the same information for microspheres with diameter of 3.0 μm. Comparison of Fig. 2b and Fig. 7b shows that including the imaginary component of the index of refraction leads to a much better correspondence between the measurements and the calculated response. The styrene absorption band at 270 nm produces a significant reduction in the scattering cross section at 270 nm. The reduction is expected because the scattering and absorption processes are mutually exclusive. The absorption of photons by the styrene molecules reduces the number of observed scattered photons. Conversely the observation of a scattered photon implies that absorption did not occur.

**Figure 6 (a) and (b) The solid and open circles show the estimated absorption cross sections of suspensions**

of 1.5 μm and 3.0 μm microspheres respectively. The estimates were obtained by dividing the measured absorbance of the samples inside the IS by parameter c in Eq. (9). The parameter c is proportionate to the microsphere concentration. The solid traces show the absorption cross section which best fits the data. The fitting was performed according to Eq. (9) in the text. (b) The imaginary component of the index of refraction for 1.5 μm (solid trace) and 3.0 μm (dashed trace) microspheres obtained from the best fit to the data shown in part (a).

The three steps of the analysis culminated in the estimate of the properties of the microspheres and the instrument which yielded a good representation of the measured data. The solid circles in Fig. 8 show the measured absorbance for a suspension of 2.0 μm microspheres divided by the fit parameter c, and the solid trace shows the calculated apparent scattering cross section. The dashed trace in Fig. 8 shows the calculated L-M total scattering cross section for 2.0 μm polystyrene microspheres in water. The calculation of the total scattering cross section (dashed trace) used the same parameters as the calculation of the apparent cross section except for the instrument acceptance angle which was set to zero (this parameter characterizes the instrument and was not needed to calculate the total scattering cross section).

Table 1 gives the results of four consecutive independent measurements performed on suspensions of 2.0 μm...
microspheres. The suspensions were made by pipetting 5 μL of stock suspension (Polysciences Cat. No. 19814, lot no. 625383) into 20 mL distilled water. The values of the cross sections in Table 1 were obtained by using the best fit parameters from Eq. (4) and Eq. (9) and then setting the acceptance angle to zero. The quantum yield (QY) was obtained with additional fluorescence measurements using Eq. (7) and Eq. (8). The real part of the index of refraction was obtained by inserting the fit parameters into Eq. (11) of paper #1.

**Figure 7 (a) and (b)** The solid circles show the estimated apparent scattering cross section

of a suspension of 1.5 μm microspheres placed outside the IS. The estimate was obtained by dividing the measured absorbance by the parameter c in Eq. (4) (the buffer contributions were subtracted). The solid trace shows the calculated apparent scattering cross section which best fits the data. The fitting was performed according to Eq. (4) in the text. For wavelengths less than 300 nm, the imaginary component of the index of refraction shown in Fig. 6b was used in the calculation of the M-L scattering cross section. The apparent scattering cross section at 266 nm is reduced from the value it would have if there was no molecular absorption. (b) The same comparison as in Fig. 7a except the diameter of the microspheres was 3.0 μm. Again, the apparent scattering cross section at 266 nm is reduced from the value it would have if there was no molecular absorption.

**Figure 8 The solid circles show the measured absorbance**

(divided by the parameter c in Eq. (4)) of a suspension of 2.0 μm microspheres placed outside the IS. The solid trace shows the computed apparent scattering cross section according to Eq. (4). For wavelengths less than 300 nm, the imaginary component of the index of refraction was similar to that shown in Fig. 6b. The total scattering cross section (dashed trace) was calculated using the same parameters as in the calculation of the apparent scattering cross section.

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(solid trace) except for the instrument acceptance angle which was set to zero. The total scattering cross section at 266 nm is reduced from the value it would have if there was no molecular absorption.

![Diagram showing scattering cross section vs wavelength](image)

**Table 1 Properties of 2.0 μm microspheres at 266 nm obtained from the fit of the L-M apparent cross section to the absorbance measurements**

<table>
<thead>
<tr>
<th>Trial</th>
<th>Diameter μm</th>
<th>n real</th>
<th>n imaginary</th>
<th>Scattering cross section, μm²</th>
<th>Absorption cross section, μm²</th>
<th>QY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.943</td>
<td>1.761</td>
<td>7.726e-3</td>
<td>5.65</td>
<td>1.56</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1.942</td>
<td>1.762</td>
<td>7.730e-3</td>
<td>5.64</td>
<td>1.54</td>
<td>0.026</td>
</tr>
<tr>
<td>3</td>
<td>1.942</td>
<td>1.762</td>
<td>7.730e-3</td>
<td>5.64</td>
<td>1.54</td>
<td>0.027</td>
</tr>
<tr>
<td>4</td>
<td>1.943</td>
<td>1.761</td>
<td>7.726e-3</td>
<td>5.66</td>
<td>1.50</td>
<td>0.029</td>
</tr>
<tr>
<td>Mean</td>
<td>1.9426</td>
<td>1.7615</td>
<td>7.7280e-3</td>
<td>5.648</td>
<td>1.535</td>
<td>0.0273</td>
</tr>
<tr>
<td>SD</td>
<td>6.75e-4</td>
<td>5.77e-4</td>
<td>2.31e-6</td>
<td>9.57e-3</td>
<td>0.0252</td>
<td>1.53e-3</td>
</tr>
</tbody>
</table>

The value of the diameter is consistent with the value (1.898±0.029) μm provided by the manufacturer of the microspheres. The reproducibility of the various properties is excellent as shown by the values of the standard deviation (SD) in the last row of Table 1. However the values of the index of refraction contain systematic uncertainties due to the uncertainty in the estimate of the collection efficiency of forward scattered light. This uncertainty leads to uncertainty in the c parameter which scales the measured absorbance to the scattering or absorption cross sections. The systematic uncertainty becomes apparent if a comparison is made between the imaginary component of the index of refraction shown in Table 1 and the average value of the imaginary part of the index of refraction, obtained from measurements on microspheres with diameters 1.5 μm, 2.0 μm, and 3.0 μm, which is 0.0060±0.0016. Thus the uncertainty due to
systematic effects is substantially larger than the uncertainty due to random variation in independent measurements on microspheres with the same diameter.

Since the L-M formalism uses only the ratio of the index of refraction of the microsphere and the index of refraction of the medium, the calculation of the total cross section can be extended to microspheres in air by simply setting the medium index of refraction to 1 and retaining the values of the diameter and the microsphere index of refraction.

4. Conclusion

An analysis of the measurement process with a spectrometer with an integrating sphere (IS) detector lead to a procedure for separating the measured absorbance into a part due to scattering and a part due to molecular absorption. The analysis hinged on the interpretation of absorbance measured for a suspension placed outside \( A_1 \) and inside \( A_3 \) the IS detector of the spectrometer. Equation (1) and Eq. (2) give the relationship between the measured absorbencies \( A_1, A_3 \) and the analyte properties \( a_s, a_m, a_{sp} \). The results suggest that the measurement model presented in this work is valid and that it is indeed possible to separate the contributions from scattering, \( a_s \), and molecular absorption, \( a_m \). The two quantities, \( a_s, a_m \), are independent characteristics of the microsphere suspension. The quantity \( a_m \), which is directly related to the absorption cross section, gives information about the electronic states of the absorbing styrene molecules, while the quantity \( a_s \), which is directly related to the scattering cross section, provides information about the diameter and the wavelength dependence of the index of refraction of the material inside the microsphere. Further work is needed to clarify the systematic errors inherent in the preparation of suspension samples, instrument response, and the measurement model. Most likely the most significant uncertainty is in the estimate of the efficiency of collection of forward scattered light, which is directly related to the partial scattering extinction \( a_{sp} \). The collection efficiency depends on the instrument configuration as well as the angular distribution of the scattered radiation. A better parameterization of the collection efficiency of forward scattered light will be addressed in future work.

5. References


Footnote

1

Certain commercial equipment, instruments, and materials are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology.

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OMNIDATA and the Computerization of Scientific Data

Source: http://nistdigitalarchives.contentdm...id/1605/rec/60 (PDF)

Prepared by John R. Rumble, Jr.
NBS pioneers computerized scientific data management

For much of its history, the National Bureau of Standards has been a leader in providing the most reliable available technical data to scientific and engineering users. The Bureau has operated large-scale data evaluation programs in a wide variety of disciplines and has distributed the results through various publication channels. With the advent of modern computers, it was natural for NBS data experts to explore how computers could be used both for internal data management activities and for the public dissemination of NBS data collections. During the 1970s, the Office of Standard Reference Data (OSRD) and the various data centers that it coordinated embarked on a number of projects aimed at utilizing the growing power of digital computers to improve the efficiency and effectiveness of the SRD program. NBS quickly became recognized as a pioneer in this area.

OMNIDATA established

At that time, there was a tendency for each data group to develop computer programs to handle the particular type of scientific data of concern to it. Since the SRD program covered such diverse classes of data, there was an incentive for OSRD to investigate the possibility of developing general purpose programs capable of managing a broad range of data. This effort led to the creation of the database management program OMNIDATA, described in the book OMNIDATA, An Interactive System for Data Retrieval, Statistical and Graphical Analysis and Data-Base Management: A User’s Manual [1], authored by Joseph Hilsenrath and Bettijoyce Breen. This represents the first major publication of the National Bureau of Standards in the area of computerized scientific data management.

In the early 1970s when the OMNIDATA project was begun, data retrieval, data analysis, and data file maintenance were largely done in the batch mode, with programmers submitting punched cards for processing on a mainframe computer and, after an indeterminate period of time, receiving a printout of results. Also, computer programs designed to run routinely were almost always inflexible, and the writing of ad hoc programs to answer specific questions often entailed expense and delay out of proportion to the urgency of the problem that motivated the question in the first place. When early commercial general-purpose data management programs began to appear, primarily intended for business applications, they had adequate and roughly comparable search and retrieval capability, file definition features, and report generators. None, however, had enough data analysis and data manipulation facilities to handle the numerical and alphanumeric data files required for scientific use, nor did they address unique characteristics of scientific information, such as Greek and mathematical symbols, uncertainties, and varying number of significant figures, all of which added to the complexity to scientific data.

OMNIDATA was designed to overcome many of these shortcomings. Programs were written to analyze and store data. Rudimentary graphics packages created visualizations of data. The 45 unique modules and the supervisory program of the OMNIDATA system could be used not only by the computer professional, but also by the novice with little or no knowledge of computers. It could be run in demand mode, interactively from a computer terminal on a time-shared computer system. In addition to handling such administrative files as personnel, training, inventory, and travel, the system was robust enough to handle diverse scientific data files, including crystal structure data, thermochemical data, chemical kinetics data, and data on physical properties. Finally, OMNIDATA was designed and written to be modular, a hallmark of truly efficient computer programming and systems design, and a visionary precursor to what is today called component-based software.
Most of the individual modules provided tools for data retrieval, analysis, and reporting. Specifically, the system had facilities for searching and reporting; plotting and graphical analysis; arithmetic operations in general, and statistical analysis in particular; file partitioning and subsequent sequential analysis on subfiles; keyword indexing of bibliographic files; flagging, coding, and decoding of data items; analysis of questionnaires and surveys; and a large variety of data management and validation routines of use to both the end user of the data and the database administrator. An important feature of OMNIDATA was its ability to convert data files from other formats for use in the OMNIDATA system and to generate data arrays that could be accessible to other programs written in languages including FORTRAN, COBOL, and XBASE. Also, the OMNIDATA system interfaced with the OMNITAB II program [2], used extensively at NBS and elsewhere, to provide a repertory of well-tested and highly accurate statistical routines.

The OMNIDATA system allowed for flexibility in file size. With it, one could profitably automate files from those with few records of a small number of data elements to elaborate databases of many records with numerous data fields. In contrast to other management information systems of the era, which limited the number of data items that could be searched or manipulated, each module in OMNIDATA was capable of operating on every data item, and the user could search on any field, even down to the character level. Its modularity, flexibility, and data analysis capabilities made OMNIDATA unique. It was a forerunner of the database management systems marketed today and the systems so essential to the functioning of the World Wide Web.

The use of OMNIDATA quickly spread to other parts of NBS, beyond the Standard Reference Data Program, so much so that there were continuing problems in providing support and extensions for a diverse group of users. The legacy of OMNIDATA was not the software itself, but the realization that scientific data projects could successfully convert to computerized operation—and that they would have to do so in order to continue as viable projects.

The lessons of OMNIDATA were critical to the push to computerize both the internal data operations and the dissemination of databases, which began in earnest in the 1980s. The effort was led by Bettijoyce Breen and John Rumble, Jr., who joined the Office of Standard Reference Data in 1980. During this decade every NBS/ NIST data activity created databases of references containing the data of importance to its area of responsibility. Many developed specialized data entry programs that captured not only this bibliographic information, but also the numeric tabular and graphical data contained therein. In addition, the data centers developed suites of software that supported data evaluation through the use of discipline specific analysis, statistical procedures, and correlation techniques. At the beginning of this effort, most of the software incorporated the ideas found in OMNIDATA, with significant extensions to take care of specialized requirements.

Use by outside organizations

Many of the data handling software packages developed at NBS were used by outside organizations. The NIST Crystal Data Center developed AIDS 80, a powerful package that evaluated and managed crystallographic data [3]. The NIST Alloy Phase Diagram Data Center created a suite of graphical digitization and database management tools that supported the international Alloy Phase Diagram Program run jointly by the American Society of Metals and NBS [4]. A similar set of graphics software was developed for handling ceramics phase diagrams under the NBS-American Ceramic Society Phase Diagram for Ceramists Program [5].
Chemical Information System (CIS)

The computerized dissemination of NBS collections of evaluated data proceeded likewise. In the late 1970s, NBS worked with the Environmental Protection Agency and the National Institutes of Health to create and operate the Chemical Information System (CIS), which was the first online system to provide scientific numerical data. The CIS featured a powerful substructure and nomenclature search system that allowed users not only to search for data on a specific substance, but also to identify classes of chemical compounds with particular structural features. The CIS integrated databases built by many groups, including NBS thermochemistry and crystallographic data centers.

The Standard Reference Data program

At the same time, the Standard Reference Data program began offering magnetic tapes of formatted data files suitable for outside users to load onto their own mainframe computers. It was the responsibility of the users to build their own search software and to manage the data. The PC revolution of the 1980s changed all that, and OSRD quickly began offering files similar to those on magnetic tapes on floppy disks. It soon realized, however, that users wanted self-contained packages that were easy to install and that included built-in user interfaces. By 1985 two systems were under advanced development. Steve Stein, then of the Center for Chemical Physics, was building an MS-DOS mass spectral data system, and Chuck Wagner of Surfex and John Rumble, Jr., of NBS were building an x-ray photoelectron spectroscopy (XPS) database on an Apple platform. The mass spectral database was released in 1987 and became an immediate success. Today it is incorporated into virtually every mass spectrometer sold. The next two years saw many other NBS databases released including the XPS database.

Computerized materials data

In 1982, NBS scientific database management efforts addressed another area, that of materials data. In November of that year, NBS cosponsored with FIZ Karlsruhe (a German government technical information center) and CODATA (the ICSU Committee on Data for Science and Technology) a workshop on computerized materials data. This Fairfield Glade meeting, named after its location in Tennessee, spawned an international activity to build an online materials data system. The proceedings from that workshop, Computerized Materials Data Systems [6], edited by Jack Westbrook and John Rumble, Jr., were widely circulated worldwide and became the “bible” for planning such an online system. The seminal meeting addressed the full range of topics related to online materials data systems, including their scope, user interfaces, system development, legal and economic issues, and barriers to be overcome. The Fairfield Glade Workshop concluded that it was not only possible to build such a system, but that one should be built as soon as possible.

Materials Property Data Network (MPDN)

Over the next five years, over 15 additional workshops were held covering the full range of engineering materials disciplines, potential user industries, and many other aspects. A prototype system was built with funding from NBS, the Department of Energy, and the Department of the Army. The Metals Properties Council, a trade association of the metals industry, worked with NBS and other groups to establish the non-profit Materials Property Data Network (MPDN). The MPDN, which soon became part of the STN dialup network of the Chemical Abstracts Service, was a successful online data system in the pre-Internet era.

http://semanticommunity.info/Data_Science/NIST_Scientific_Data_for_Data_Science
Updated: Sat, 19 Sep 2015 07:29:15 GMT
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One offshoot of this effort was the establishment of ASTM Committee E49 on Computerization of Materials Properties Data. This committee, which was chaired by John Rumble from 1988 to 1993, rapidly became the international focal point for standards relating to all aspects of the computerization of materials data, and these standards are in wide use today.

**Microsoft Windows operating system and the Internet explosion**

The blossoming of NBS/NIST computerized data dissemination continued unabated until about 1994, when two concurrent changes hit the computer world. These were the release of the Microsoft Windows operating system and the Internet explosion. In one short period, the NIST PC databases and older online systems such as the MPD Network became obsolete as users demanded Windows versions of existing MS DOS data products. In addition, the Internet, and especially the World Wide Web, revolutionized online data delivery. Where previous online systems required years of development, the Web required only months of work. At the present time, NIST operates 15 Web-based data systems that receive thousands of users every day.

**The forefront of computerizing scientific data**

Today’s scientific database environment is a long way from the mainframe world of 1976 when Hilsenrath and Breen issued their first manual for OMNIDATA, and even of 1986, when the first MPDN prototype came online. These changes have made the creation of databases considerably easier and have brought easy access for users worldwide to the full range of NIST evaluated data. The ideas in OMNIDATA and Computerized Materials Data were germinal in articulating the core principles of scientific database management and online dissemination. The distance traveled since then is a tribute to Hilsenrath, Breen, and Rumble and their foresight in leading NBS to the forefront of computerizing scientific data.

**Joseph Hilsenrath**

Joseph Hilsenrath began his career at NBS in 1948, first as a scientist/mathematician specializing in employee training, then as an experimental researcher in high pressure physics, after which he became Chief of the Equation of State Section of the Heat Division. As the first computers became available at NBS, he became interested in the preparation of tables of thermodynamic data and in putting computer know-how in the hands of Everyman. His OMNITAB statistical packages received wide use in NBS and other Government agencies. He moved to the Office of Standard Reference Data in 1967, where he led the development of computerized typesetting methods that saw use throughout the Government. He retired in 1974, but for many years remained active in NBS reference data activities.

**Bettijoyce Breen**

Bettijoyce Breen joined NBS in 1969 as a computer programmer for the Office of Standard Reference Data after receiving her B.S. in chemistry from William and Mary College. After completion of the work on OMNIDATA, she supervised the introduction of the next generation of computerized typesetting technology into NBS and later became head of the OSRD Data Systems Development Group. This group helped the various data centers in NBS and elsewhere to automate their operations and oversaw the preparation of database packages for public dissemination. She received an M.S. in Chemical Information from American University in 1975 and became active in the Chemical
Information Division of the American Chemical Society, serving as both Treasurer and Chair of the Division. In 1990, as Bettijoyce Breen Lide, she joined the NIST Advanced Technology Program (ATP), where she set up the first ATP management information system. As an ATP program manager, she established the program on Information Infrastructure for Healthcare and later headed the Information Technology and Applications Office. In 1999 she received the George Uriano Award of NIST for fostering industrial-government interactions.

John Rumble, Jr.

John Rumble, Jr. joined NBS in 1980 as the OSRD program manager for materials data. In addition, he played a strong role in computerizing NBS/NIST data activities in all disciplines. Rumble became Chief of the Office of Standard Reference Data in 1994. He has been active in many activities related to standards for scientific and technical information and was elected President of CODATA in 1998. He is also a Fellow of the ASM International and the American Society for Testing and Materials.

Bibliography

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